CARDIFF UNIVERSITY
SCHOOL OF ENGINEERING

Combustion of Green Fuels for Power Generation in Gas Turbine

By

Hua Xiao

Supervisors:
Professor Philip J Bowen
Doctor Agustin Valera-Medina

A Thesis submitted to Cardiff University
For the Degree of Doctor of Philosophy
In Sustainable Energy and Architecture, 2018

DECLARATION

This work has not been submitted in substance for any other degree or award at this or any other university or place of learning, nor is being submitted concurrently in candidature for any degree or other award.

Signed ……………………………………. (Hua Xiao) Date …............................

STATEMENT 1

This thesis is being submitted in partial fulfilment of the requirements for the degree of PhD

Signed ……………………………………. (Hua Xiao) Date …............................

STATEMENT 2

This thesis is the result of my own independent work/investigation, except where otherwise stated, and the thesis has not been edited by a third party beyond what is permitted by Cardiff University's Policy on the Use of Third Party Editors by Research Degree Students. Other sources are acknowledged by explicit references. The views expressed are my own.

Signed ……………………………………. (Hua Xiao) Date …............................

STATEMENT 3

I hereby give consent for my thesis, if accepted, to be available online in the University's Open Access repository and for inter-library loan, and for the title and summary to be made available to outside organisations.

Signed ……………………………………. (Hua Xiao) Date …............................

ACKNOWLEDGMENTS

I would fist like to express my deep gratitude to my supervisors, Dr Agustin Valera-Medina and Prof Philip J Bowen. I would not be in this department and have this wonderful educational experience if Prof Bowen and Dr Valera-Medina did not recruit me three years ago. Their illuminating guidance and enthusiastic encouragement contributed a lot to the completion of my thesis.

I also would like to thank the staffs of the Gas Turbine Research Centre, Dr Daniel Pugh, Mr Steve Morris, Dr Richard March, Dr Tony Giles, Gina Goddard, etc. I wish also to thank all the staff of the Research Office, Finance Office and the IT staff in School of Engineering for their help during my study period.

My great thanks also go to all my friends and colleagues in Cardiff especially those helped me a lot in using High-Performance Computing (HPC) cluster, Oula, Xiude, Peng, Zaid, Yue, etc. Their advice, expertise and good spirits have greatly helped me.

I would like to extend my thanks to Cardiff University and the China Scholarship Council for sponsoring my PhD study.

Lastly, but most importantly, my thanks go to my parents, especially my mother Victoria(Yongping) Wang, and my dear relatives for their persistent love, support and sacrifice.

ABSTRACT

The main objective of this thesis is to investigate the fundamental combustion process of ammonia-based fuels and the application on swirl-stabilised flames in the context of engineering type gas turbine combustion. The present study begins with a fundamental validation and mechanism reduction for chemical kinetics of ammonia/methane combustion. Different-sized reduced mechanisms of the well-known Konnov's mechanism were compared at high-pressure conditions relevant to gas turbine devices. The reduced models can benefit the future simulation work with considerably less computational cost. Then characteristics of ignition delay time, laminar flame speed and emissions were obtained over a wide range of equivalence ratios and ammonia fractions. Prediction results showed a good potential of ammonia/methane to be used in gas turbine engines with relatively low emission.

In the second part of this dissertation, in order to identify reaction mechanisms that can accurately represent ammonia/hydrogen kinetics at industrial conditions, various mechanisms were tested in terms of flame speed, combustion products and ignition delay against experimental data. It was preliminarily found that the Mathieu mechanism and Tian mechanism are the best suited for ammonia/hydrogen combustion chemistry under practical industrial conditions. Based on the Mathieu mechanism, an improved chemical mechanism was developed. Verification of the established model was quite satisfying, focusing particularly on elevated conditions which are encountered during gas turbine operation.

Finally, a first assessment of the suitability of a chosen 70%NH_3-30%H_2 (%vol) blend was performed for utilisation within a gas turbine environment. It was found that stable flames can be produced with low NO_x emissions at high equivalence ratios. Also, results showed that high inlet temperature conditions representative of real gas turbine conditions can significantly improve the combustion efficiency and reduce NO_x emissions. A numerical gas turbine cycle calculation was performed indicating more research are required to enable higher efficiencies using ammonia/hydrogen.

PUBLICATIONS

[1] Xiao, H., Valera-Medina, A. and Bowen, P.J., 2017. Study on premixed combustion characteristics of co-firing ammonia/methane fuels. Energy, 140, pp.125-135.

[2] Xiao, H., Valera-Medina, A. and Bowen, P.J., 2017. Modeling combustion of ammonia/hydrogen fuel blends under gas turbine conditions. Energy & Fuels, 31(8), pp.8631-8642.

[3] Xiao, H. and Valera-Medina, A., 2017. Chemical kinetic mechanism study on premixed combustion of ammonia/hydrogen fuels for gas turbine use. Journal of Engineering for Gas Turbines and Power, 139(8), p.081504.

[4] Xiao, H., Valera-Medina, A., Marsh, R., & Bowen, P. J. (2017). Numerical study assessing various ammonia/methane reaction models for use under gas turbine conditions. Fuel, 196, 344-351.

[5] Xiao, H., Howard, M., Valera-Medina, A., Dooley, S., & Bowen, P. J. (2016). Study on reduced chemical mechanisms of ammonia/methane combustion under gas turbine conditions. Energy & Fuels, 30(10), 8701-8710.

[6] Xiao, H., Howard, M.S., Valera-Medina, A., Dooley, S. and Bowen, P., 2017. Reduced chemical mechanisms for ammonia/methane co-firing for gas turbine applications. Energy Procedia, 105, pp.1483-1488.

[7] Xiao, H., Valera-Medina, A., Bowen, P. and Dooley, S., 2017. 3D simulation of ammonia combustion in a lean premixed swirl burner. Energy Procedia, 142, pp.1294-1299.

[8] Xiao, H., Wang Z., Valera-Medina, A., Bowen, P. Study on characteristics of co-firing ammonia/methane fuels under oxygen enriched combustion conditions. (Accepted by Journal of Thermal Science)

[9] Valera-Medina A., Gutesa M., Xiao H., Pugh D., Giles A., Goktepe B., Marsh R., Bowen P. Premixed ammonia/hydrogen swirl combustion under fuel-rich conditions for gas turbines operation. (Submitted to Proceedings of the Combustion Institute)

[10] Valera-Medina A., Xiao H., Owen-Jones M, David W.I.F., Bowen P. Ammonia for power. (Submitted to Progress in Energy and Combustion)

TABLE OF CONTENTS

LIST OF FIGURES

LIST OF TABLES

NOMENCLATURE

Alphabetic Symbols

A_i	Pre-exponential factor	cm^3/(mol·s) (for 2nd order reaction) and 1/s(for 1st order reaction)
c_p	Constant-pressure heat capacity	J/(kg·K)
c0	Mixture concentration of the feed	mol/m^3
c	Mixture concentration in the reaction zone	mol/m^3
c1	Mixture concentration at the exit	mol/m^3
${D_k}^T$	Thermal diffusion coefficient for species k	m·m/s
$D_{k,j}$	Ordinary multicomponent diffusion coefficients	m·m/s
E_i	Activation energy of the reaction	cal/mol
e	Mixture internal energy	J/kg
F	Residual vector	
h_k	Specific enthalpy of the kth specie	J/kg
k_{f_i}	Forward rate constant of the ith reaction	mol/(L·s)
k_{r_i}	Reverse rate constant of the ith reaction	mol/(L·s)
K_{c_i}	Equilibrium constant of the ith reaction	dimensionless
$\dot{M}$	Mass flow rate	kg/s
P	Pressure	Pa
$\mathbf{q}$	Heat flux	J/m^2
q_i	Rate of progress variable for the ith reaction	mol/(m^3·s)
Q	Reactor heat loss	J
R_c	Universal gas constant	kJ/(kmol·K)
$\tilde{S}_{ij}$	Filtered strain rate tensor	dimensionless
T	Temperature of the reaction	K
T_{ad}	Adiabatic flame temperature	K
$\mathbf{u}$	Velocity vector	m/s
V	Reactor volume	m^3
ν_k	Ordinary diffusion velocity	mol/(m^2·s)
$\bar{W}$	Mean molecular weight of the mixture	kg/mol
w_k	Thermal diffusion velocity	K/(m^2·s)
x	Spatial coordinate	m
X_k	Molar concentration of the kth species	mol/m^3
Y_k	Mass fraction of the kth species	dimensionless

Greek Symbols

κ	Mass fraction of the reacting zones	dimensionless
β_i	Temperature exponent of the ith reaction	
λ	Thermal conductivity of the mixture	m^2/s

ρ	Density	kg/m^3
τ_{res}	Residence time	s
τ_{ij}	Viscous stress	Pa
τ_c	Chemical time scale	s
τ_{mix}	Characteristic time for turbulence	s
ν	Kinematic viscosity	m^2/s
χ_k	Chemical symbol for the kth species	
$\overline{\omega}_k$	Filtered chemical reaction rate	$mol/(m^3 \cdot s)$
$\dot{\omega}_k$	Net rate of production the k th species	$mol/(m^3 \cdot s)$
Δ	Filter width	m
ϕ	Solution vector	

LIST OF ABBREVIATIONS

atm	A unit of atmospheric pressure
CO	Carbon monoxide
CO_2	Carbon dioxide
CFD	Computational fluid dynamics
CRN	Chemical reactor network
CRZ	Central recirculation zone
CH_4	Methane
DLN	Dry low NO_x
DNS	Direct numerical simulation
DRG	Directed relation graph
E.R.	Equivalence ratio
EXP.	Experimental data
GTRC	Gas turbine research centre
HPOC	High pressure optical chamber
H_2	Hydrogen
LES	Large eddy simulation
LDV	Laser Doppler velocimetry
MILD	Moderate or intense low oxygen dilution
NH_3	Ammonia
NO_x	Nitrogen oxides
PaSR	Partially stirred reactor
PIV	Particle image velocimetry
PSR	Perfectly stirred reactor
ppm	Parts per million
RANS	Reynolds-averaged Navier-Stokes

CHAPTER 1

Introduction

Chapter 1

1.1 Future Energy Challenges

Since the Industrial Revolution the demand for energy has been growing rapidly mainly due to the development of industry and the increase of population. At the present time, the world's energy consumption is still highly dependent on traditional fossil fuels. For instance, about 70% of the world's electricity production is from carbon-intensive fossil fuels like coal, petroleum, natural gas, etc. [1, 2] However, it is predicted that production rates of traditional fossil energy are limited whilst the ever-rising demand for fossil fuel worldwide will keep increasing. Thus, a growing mismatch will possibly emerge in the future between the demand and supply of fossil fuels [1]. Also, since conventional fuels are non-renewable, the expense is becoming much higher than ever. As power generation, transportation and many other industries highly rely on fossil energy sources, the challenges and uncertainties of energy supply can threaten the energy security of a country.

On the other hand, combustion products of fossil fuels have caused serious environmental pollution problems, such as acid rain, photochemical smog, ozone layer depletion, etc. Also, it is considered that climate changes are caused by carbon dioxide emissions which are mainly from the excessive consumption of traditional fossil fuels since the industrial revolution[3]. The adverse impact of excessive fossil fuels, which can even lead to gloomy prospects of our whole planet's ecosystem, is now the main topic of study.

A possible solution to these problems is to replace current fossil fuel systems with new systems capable of utilising novel and renewable fuels. In this way, stable energy sources can be used to achieve less emission discharges. Thus, requirements for new generation of both fuels and power equipment are becoming stronger.

1.2 Ammonia as a Green Fuel

As discussed above, under such severe situations, in order to satisfy the growing demand for energy consumption all over the world and simultaneously protect our ecosystem from pollution and global warming, it is estimated that more than 10^6 W of carbon-free power needs to be produced by the middle of the century [4]. Options include decarbonisation of fossil fuels, nuclear energy and many kinds of renewable sources. Among these hydrogen energy [5] is quite attractive, as many relevant studies have suggested using hydrogen from renewable energy resources as an ideal future fuel. In fact, hydrogen has a high heating value and its advantage in burning efficiency makes it one of the best alternative fuels. Besides, hydrogen itself is not pollutant and its main combustion product is only water, which is totally environmentally friendly. However, several technical difficulties still lie in storage, transportation and distribution of hydrogen, which are still tough to overcome for the implementation of using hydrogen as a fuel at large sales. Issues associated with hydrogen have led to consideration of other molecules such as ammonia as a potential energy carrier candidate.

Ammonia, as an excellent hydrogen carrier, has attracted lots of attention due to its advantages in aspects like storage and delivery compared to hydrogen [6, 7]. Ammonia's hydrogen content is high (17%) and it can also be utilised through decomposition into hydrogen and nitrogen using low energy. Unlike hydrogen, ammonia can be compressed to liquid form at ambient temperature, which is a convenient way of storing hydrogen and a good choice for transportation. In fact, as a major product of chemical industry, the yield of ammonia is over 176 million tons every year [7, 8]. Thus, it is widely used as fertilizer, refrigerant, cleanser, fermentation agent and there are already experience and facilities for its storage, safe handling, transportation and distribution networks available worldwide. Specifically, anhydrous ammonia is distributed across the world via pipelines, railroads, barges, ships, road trailers and storage depots. Long term experience of ammonia distribution from the first quarter of the twenty-first century has facilitated the global deployment of this chemical, ensuring that well established distribution networks exist across the planet. For instance, in the USA, the NuStar Line (3,070 km long) moves ammonia from Mississippi into the heart of the corn-belt region of the central and northern States of the union, where it is distributed even further via the Magellan line (~1,900 km long). Both lines approximately deliver 2.9 million tons of ammonia per year [9]. In Eastern Europe, a line that runs from TogliattiAzot's plant (Tolyatti, Samara) to Odessa in the Black Sea is one of the largest (~2,400 km long) with a capacity of 3 million tons per year[10]. Also, Western Europe alone moves around 1.5 million tonnes of ammonia by railway every year. Greater quantities are transported by this mean in the United States using insulated tank cars capable of storing up to 33,500 gallons of the chemical [11].

Besides the advantages in storage and transportation of ammonia as hydrogen vector, the potential of utilising ammonia directly as a fuel has been drawing more and more attention in recent years. Just like hydrogen, ammonia (NH_3), has the potential to replace fossil fuels in many areas such as transportation, power generation, etc. For instance, it has a high octane number of 110 –130 so it is a good fuel for internal combustion engines. Ammonia yields only water and nitrogen as combustion products when it is completely burned. There is also no carbon dioxide or soot emissions when burnt, indicating combustion of ammonia can have certain advantages over fossil fuels. Currently ammonia can be produced with Haber–Bosch process with methane as feedstock and also by gasification of coals in Synthetic NH_3 industry. Studies are also being performed to synthesize ammonia from water and air using alternative energies (e.g. wind, solar, nuclear) in which carbon-free hydrogen feedstock can be used for ammonia manufacturing. These technologies can also take advantage of current fuel infrastructure to have little environmental impact. In addition, in terms of practical implementation, it is safer than hydrogen and various fuels in many aspects. It has a narrow flammability range so it is generally considered non-flammable. It is also easy to be detected by smell at concentrations as low as 5 ppm [12] when there is any leakage. Moreover, it dissipates rapidly in atmosphere since its density is lower than air. These safety related properties will help to utilise ammonia as a realistic energy solution that makes sense. In sum, the various advantages in production, storage, transport and utilisation of ammonia will offer it a quite promising prospect of playing an important role in future energy systems as a green sustainable fuel.

1.3 Gas Turbine for Power Generation

Gas turbines are a type of internal combustion engines that convert chemical energy into mechanical energy. A typical gas turbine is composed by three components: an upstream compressor coupled to a downstream turbine and a combustor in between. When a gas turbine is working, pressure of incoming atmospheric air flow is firstly increased through a compressor. Then the air is mixed with fuel and the air/fuel mixture is ignited to increase the temperature in a combustor. In this way, chemical energy of the fuel is converted into heat of the air/fuel mixture. The high temperature and high pressure gas then expands through a turbine shaft generating a work output, while the energy not converted comes out of the turbine in the exhaust gases with exhaust pressure and temperature. Part of the turbine shaft work is then used to drive the compressor and the remaining part is useful for other devices such as an electricity generator.

When it is used for electricity generation, a gas turbine is at the heart of a power plant. Gas turbines for power generation can utilise a range of gaseous and liquid fuels such as natural gas, oil and even low calorific value fuel. It also has advantage in higher fuel efficiency and lower emissions than traditional coal fired steam turbine generation systems. Typically, a large single-cycle gas turbine producing 100 to 400 megawatts of electric power has a thermal efficiency of 35–40% and by recovering waste heat with a combined cycle configuration, the efficiency of gas turbine power plant can reach up to about 60 percent. Also, comparing with renewable energy sources such as wind power and solar energy, gas turbine power generation has the advantage in providing stable and controllable electricity output, which is a weakness for renewable energy systems due to their intermittency and the non-dispatchable nature. At the same time, those near disaster nuclear scenarios experienced or witnessed in the world have led to decisions in countries like Germany to move away from nuclear facilities whilst being in favour of much safer and controllable gas turbines. As a consequence, gas turbines have become one of the most widely-used technologies in power generating sector increasing dramatically worldwide. Actually, nowadays stringent emission reduction targets to reduce greenhouse gas emissions are further stimulating the growth of the gas turbine industry. Many countries such as the U.S. and UK etc. have already made various action plans to meet their growing electricity energy demand using cleaner sources. For instance, natural gas has fuelled about 25 percent of the total electricity generation in U.S. and the government is targeting to increase the power from gas fired stations to 30% by 2025 while the UK government is targeting to shut down all the coal fired power plants by 2025 in order to fulfil its clean energy commitment [13]. Thus the strong stimulus will continue to bring a significant development for gas turbine electric power generation industry over the forecast timeline as shown in Figure 1-1. Quantitatively, it is predicted that a world market for 5,480 industrial power generating gas turbine units will be produced over the next 10 years [14].

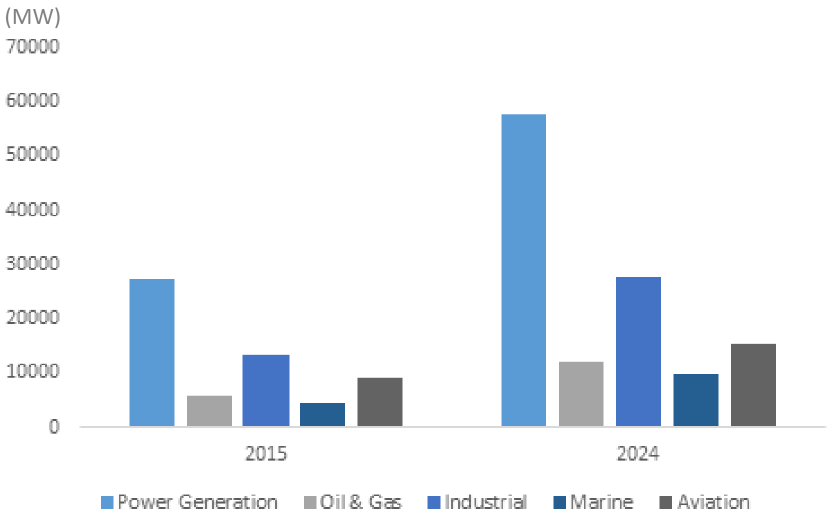


Figure 1-1 Global gas turbine market, by application, 2013 - 2024 (MW) [13]

1.4 Ammonia for Power using Gas Turbine

As the power generation sector is still faced with great pressure to reduce pollution and carbon dioxide emissions, gas turbine power generation industries are also seeking to expand the capabilities of utilising novel renewable fuel sources. Besides, the problem of fuel shortages, supply interruptions and price constraints can cause considerable economic and electric reliability risks for countries and regions. To mitigate the energy security risks many countries are taking fuel flexibility as a significant concern to ensure dependable source of electricity, thus also requiring multi-fuel capability for new gas turbine power plants. Nowadays, acceptable fuels for gas turbine mainly include conventional petrol, natural gas, propane, kerosene, diesel as well as renewable sources such as biodiesel, syngas, E85, biogas, etc. In this study, ammonia is proposed as a novel alternative fuel source for gas turbine use.

Actually, it is already proposed and verified the possibility of employing ammonia as a primary fuel in engines, with a vast number of application cases of internal combustion engines [15-17]. However, power obtained from such units is relatively modest, typically in the 0.1 – 1 MW range. While as discussed in the previous section, ammonia is a green fuel that can be used for cooling, transportation and storage of integrated systems based on combustion processes, therefore potentially it can deliver good amounts of energy for industrial applications on a large scale.

Thus similarly responsive as internal combustion engines but larger power generators will be required to meet the demands of electrical grids for ammonia application as a fuel. In this situation, considering the status of gas turbine in electric power generation, using “green” ammonia in gas turbines for power generation is supposed to be an interesting proposition. As mentioned in previous sections, the great advantages and potential as a green fuel has already indicated the feasibility of ammonia for power generation application in gas turbine industry.

The general goals of ammonia’s combustion in gas turbine are high combustion efficiency, high combustion temperature, good flame stability and as less emissions as possible. However, the design of modern gas turbine for power generation is mainly dependent on the operating experience of natural gas, therefore there are still challenges associated with achieving good combustion performance for the design and study of gas turbines using ammonia. Ammonia is technically considered non-flammable with a high auto-ignition temperature (650 ºC), which reduces the direct use of pure ammonia combustion in gas turbines. Therefore combustion promoters are needed to enhance the ammonia combustion. However, when using ammonia and combustion promoters typical stability issues will arise such as flashback, blow-off and thermo-acoustic oscillations. Besides, gas turbine operation is a highly complicated process. Pressure drop, corrosion of metals, inlet temperature distribution of turbine, toxicity, etc. are also practical considerations for ammonia-fuelled combustor. Pollutants are also an essential concern of modern equipment for the more stringent environment protection regulations nowadays. Importantly, to use ammonia in gas turbines, emissions reduction is a key issue, mostly for NO_x. In fact, the emission formation in a specific combustor is highly complex. Factors such as flow field, temperature, pressure, combustion kinetics, heat transportation, etc. are coupled with each other highly nonlinearly. Thus a large amount of studies are needed to explore factors influencing the emission of combustion using ammonia blends in gas turbines, so that strategies can be developed to reduce the pollutants and improve reliability in this equipment. Nowadays, there are also some novel low emission combustion technologies available for gas turbine such as steam injection, lean premixed combustion, catalytic combustion, etc. In sum, many aspects of research are needed for the application of ammonia for power in gas turbines.

1.5 Objectives and Scope

In this study ammonia is explored to be used in gas turbine combustor as a novel green fuel for power generation. The general goal of the study is to achieve satisfying performance of gas turbine combustors using ammonia as the primary fuel in various blends. To achieve this goal, different levels of investigations were performed including chemical kinetics analysis of combustion, numerical modelling and experimental campaigns for premixed ammonia-based fuel blends in laboratory scale gas turbine combustors.

Objectives of this study:

1 To verify and optimise the performance of prediction accuracy and efficiency for detailed chemical kinetic mechanisms, and use them to study combustion characteristics of ammonia as a renewable fuel for gas turbine use.

2 To gain a deep understanding on the characteristics of fundamental combustion properties of ammonia-based fuel mixtures. Numerical simulations are used to investigate ammonia-based fuel mixture flames providing spatial and temporal information experimentally inaccessible. Combustion simulations with a proper detailed chemical reaction mechanism can help to find the way and feasibility of implementing ammonia as a primary fuel.

3 To obtain detailed and reliable experimental data for stable and clean combustion of ammonia-based fuel blends in a gas turbine combustor. A generic tangential swirl burner is used to determine flame stability and emissions produced at different conditions such as equivalence ratio (ratio of the actual fuel/air ratio to the stoichiometric fuel/air ratio), fuel blends, inlet temperature, etc.

1.6 Outline of this Thesis

Chapter 1 is to state the background and objectives of this thesis.

Chapter 2 provides the presentation of literature review on ammonia combustion related to gas turbine applications and chemical kinetics studies.

Chapter 3 provides the basic theory for chemical reaction mechanism, numerical models of premixed flames and experimental setup of gas turbine combustors all used in this project.

Chapter 4 shows numerical analysis on ammonia/methane flames.

Chapter 5 shows numerical analysis on ammonia/hydrogen flames.

Chapter 6 describes the experimental investigation results of ammonia/hydrogen blends in a swirl burner. Flame stability and emission characteristics under different conditions are discussed in this chapter.

Chapter 7 makes a general discussion of all the results in order to provide guidance for future works.

Chapter 8 provides some conclusions and suggestion for future works.

CHAPTER 2

Progress in Ammonia Combustion Research

Chapter 2

2.1 Fundamental Ammonia Combustion

To develop combustion-based technologies for ammonia utilisation, it is essential to have a deep understanding of the detailed chemical process in the ammonia combustion phenomenon. Therefore, research has been dedicated to understand the fundamental characteristics of ammonia and the reactions that occur throughout the combustion process.

As early as 1960s, studies [18, 19] started to be performed to understand the chemical reactions of flames containing ammonia. Then a wider range of compositions and conditions were investigated to gain more insight into kinetics of ammonia contained flames [20-22]. For instance, Soete et al. [23] from measurements carried out on flat premixed hydrocarbon/oxygen/argon added small amounts of ammonia, overall reaction rates of formation of NO and N_2 were determined and the importance of HCN molecules were identified as intermediates in the fuel NO. Davidson et al. [24] explored the mechanism of ammonia pyrolysis over a wide range of conditions behind reflected shock waves. In their work, quantitative time-history measurements of the species NH and NH_2 were made.

The first complete description of detailed chemical mechanism for ammonia oxidation was proposed by Miller and Bowen [25] based on ammonia combustion experiments. The comparison between the theoretical kinetic model and experimental data illustrated good performance of the Miller mechanism for ammonia combustion over a range of temperature, equivalence ratios and pressures, especially for the NO_x chemistry. Actually in this study, mechanisms for NO_x formation and removal process are carefully considered of which important elementary reactions and their coefficients are provided. It is analysed that the NO/N_2 production is mainly depended on the fate of NH_x radicals, which is oxidised to NO through nitroxyl (HNO). Miller's mechanism has been proved in several ammonia combustion studies [26-28].

Based on the Miller [25] mechanism, Lindstedt et al. [29] developed a chemical kinetic mechanism model for ammonia oxidation in a wide range of flat laminar flames. Important elementary reactions were recognised in NO formation process for neat ammonia and doped lean hydrogen flames. It is found that Zeldovich mechanism is responsible for the NO formation and conversion with more fuel concentration of ammonia/hydrogen flames while reaction NH+OH is playing a more significant role in NO formation of neat ammonia flames.

Skreiberg et al. [30] established a detailed chemical kinetic model for ammonia oxidation in the presence of hydrogen, carbon monoxide, and methane. The H/N/O submechanism draws primarily on Miller's work on ammonia flames. In the mechanism, several reactions were characterised more accurately and the mechanism model satisfactorily predicts flow reactor measurements data. It summarised low temperature will promote the reaction path $NH_3 \rightarrow NH_2 \rightarrow N_2$, whilst $NH_3 \rightarrow NH_2 \rightarrow NH \rightarrow N$ is important at higher temperatures. Lindstedt's model has also been employed in several ammonia combustion studies [26, 31, 32].

Among the detailed mechanisms proposed for ammonia combustion, Konnov's kinetic model [33] was a widely used and verified one, proving a better performance on the prediction of NO_x emission and propagation among many mechanisms available [32, 34-37]. This detailed chemical kinetic mechanism [38] was originally developed for the combustion of small hydrocarbon fuels considering the presence of ammonia. The mechanism model has been updated continuously and in the latest version the model was much improved compared to previous versions, in which particular attention has been paid to the upgrading of the H/N/O submechanism in the development of the model. Specifically, with the improved implementation of NCN pathway, a more accurate calculation result of NO formation and NCN radicals in the flame were obtained. It has been tested against experimental data available for oxidation, ignition, and flame structure of mixtures of nitrogen-containing species, hydrogen, carbon monoxide and hydrocarbons in his model establishment study.

Duynslaegher et al. [39] found in their stabilised flame experiments of ammonia–oxygen–hydrogen mixtures that using the Konnov mechanism will overestimate the mole fraction profiles of radical NH_2 while underestimate the ones of N_2O. In this situation, Duynslaegher et al. [40] improved Konnov's ammonia combustion mechanism model by modifying the reactions containing nitrous oxide (N_2O) and amidogen radical (NH_2). In the work Duynslaegher et al, rate constants modifications for four elementary reactions $NH + NO = N_2O + H$, $N_2O + H = N_2 + OH$, $NH_2 + H = NH + H_2$, $NH_2 + NH_2 = N_2H_2 + H_2$ were performed on the base of the Konnov mechanism. As NH_2 is the main intermediate in the oxidation of ammonia and therefore the precursor related to the formation of almost all the combustion products, the improvement of NH_2 radical profile prediction lead to a significant prediction improvement on radicals such as nitrous oxide, nitrogen monoxide and the amidogen radical. In this study a reduction version of the mechanism model was also provided for the use in internal combustion engine conditions.

The Tian mechanism [41] was developed based on $NH_3/CH_4/O_2/Ar$ flame data under low pressure conditions. In Tian's research, profiles of combustion intermediates and products were determined in 11 premixed flames of different mole ratios of NH_3/CH_4. The updated chemical mechanism model by Tian et al. satisfactorily identified detailed flame structure features. The model and experiments showed that with more ammonia fraction in the fuel mixtures the products of H_2O, NO and N_2 increase whilst those of H_2, CO, CO_2 and NO_2 indicate reverse tendencies. The pathway analyses performed with the mechanism model have demonstrated the key reactions in the mechanism such as $H + O_2 = O + OH$, $NH_2 + O = HNO + H$, $NH_2 + NO = N_2 + H_2O$ and $NH + NO = N_2O + H$, which have prominent effect for NO and N_2 conversion. Also key species such as CH_3, CH_2, CH_2O, NH_2, NH and HNO were identified in the oxidation of CH_4/NH_3 mixtures. Tian's mechanism has been more widely used recently over a wide range of conditions [35, 42].

Mendiara and Glarborg [43] also conducted an experimental study in a laminar flow reactor and developed a chemical kinetics model for NH_3 oxidation in oxy-fuel combustion of CH_4/NH_3 with a temperature range from 973 to 1773 K. The reactor in the experiments was operated under atmospheric pressure conditions and stoichiometries between 0.13 and 0.55 equivalence ratio. The kinetic mechanism model is based on the Tian mechanism describing CH_4/NH_3 oxidation especially extending hydrocarbon/amine interaction subset. Through pathway analysis it was identified that the formation of NO is mostly related to HNO as intermediate of which the primary source is from NH_2+O. This detailed chemical mechanism also successfully captured experimental trends for the effects of high CO_2 concentration.

Mathieu and Petersen [44] studied the oxidation of ammonia under high temperatures (1560–2455 K) and high pressures (around 1.4, 11, and 30 atm) conditions. A detailed mechanism model was established for ammonia oxidation of shock tube experiments.

It also provided a state-of-the-art NO_x sub-mechanism which can be used for a wide range of conditions. The established chemical mechanism has proved satisfying accuracy in predicting ignition delay times of ammonia oxidation under elevated conditions, which are more relevant to many industrial applications.

There are some other detailed chemical mechanisms, which are originally developed for hydrocarbon fuels, also potentially able to be used in ammonia combustion study. For instance, the famous GRI Mech 3.0 mechanism [45] is extensively used for combustion of natural gas, which includes the formation of NO_x and reburn chemistry. GRI-Mech 3.0 mechanism is also used as reference for NH_3 oxidation [32, 35, 46], since ammonia-doped methane/air flames using this mechanism have also been studied in the past with satisfactory results [47]. Åbo Akademi (ÅA) kinetic reaction scheme [48] was created for the combustion of biomass-derived gases under moderate temperature and validated in the flameless ammonia chemistry study in [49].

In addition, in recent decades numerous studies have been performed investigating various properties for different types and conditions of ammonia related combustion and flames. As for the combustibility of ammonia, in the experiments of Shebeko et al., [50] flammability limits for ammonia/oxygen and ammonia/hydrogen/oxygen mixtures were studied at temperature and pressure of up to 70°C and 1.0 MPa respectively. It was identified that the lower concentration limit of ammonia/oxygen flame decreases significantly at elevated temperature and pressure. Pfahl et al. [51] also studied the flammability limits, ignition energies, and flame speeds of different ammonia contained mixtures experimentally. The experiments were carried out in a closed combustion vessel at initial pressures of 100 kPa and temperatures of 295 K. The ignition energy experiment results of lean ammonia–nitrous oxide mixtures indicate that under high ignition energies (higher than 5000J) the initiation of combustion occurs independent of fuel amount of ammonia, while there is an obvious minimum concentration of ammonia fuel for low ignition energies (up to 10J). It is also shown that increasing the initial amount of nitrous oxide in ammonia–air–nitrous oxide gases increases the laminar flame speed clearly.

Laminar flame speed is an important combustion property, i.e. a combination of the burning rate and density ratio as an important parameter in understanding the fundamentals of a particular flame. Takizawa et al. [52] measured the flame speed for

NH_3/air mixtures of different stoichiometry by the spherical vessel method under atmospheric conditions, obtaining a maximum value of 7.2 cm/s at equivalence ratio of 1.10.

To determine the impact of practical conditions such as elevated ambient temperatures and pressures on the combustion of ammonia, analysis using premixed ammonia–air mixtures with equivalence ratios around unity, at conditions which are encountered during spark-ignition (SI) engine operations have also been performed. Duynslaegher et al. [31] numerically investigated laminar flame speed and NO_x emission concentrations of premixed ammonia combustion using Konnov's mechanism at elevated pressure and temperature conditions (1–49 atm., 298–732 K) which are relevant to engine operational conditions. In this study, corresponding to a 40% increase in compression ratio, the laminar flame speed increases up to 30% whilst a difference of 100K is noted for the adiabatic flame temperature. It is suggested that both equivalence ratio and compression ratios have an important impact on the adiabatic flame temperature and laminar flame speed while equivalence ratio is the major factor influencing the NO formation.

Then Hayakawa [32] evaluated the flame speed for spherically propagating premixed flames of ammonia/air under elevated conditions. It was the first experimental work that clarified the decrease of flame speed under high pressure condition up to 0.5 Mpa. At the same time, Li et al. [53] numerically investigated the ammonia combustion characteristics under oxygen enriched conditions and proposed it as a potential method to improve ammonia combustion performance such as flame speed.

As characterisation of emission profiles of species such as NH_3, O_2, H_2O, N_2O and NO [182] are crucial in gaining understanding and confidence in the behaviour of reaction mechanisms with ammonia fuels, in the work of Brackmann et al. [54] data were provided of OH, NH and NO profiles for premixed ammonia/air flames using contemporary laser-induced fluorescence at atmospheric pressure. The kinetics analysis with the experimental data showed that the Mendiara mechanism performes best prediction for temperature, radical profiles and flame front positions.

As for ignition characteristics of ammonia, Nakamura et al. [55] performed an experimental study for stoichiometric ammonia/air mixtures in a micro flow reactor.

In this study ignition characteristics at low temperatures (ambient temperature to 1300 K) were specifically examined as previous experimental work [44] only investigated ammonia oxidation under high temperature conditions around 2000K.

It is well known that the slow reaction of ammonia requires promotors to improve its combustion performance. Doping ammonia with faster reactants has always been considered the most practical solution to counter the low reactivity. Hydrogen is a famous alternative green fuel with unique features such as carbon-free, high reactivity and flame speed. Thus, doping hydrogen has been widely investigated to determine fundamental flame characteristics especially in the recent decades.

As for the flammability, extinction limits and structure of hydrogen doped ammonia/air flames, Ciccarelli et al. [56] explored the flammability map of ammonia and ammonia/hydrogen mixtures in air at the initial temperature up to 600 °C and atmospheric pressure conditions. The flammability map showed to widen linearly with increased initial temperature. It was also shown that as the mixture fraction of the ammonia dissociation products increased in mixtures of ammonia and hydrogen and nitrogen - the ammonia dissociation products, the flammability limits tend to widen. Shmakov [37] also provided updated experimental data of flat premixed burner-stabilised $H_2/O_2/N_2$ flames, doped with 300–1000 ppm of ammonia, figuring out that further attempts need to be paid to kinetics model improvement. Lee and Kwon [57] numerically studied counterflow nonpremixed ammonia/hydrogen/air flames at normal temperature and pressure to improve the safety of hydrogen use. Effects of ammonia on reducing high-stretch extinction limits of hydrogen/air flames were identified. Um et al. [27] experimentally examined the combustion stability limits and nitrogen oxide emissions of non-premixed ammonia/hydrogen/air flames at normal temperature and pressure conditions. It justified the potential of NH_3 substitution for improving the safety of H_2 combustion with significant reduction observed in stability limit. Choi [58] explored the potential of using H_2 as an additive for improving the reactivity and ignition of nonpremixed NH_3/air flames. The extinction limits, flame temperature and morphology of the counterflow nonpremixed ammonia/hydrogen/air flames are experimentally determined at elevated temperatures and normal pressure. Results showed enhanced blow-off limits and the maximum flame temperature with hydrogen substitution in ammonia /air flames.

When using ammonia as a potential alternate with hydrogen added, the characteristics of flame propagation and NO_x emissions are essential concerns in ammonia-based flame studies. Lee et al. [26] tested laminar premixed hydrogen-added ammonia/air flames in terms of flame speed and NO_x and N_2O emissions. The results suggested hydrogen as a promising additive for improving the combustion performance with low NO_x and N_2O emissions under fuel-rich conditions. Furthermore, studies [28] were performed by the same group on the effect of ammonia substitution on ammonia/hydrogen/air flames both experimentally and computationally. The results showed that ammonia substation will significantly reduce laminar flame speed and increase nitrogen oxide emissions of hydrogen/air flames. It was also found that nitrogen oxide emission of fuel rich conditions is much lower than fuel lean conditions. Joo et al. [59] studied burner stabilised premixed flames of ammonia/hydrogen/air mixtures in experiments by measuring combustion stability limits and nitrogen oxide emissions at normal temperature and pressure conditions. The substantially reduced combustion stability by ammonia substitution suggested the potential of ammonia as additive in hydrogen combustion to improve safety. Kumar and Meyer[35] performed a series of measurement of laminar flame speed for ammonia/hydrogen/air jet flames. In this study, ammonia fraction within the fuel was varied in step increases of energy delivered up to a maximum of 80% for equivalence ratios between 0.5 and 1.1. Computational models were developed using the GRI-Mech 3.0, Tian, and Konnov reaction mechanisms. Numerical calculations on laminar flame speed considering heat loss showed that Konnov mechanism and Tian mechanism have good prediction accuracy against experimental data, highlighting production of the OH radical as the key performance variable in modelling laminar NH_3 decomposition. Duynslaegher et al. [39] studied the structures of diluted ammonia/hydrogen/oxygen/argon flames experimentally and numerically under low pressure conditions. The simulation work using the Konnov mechanism gives satisfying predictions against experimental data. It was also determined that the impact of hydrogen fraction varying from 5% to 12.5% is not significant on the composition of burned gas. Li et al. [60] experimentally investigated premixed hydrogen/ammonia combustion at a wide range of equivalence ratios and initial hydrogen concentrations in the fuel mixture. It identified that hydrogen has an accelerant role in hydrogen/ammonia/air combustion, while ammonia has a major detrimental effect in laminar flame speed. In addition, fuel-NO_x has a dominant role and thermal-NO_x has a negligible role in hydrogen/ammonia/air combustion. It was observed that thermal-NO_x decreases in hydrogen/ammonia/air combustion compared with pure hydrogen/air combustion, while NO_x concentration reached its maximum at the stoichiometric condition. Ammonia was also found to be completely bunt with the addition of hydrogen. In the research of Ichikawa et al. [61], hydrogen/ammonia/air flames were experimentally and numerically investigated and found that flame speed increased exponentially as the hydrogen fraction in the blend was increased, reaching a similar order of magnitude observed for conventional hydrocarbon flames when the hydrogen fraction in the fuel is 0.4.

Numerically, Nozari and Karabeyoglu [62] developed a reduced chemical mechanism for the combustion of ammonia/hydrogen based on the Konnov mechanism, which is aiming to expedite the design of future ammonia combustors. Li et al. [63] numerically analysed the enhancement of hydrogen addition in ammonia flame speed and ignition. Reactions of $O+H_2=OH+H$, $H+O_2=OH+O$ and $H_2+OH=H_2O+H$ were identified as playing the most important role in the increased reactivity by hydrogen. At high temperature, these findings suggest that blow-off limits, the concentration of radicals H, OH and O and the maximum flame temperature are enhanced with H_2 substitution in benchmark NH_3/air flames, demonstrating that hydrogen doping could potentially facilitate the use of ammonia as a reliable alternative fuel, with increased laminar flame speed, reduction of emissions and positive changes in Markstein length.

As the main ingredient of natural gas, methane is also a possible promotor for ammonia combustion utilisation, which can be found in some previous combustion studies. Pfahl et al. [51] have measured the laminar flame speed of various ammonia-methane-hydrogen-nitrous oxide-nitrogen mixtures in air. It was found that increasing the initial concentration of fuel mixture or amount of nitrous oxide will lead to a higher laminar flame speed generally. Sullivan et al. [49] performed both experimental and modelling studies of a laminar ammonia-seeded methane diffusion flames. Within the conditions of this investigation, it was identified that with higher ammonia concentration, more percentage of ammonia is converted to N_2 rather than to NO. In the work from Henshaw et al. [64] the flame speed and combustion products of premixed NH_3-CH_4-air flames at atmospheric ambient conditions were measured using an adiabatic flat flame burner, complemented by CHEMKIN-PRO simulation.

This study was undertaken for equivalence ratios between 0.5 - 1.5 and for NH_3 fractions of 0% to 5% by volume in the fuel, as observed in some industrial processes. The measured flame speed agreed well with simulated results and the addition of 4% ammonia was seen to result in a 10% - 20% decrease in flame speed. Both simulations and experiments showed that adding NH_3 to CH_4-air mixtures resulted in an increase in NO_x concentration, especially at stoichiometric conditions, with a minimal effect on CO formation. Near the flammability limits, less than 0.1% of the incoming NH_3 penetrated the flame. Konnov [65] conducted an experimental study of methane/oxygen/nitrogen flames doped with ammonia (0.5% of the fuel), in which flame speed with different equivalence ratios was measured. Li et al. [66] studied ammonia-doped methane/air flames on a perforated plate burner at atmospheric pressure using laser-saturated fluorescence (LSF) and probe sampling for NO concentrations measurement. It is suggested that the results of ammonia conversion disagree with some other earlier experiments due to their lack of proper coating in cylinders. Also, the experimental results of NO_x formation were accurately reproduced by the flame modelling with the Konnov mechanism, which verified the capability in predicting ammonia conversion both in lean and in rich flames. Okafor et al. [67] provided data on the unstretched laminar flame speed of methane/ammonia/air mixtures with experiments using a constant volume chamber at 298 K and 0.10 MPa. Numerical results also identified it is through the H and OH radicals' concentration that ammonia chemistry impacts on the flame speed of ammonia/methane flame. As it can be seen from the review, most relevant studies take ammonia as a small amount of additive in the methane flames. Thus, more investigation will be needed if ammonia is going to be used as a primary fuel combusted with methane.

It is clear from all the current research that it is still the concern that knowledge gap exists related to the interaction of species and radicals at different conditions and fuel blends, thus prompting the research in these areas to create models that can accurately predict the behaviour of ammonia doped flames under conditions relevant to various conditions and practical industrial environments.

2.2 Ammonia as a Fuel in Internal Combustion Engines

As a potential chemical in combustion applications, ammonia can be used as fuel in internal combustion engines (ICE) for compression or spark ignition units. Similar to other alternative fuels such as ethanol, methanol, hydrogen and gasoline/diesel blends, the high octane of ammonia (~130) can improve combustion properties and reduce undesirable effects such as knocking [68].

The use of ammonia as vehicular fuel for motorised applications goes back as far as 1822 with a proposal from Sir Goldsworthy Gurney [69] where he developed an engine to drive a small locomotive. However, it was not until 1905 that the first small scale motor was developed by Ammonia Casale Ltd., who took out patents in Italy in 1935 and 1936 [70]. As early as 1933, Norsk Hydro operated an internal combustion engine vehicle on hydrogen produced from on-board reforming of ammonia [71]. Other devices followed with minor success. During World War II the scarcity of fossil fuels in some regions led to the search for alternative fuels for use in public transportation. Due to the lack of diesel in Belgium in 1942 Ammonia Casale was commissioned to implement their new patent based on a process that employed compressed gas and ammonia to replace diesel in the Belgian bus service. The so-called Gazamo process, was implemented in ~100 vehicles and continued until diesel fuel became plentiful enough [70].

In the 1960s, further developments ensued in the quest for alternative fuels for IC-Engines, driven by new environmental legislations and early signs of the energy crisis which would impact on economies the following decade. Development work on spark ignition reciprocating engines, fuelled by ammonia, was undertaken for military applications, as conventional engines had been shown to perform poorly with pure ammonia. In order to improve performance, propositions included increasing spark energy, compression ratio, supercharging the engine and adding hydrogen into the fuel through dissociation of NH_3 [72-74]. These developments showed that ammonia needed to be vaporised with at least 4-5% (by weight) H_2 for good performance. Use of CI engines also received considerable attention at that time [75-77]. Ammonia vapour and liquid ammonia were studied in diesel and spark ignition engines respectively, at high compression ratios. Although the tests at 30:1 compression ratio using the spark ignition engine were unsuccessful, the results using ammonia vapour and diesel (for ignition purposes) generated optimism for the success of using ammonia as fuel in IC engines. Then surprisingly, very little research and development was undertaken during the 1970-80s in this field. The literature concerning development of ammonia based engines is very sparse during this period, with the exception of the AMC GREMLIN at the University of Tennessee in 1974 [78]. The field experienced a revival in the 1990s, followed by a considerable increase in publications from 2004 onwards, with the first ammonia conference in the USA [18].

Up to now, ammonia fuelled engines have attracted the attention of various countries around the world as a promising technology that could contribute to a sustainable future. For instance, Boothroyd [79] recently proposed the use of ammonia storage from stranded energy resources in rural areas to power large scale manufacture near cities for Australia. Since ammonia distribution is still conducted in Australia by trucks, it has been proposed to replace long distance trucks by a fleet of ammonia-inflated airships. Similarly, Leighty [80] proposed the use of stranded, renewable energy sources in Alaska to produce ammonia that can be used as fuel for ICE/Fuel Cells/GTs for on-demand energy production and transportation.

Analyses of the feasibility of ammonia as a sustainable fuel in internal combustion engines based on thermodynamic performance, system effectiveness, driving range, fuel tank compactness and cost of driving have also been performed [12], [81]. Not surprisingly, the studies concluded that to make ammonia a viable fuel in ICEs, ammonia needs to be mixed with other fuels as combustion promoters due to ammonia’s low flame speed and high resistance to auto-ignition. This was confirmed from previous studies where a dual-fuel approach was usually chosen to implement ammonia combustion in IC engines [17, 82]. These works and others carried by Liu et al. [83] showed that ammonia fuelled engines have low power losses, no more corrosion and no more lubricant consumption than conventional fuels. Thus, due to the high interest in developing this technology, patents are under test evaluation for commercial release in the near future. A good reference to previous ammonia patents dating back to 1937 can be found in a patent submitted by Caterpillar Inc. in 2008 for an engine fuelled using ammonia [84]. Specific to this particular patent, ammonia has been used as primary fuel with electrical supplements to the mechanical power to drive a new power system capable of providing good combustion efficiency. The publication of ammonia energy has recognised other stakeholders in the development of ammonia fuelled engines, separating them into different categories [85]: Spark Ignition carbon based dual fuels, i.e. Biogas International (Italy), the Savia Coalition

(Italy), Green Transportation Technology Group (South Korea), Xiamen University (China), etc. Compression Ignition carbon based dual fuels, i.e. Sturman Industries (USA), Hydrofuel Inc (Canada) and Iowa State University (USA); Hydrogen doped ammonia engines, i.e. Toyota (Japan), Siemens (UK), etc.

2.2.1 Ammonia Blending with Carbon based Fuels

As previously presented, doping ammonia with other fuels has been considered one of the best solutions to improve ammonia combustion in ICEs. It has been demonstrated [86, 87] that high performance can be achieved using ammonia/gasoline fuelling, a three-way catalytic converter capable of cleaning emissions under stoichiometric and rich conditions over short and long distances [88]. Replacement of diesel with diesel/ammonia has also been attempted [16] showing promising results with modification to current diesel engines. Some of the results demonstrated that peak engine torque could be achieved by using different combinations of diesel and ammonia, with a monotonic CO_2 reduction for the same torque output for systematic NH_3 increase. Additionally, lower NO_x emissions were measured for ammonia fuel mixes not exceeding 60% NH_3 [89]. Combinations such as gasoline/ammonia and ethanol/ammonia [90], ammonium nitrate/ammonia [91] and even pure oxygen using 100% ammonia [92] have been also attempted, showing that these fuel mixtures can provide elevated power outputs under stable conditions, although mainly conditioned by the NO_x emissions product of the combustion process.

Direct gaseous ammonia injection has also been assessed in recent studies by Ryu [93] who showed a high correlation between the timing and duration of the injection of ammonia in a spark-ignition-engine. It was noted that the injection timing should be in the range of 320 to 370 BTDC for gasoline-ammonia fuel mixes. Due to slow flame-speed propagation of NH_3, the engine efficiencies were observed to be lower than the baseline performance. Finally, it was found that the emissions were slightly reduced for some species, i.e. carbon monoxide, though accompanied with an increase in NO_x and NH_3, as expected. Similar work has focused on blends of ammonia with commercially available emulsifiers such as ethanol or methanol that can enhance solubility of the blend [94]. Results proved that pure, liquid phase gasoline is capable of dissolving only 4.5% (vol) of ammonia at 345 kPa and 286.65 K, while the use of 10%(vol) of ethanol or methanol increased the solubility of ammonia to 11% (vol).

Further studies showed that gasoline with 30% ethanol or methanol can retain up to 17.35%(vol) ammonia [95]. At higher engine speeds, better engine performances in terms of increased torque and power output were observed for ammonia rich fuels compared to those for pure gasoline fuels. Thus, it was concluded that hydrogen can be stored as an ammonia-gasoline fuel blend and successfully recovered without major modification to the existing infrastructure of the engine [96]. The Korean Institute for Energy Research (KIER) has developed one of the most interesting new concepts for ammonia fuelled engine technology, which is to convert existing vehicle fleets into 70% NH_3 /30% gasoline vehicles [97]. The developers have converted an LPG-gasoline unit by adding a control system and removing the corrodible, copper containing metals - specifically the so-called ‘yellow metal’ high zinc brass. If the system was installed across 20% of the current Korean fleets, the country could reduce CO_2 emissions by 10 million tons annually, thus aiding their future targets on climate change mitigation.

Numerical simulations of co-fuelling reciprocating engines with ammonia have also been conducted to determine best operating conditions of industrial and transportation engines. Zhong et al. [98] used CFD analyses to model compression ratios, air inlet temperatures and air/fuel ratios using ammonia with n-heptane. The results demonstrated that compression ratios of 16:1 and inlet air temperatures of 800 K allow ignition of ammonia blends through compression. Moreover, it was shown that as n-heptane increases, the ignition temperature required reduces from 800 to 360 K. A very comprehensive compilation of data has been gathered by Dincer et al. [99] with regards to co-fuelling ammonia blends for diesel locomotives using integrated heat recovery, hydrogen production and emission reduction subsystems. Economic considerations such as carbon-tax rates and fuel costs were considered. Further work has compared a conventional diesel-electric locomotive through energy and exergy efficiency, fuel consumption and environmental impacts. Results showed that a blend with 50% of fuel energy supplied by ammonia can improve heat recovery with a slight increase in energy and exergy efficiencies. Moreover, there is a considerable reduction of greenhouse gases of up to 53% with pollutant production (NO_x, CO, particulate matter, hydrocarbons) below the standards required by 2012-2014 [100].

Dimethyl ether (DME) fuels were also assessed using liquid ammonia–DME mixtures in a compression-ignition engine with a direct-injection strategy. The cost analysis showed a comparable fuel energy cost to diesel fuel with ammonia/DME, although the inclusion of ammonia in the fuel mixture was shown to increase CO, HC and NO_x emissions, with lower power outputs [101]. Injection strategies were developed to enable the use of ammonia-DME in direct-injection compression-ignition engines [15], the corresponding engine performance was also linked to increased CO, HC and NO_x emissions, thus suggesting that post-exhaust treatment would be required for these systems.

As for all combustion systems, emissions from ammonia combustion play a crucial role in deployment; thus dedicated research has focussed in this area. Further investigations [102] depicted gasoline–ammonia combustion in a spark-ignition engine in terms of the combustion characteristics and exhaust emissions with direct injection. CO emissions were found to decrease but emissions of NO_x and hydrocarbons were increased with ammonia, as expected due to the high nitrogen content of the ammonia molecule. Notwithstanding the emissions challenges, however, direct injection of gaseous ammonia with carbonaceous fuels was proven to be feasible in engine combustion.

2.2.2 Ammonia and Hydrogen

Of particular interest is the use of hydrogen in the ammonia blends, as the molecule is also a carbon-free fuel and can be recovered through splitting of ammonia, with the previously stated improvements in combustion performance. Studies show that ammonia can be blended with hydrogen at levels as low as 5% hydrogen [103], still providing good power response. Higher doping ratios have also been deployed [104], showing, for example, that 10% hydrogen addition provided optimum efficiency and effective power. High NO_x emissions were present under lean conditions, thus suggesting the need for selective catalytic reduction (SCR) of exhaust gases under these conditions.

Further studies of reciprocating engines have also been extended to more practical applications e.g. 2009 Duynslaegher et al. [34] conducted a preliminary experiment using ammonia in a spark ignition engine trying to obtain the satisfying efficiency and as less emission as possible in exhaust gases. In Italy, where implementation of ammonia ICE technology has been performed by DESTEC in Pisa [105, 106], showing good results for the conversion of a Lombardi 505cm^3 gasoline engine into a hydrogen/ammonia system for waste collection buses. Since liquid ammonia contains 1.7 times as much hydrogen as liquid hydrogen itself [107], an ammonia tank (1 MPa) is expected to contain 2.5 times as much energy as a hydrogen tank (at 70 MPa) by volume, i.e. a hydrogen tank of 770 L (350 kg) could be replaced by an ammonia tank of 315 L (172 kg) [68]. Consequently, the smaller tanks required for liquid ammonia were presented as an opportunity for the local Region of Tuscany [105].

The key mechanical modification to the engine required the addition of electro-injectors for hydrogen and ammonia to the intake manifold [108]. One of the main features of these devices was the development of a new patented device capable of cracking ammonia into hydrogen and nitrogen at the concentration required for the engine [107]. The experimental results confirmed the need to dope the ammonia blend with hydrogen and that observed brake power was less than that for gasoline as a consequence of the poor heating value of the mixture. The maximum observed NO_x emission was 11.5 g/kWh at half load and 4500 rpm, without catalytic reduction [108]. Similar thermal ammonia reformers have been also evaluated by other research groups to obtain hydrogen to increase the reactivity of an ammonia fuel blend [68], showing that a 40% hydrogen fraction improves combustion properties close to those observed for gasoline.

Recent studies [109] also evaluated the implementation of hybrid systems. Developments showed two systems using ammonia-hydrogen fuel for either an internal combustion engine or a combination of an ICE with PEM fuel cells to power a vehicle. The results from the theoretical study show that although the energy efficiency of the configuration without fuel cells is considerably higher, 61.89% compared to 34.7%, the amount of exergy that is destroyed by the ICE is significantly greater, with values that go from 197.5 kW without fuel cells compared to 142.8kW with them. It must be emphasised that integration of heat recovery for dissociation units played an important role in the improvement of these systems, concepts that can be expanded to other combustion technologies to increase efficiency while minimizing exergy destruction.

Regarding emissions, research groups have investigated mechanisms governing the nitrogen based emissions in an ammonia/hydrogen fuelled SI-engine [110]. Applications with flue gases exhaust treatment showed lower levels than legally required when a SCR catalyst was used to eliminate all NO_x emissions. Gill et al. [111] compared the combustion and emissions characteristics of using hydrogen, ammonia and dissociated ammonia as a dual fuelling approach with diesel fuel in a compression-ignition engine. The study showed that pure NH_3 performed better than dissociated NH_3 at high load in terms of engine stability and brake thermal efficiency -possibly a consequence of increased heat loss from the combustion chamber, changes to combustion characteristics and changes to the efficiency of H_2 combustion under different loads and concentrations, while at low loads the fuels behaved similarly, although it should be noted that using dissociated NH_3 was found to have lower exhaust NH_3 emissions and significantly low N_2O formation compared to un-dissociated NH_3 addition.

In terms of emissions, all modern combustion vehicles are now required to operate SCR catalyst systems and/or fuel additive systems to reduce nitrogen oxides to N_2 gas. Interestingly, these systems work through the addition of chemicals that decompose to ammonia [112], and ammonia then reduces the NO_x within the gas flow. Therefore, as proposed in [113] NO_x emissions from ammonia fuelled combustion devices may be mitigated in a similar fashion. However, it should be noted that for devices fuelled by ammonia a ready reservoir of ammonia for NO_x reduction will exist and therefore it may be possible to design ammonia fuelled systems that do not require secondary exhaust clean-up or high cost catalyst systems to achieve emission free exhaust. Furthermore, ammonia combustion is often improved through preheating or partial decomposition of the ammonia prior to combustion and it may be possible to parasitically use the waste heat from exhaust systems to pre-heat or decompose ammonia while simultaneously removing NO_x pollutants.

In summary, clearly further research developing internal combustion technologies fuelled by ammonia is necessary. There is now increasing interest in these systems and considerable competition to produce the first commercially viable devices. However, as described previously, the challenge of reducing further NO_x and unburned ammonia remains at the heart of this research and technological field.

2.3 The Use of Ammonia in Gas Turbine Application

Gas turbine is another power-generating device which offers the potential benefits through ammonia fuelling as described earlier. Hence, a gas-turbine combustor that burns a combination of NH_3 and other fuels with controlled emissions and combustion characteristics is highly desirable. Studies that have contributed to improving understanding of ammonia fuel blends for gas turbine power generation are summarised in this section. It is noted that this is an immature field, with relatively few publications concerning the development of ammonia gas turbines.

Early research on the development of ammonia fuelled gas turbine combustion systems was undertaken during the 1960's [114-116]. Those studies demonstrated that ammonia's ignition energy was considerably higher compared to fossil fuels due to the low reactivity of ammonia. Moreover, at stoichiometric conditions, the quenching distance for ammonia-air (0.275 in) was 3.5 greater than for propane, with ammonia burning at narrower equivalence ratio ranges [114]. However, it was also found that dissociation of ammonia could produce faster flames, which could attain similar properties to some common hydrocarbons. Thus, it was concluded that 28% dissociated NH_3 could be used as a substitute fuel in gas turbine combustion systems sized for hydrocarbon fuels. Further experiments demonstrated that the fundamental problem with ammonia-air as a turbine fuel is the relatively slow chemical reaction rate, giving a laminar flame speed of ~0.06-0.08 m/s [117]. As air flow is reduced to allow sufficient residence time for the reaction to progress, diminished Reynolds number effects lead to reduced turbulence and hence less effective mixing, which in turn decreases combustion efficiency [115]. Other studies have been conducted to demonstrate the concept of using ammonia as an engine fuel, with success in terms of power production that unfortunately fell short in terms of emissions performance for NO_x [118, 119].

In the 1960's, Solar and UC Berkeley investigated a 250HP T-350 single can ammonia burner turbine [120]. Performance of the engine using vapour NH_3 was found to be similar to JP-4. Moreover, the ammonia fuel provided increased efficiency when temperatures were matched to those produced with hydrocarbons. In 1991, the Italian power generator ENEL undertook a research programme that included ammonia for power generation. Their conclusions led to positive power production performance that was compromised by the high emission of NO_x [121]. Grcar et al. [122] combined experimental and modelling investigations of ammonia chemistry in a hot combustion environment below adiabatic flame temperatures. The final products of NH_3 oxidation remained sensitive to mixing even at temperatures below those of self-sustaining flames. At these low temperatures, NH_3 oxidation occurred in a premixed reaction zone, as sufficiently high temperatures led to the development of a non-premixed reaction zone that produces significantly less NO than the equivalent premixed system developed.

More recently, a number of different approaches have been pursued to use ammonia as a flexible fuel in gas turbines, with most of them finding that emissions are the main limitation of such technologies [123]. SPG Advanced Propulsion and Energy [120, 123] is one of the few companies claiming the development of commercial systems. They have presented through series of papers that have summarised the main challenges for the development of a reliable technology are: a) Lower flame temperatures and slower kinetics of NH_3; b) unstable combustion; c) reliable ammonia vaporization to improve efficiency; d) pre-cracking of the molecule required to increase flame speed and burning ratios.

Swirl stabilised combustion of ammonia with other molecules has been briefly analysed at the Iowa State University by Meyer et al. [124] in a 40kW burner, with nozzles, swirl stabilisers and a self-sustained heat exchanger. Stabilisation was achieved using different swirlers with different concentrations of ammonia, hydrogen and methane. For those experiments where ammonia and hydrogen were mixed, it was found that the use of a flame holder increased the combustion efficiency, with a demonstrable reduction in NO_X emissions.

The Fukishima Renewable Energy Institute (FREA), has developed fuel flexible platforms to burn liquid NH_3 produced from renewable sources, i.e. wind and solar, in combination with kerosene in a 50 kW micro-gas turbine[125]. Diffusion combustion has been employed in the prototype by-fuel combustor due to its flame stability and it has been demonstrated that the equipment can be run using ammonia-kerosene blends at different concentrations. The gas turbine was started with kerosene that was replaced by ammonia and an output power of 17 and 21kW was achieved with 38% and 30% replacement of kerosene by supplying NH_3, respectively. However, the production of NO_x increased considerably based on the amount of ammonia injected, reaching levels up to 600 ppmV. The NO_x emissions challenge for ammonia fuelled turbines has been investigated since the first development of the technology. Currently, the best solution is the use of selective catalytic converters (SCR) to reduce the emissions produced by a micro-gas turbine up to levels of 10ppmV [126-128]. Further works on this system have been performed using other blends such as ammonia-methane blends, and the implementation of rich-lean combustion systems for NO_x reduction has also been demonstrated with good performance and the reduction of emissions to half of those measured without this combustion technique [129]. Recently, the study of Kurata et al. [130] provided demonstration of power generation using a 41.8 kW micro gas turbine fuelled with ammonia. It is a successful attempt to use ammonia in gas turbine power generation system without any additive for the first time. Some other findings [131] show that additions of hydrogen can improve flame stability and mitigate even further NO_x production, encouraging the use of ammonia for power generation at low nitrogen oxide concentrations. Co-firing could be achieved using ammonia and methane/hydrogen to support power production of high energy intensive industries. With that aim, groups at Cardiff University (UK) and Tohoku (Japan) are currently investigating the development of new gas turbine combustion systems capable of providing large power quantities with low emission rates [132]. The work at Tohoku has determined the exhaust gas compositions of a particular burner under atmospheric pressure and fuel lean conditions. It has been demonstrated that as the equivalence ratio increases towards stoichiometry, unburnt species such as NH_3, CO and total hydrocarbons decrease in contrast to NO_x and that the burner achieves combustion efficiencies above 97% for ammonia-mixing-ratios below 50%. It has been reported that it was difficult to achieve low emissions and high combustion efficiency in a single-stage combustor, and hence a two-stage combustion system has been conceptualised and demonstrated, with studies suggesting lower NO_x and unburnt gas species emissions while maintaining high combustion efficiencies [133].

In terms of the specific investigation of ammonia combustion in gas turbine combustor, Valera-Medina et al. [134, 135] presented a series of studies using a generic swirl burner that was fuelled using ammonia and hydrogen/methane at different concentrations. The results showed the complexity in stabilising premixed ammonia blends, identifying a particular pattern of oxygen consumption that was followed by flame speed reduction, retarding the combustion process and eventually pushing the flame back into the combustion chamber with an inherent aeration. Also, it was recognised that the use of hydrogen injection required a new injection strategy to ensure stable combustion, as premixing eventually led to early flashback. NO_x and CO were considerably lower at high equivalence ratios >1.10, depicting a region of chemically reactive balance between methane and ammonia combustion. Hayakawa et al. [136] performed experimental studies on flame stability and emission characteristics of ammonia/air premixed flames in a swirl burner. It was found that with swirling flow, ammonia/air premixed flames can be stabilised within a wide range of equivalence ratios and inlet velocity conditions. Somarathne et al. [137] numerically studied emission characteristics of turbulent premixed ammonia/air flames in a gas turbine swirl combustor under high pressures up to 0.5MPa. It was found that with secondary air injection it is possible to realise lower nitrogen oxide and zero ammonia emissions.

Companies such as NUON have also started ambitious programmes to develop their capabilities in terms of ammonia fired systems. The most notable is the “Power-to-Ammonia” programme in which NUON collaborates with TU Delft, Proton Ventures, OCI Nitrogen, AkzoNobel, ISPT and the University of Twente [138, 139]. The NUON project perceives ammonia as a “superbattery” that stores excess renewable power at large scale over long periods. The new Magnum-plant in Eemshaven, officially opened in 2013, is proposed to be converted into a green ammonia fuelled facility instead of a coal plant, thus reducing CO_2 emissions considerably [140, 141]. Furthermore, it has recently been announced [142] that Chugoku Electric Power Company has conducted a series of trials at its Mizushima power plant in July 2017, where ammonia was added to the 155MW coal-fired plant at a rate of 450 kg/hr. The company confirmed that the addition of the ammonia did not cause the plant’s power efficiency to reduce. On the basis of energy content, the ammonia added represented 0.6-0.8% of total fuel. At this ratio, a decrease in carbon dioxide emissions was observed. The Chugoku demonstration has been the first where ammonia has been burned in a commercial power plant in Japan.

2.4 Other Ammonia Combustion Applications

Pioneering studies on propulsion technology with ammonia were undertaken during the middle of the 20th century by NASA, who identified through their XLR-99 programme the need for “combustor enhancers”, i.e. hydrogen, kerosene, fossil fuels, etc. during start-up and idle for their propulsion engine [143]. According to some documents and “in field” research [78], Reaction Motors, the company that took over the XLR-99 programme, decided to use ammonia on their Viking engine (XLR-10). The rationale behind the use of ammonia and liquid oxygen (LOX) was the need for a stable fuel with good volumetric energy density, easy to store, working in the required temperature range, with cooling properties and also potential for hydrogen engine development. However, due to the lack of motivation and no clear understanding of the need for using ammonia and the need for gravimetric energy density based fuels, the programme stopped. During the period that the project ran, the X-15 aircraft was developed. The aircraft, a powerful device commissioned by NASA, set unofficial world records in speed and altitude [78].

Thomas et al. [144, 145] discussed the use of methane-ammonia-oxygen blends in terms of their potential to allow deflagration to detonation transition in small piping lines, a technique that can be used for propulsion applications. Compositional ranges were obtained by varying the oxygen content whilst maintaining methane/ammonia ratios of 1.00:1.18. The results showed that flame speeds were modest for all mixtures where the oxygen percentage was 39% or less. Similarly, violent pressure transients were not observed for mixtures with less than 40% oxygen. Beyond these values, violent and sometimes detonating transitions were observed for the cases analysed, especially for initial pressures above ambient.

Micro-thrusters fuelled with ammonia, a revolutionary concept for propulsion of small space vehicles, has also received some interest especially in Russia, China and the USA. Blinov et al. [146, 147] presented some work in terms of the design features and performance of ammonia electrothermal micro-thrusters, showing that they can become a competitive, cost effective option due to their specific impulse increase ~20%. Fatuev et al. [148] have also presented work on the development of ACETAM, a rocket fuel based on the fluidization of gaseous acetylene by a highly concentrated dilution in liquefied ammonia. The characteristics of the fuel show improvement and higher stability when compared to other blends at various operating pressures, nozzle expansion degrees and efficiency through various stages during space launching. Ammonia and acetylene mixtures have also been studied in terms of the thermodynamic properties and potential of propellants [149]. Various concentrations of acetylene-ammonia with LOX and other fuels such as rocket kerosene and methane were evaluated thermodynamically. The results indicated that a 25% acetylene content was the best in terms of specific impulse and security, with properties that were superior to LOX and rocket kerosene.

Some published work can also be found for the development of ammonia microresistojets (MRJ) for micro-satellites. Robin et al. [150] evaluated the use of ammonia MRJs to cope with weight and complexity constraints whilst creating a high thrust/power system. Moreover, they showed that at ambient temperature and a vapour pressure of 0.85 MPa, ammonia can also serve as propellant for altitude control, with a specific impulse of approximately 80 seconds. The research described the device that provides a specific impulse of 150-210 seconds and thrust of 5-12 mN. Due to the small nature of the system and its innovative design using platinum tubes, the total device weight is about 15 grams. A successful 100 hour Engineering Model (EM) was carried out, leading to further plans for development.

Potential beneficiaries of the research undertaken include the steel industry where ammonia is available as a waste product which could be considered as fuel to be used in co-fired facilities. Teng [151] experimentally investigated the ammonia combustion ovens in steel plants. It was found that NO_x emission can be reduced significantly by adjusting the total air rate, staging the air injected and adding by-product fuel gases to the oven. Recently, Murai et al. [152] measured the total radiative heat flux and the radiation spectra of a 10 kW test furnace combusting ammonia fuels. It was suggested that 30% of oxygen enriched ammonia combustion can result in the higher temperature than that in the methane/air combustion and even have 1.4 times total radiative heat flux.

Research topics that has contributed to the progression of combustion/power applications also includes the use of combustion through catalytic materials at small and medium scales. Recent research has shown that using porous blocks is an advantageous and practical way to stabilise premixed flames [153, 154]. In summary, porous media improves the fluid properties to enhance flame speed, thus increasing flame stabilisation. These characteristics can have considerable advantages for the consumption of ammonia for combustion purposes. In addition, the high thermal conductivity of some materials such as SiC increase the heat conduction from the flame to the surrounding zones, thus decreasing undesirable emissions [155] .

Researchers in Turkey and Japan have started working on the concept of catalytic combustion of ammonia. Although the literature that exists on the topic is extremely limited, Hinokuma et al. [156] have recently published the use of copper oxides and silver catalysts supported on aluminium oxides for the combustion of NH_3. The concept allows low temperature combustion that minimizes NO_x production, as thermal NO_x are minimized. Although thermal NO_x is a minor contributor to all nitrogen oxides produced in ammonia flames, nevertheless, their reduction contributes to emissions control. The use of novel thermal pre-treatments have ensured that these materials can withstand the elevated temperatures of operation (~900˚C). Similarly, research conducted by Nozari et al. [157, 158] showed the high efficiency of burning ammonia via SiC porous media with a large operational range. Simulations and experiments provided validated results that demonstrate the potential of burning ammonia at low power rates using these configurations.

2.5 Summary

Ammonia is an energetic chemical energy store with favourable physical properties, especially when compared to other chemical energy storage media. Consequently, its energy content has been explored as a chemical for power generation globally in recent years. Although considerable research into its use as a working fluid in cycles, fuel for combustion engines, electrochemical devices and turbines presents many challenges, these technologies can become widely adopted and commercially viable with the appropriate research and investment. While significant empirical and theoretical progress has been made on optimising fuel/co-fuel/oxidant ratios and the nature and process of the combustion processes, more work is still required to develop optimised systems for specific applications, starting with the development of models that are accurate at specific, practical operational conditions. Moreover, the excessive NO_x production using this molecule requires that models focus on developing chemical kinetic models that can be integrated within a more general model for use in the design and control of ammonia-based fuel systems for power generation.

Despite the long period since its inception, it is only now that ammonia is being seriously considered as fuel both for mobile and large renewable energy storage applications, thus supporting reduction of CO_2 with high flexibility of supply. Thus, ammonia can be produced using renewable sources which enables combustion systems to be employed using a chemical that, once better understood and characterised, has the potential of operating at high power whilst producing tolerable levels of emissions. It must be emphasised that researchers around the world are now trying to characterise the complex nature of the interaction of the species and radicals that are formed during the combustion process of ammonia and the different combustion characteristics of the flames, thus focusing research on creating more accurate and simpler models that can be used for practical applications.

In practical power generators such as engines and gas turbines, the recovery of hydrogen from a chemical capable of distributing it easily and economically provides great advantages, with longer operability ranges and feasibility to produce medium to large power outputs. However, the main issue with these technologies still relies on the NO_x emissions produced through the combustion process along with unburned ammonia that usually appears in the flue gas streams. Promising results appear in the range of rich fuel combustion, where the recombination of species seems to have positive effects on NO_x reduction through the production of OH radicals, a concept that requires furthers investigation. Ammonia can also enable advanced propulsion systems to be developed with smaller tanks, and the capacity to use a chemical with wider accessibility. Previous developments produced highly advanced systems that compete with currently available technologies. Thus, the future for ammonia in propulsion systems could return to its development for commercial use in large propulsion devices. However, nowadays the use of ammonia appears to be focussed on smaller propulsion thrusters for satellites and rockets, which requires energy for splitting the ammonia molecule into its hydrogen components.

Thus, as industry, governments and society turn to more sustainable technologies for power generation, and the use of fossil fuels becomes ever more constrained "Hydrogen through Ammonia" economy via Ammonia for Power – with supporting research - provides an attractive, practical proposition which seems to have increasing industrial support. However, as emphasised through the review in this section, there are still many fields that require further development and understanding, some fundamental in nature while others practical in essence.

CHAPTER 3

Research Methodology

Chapter 3

3.1 Numerical Methodology

3.1.1 Chemical Kinetics Fundamentals

Chemical kinetics lie in the heart of fundamental combustion processes, as chemical kinetics govern the behaviour of reacting chemical species in combustion. In many practical combustion situations, it is found that chemical reaction rates can determine the combustion process, emission formation, decomposition, etc., as a combustion reaction usually proceeds over many reaction steps, in which production and consumption of intermediate reactants is characterised. In general, elementary reversible (or irreversible) reactions involving K chemical species can be written in the form

$$\sum_{k=1}^{K} \nu'_{ki}\chi_k \Leftrightarrow \sum_{k=1}^{K} \nu''_{ki}\chi_k \ (\mathrm{i}=1,\ldots,\mathrm{I}) \qquad 3\text{-}1$$

The stoichiometric coefficients ν_{ki} are integer numbers and χ_k is the chemical symbol for the kth species. The superscript ' indicates forward stoichiometric coefficients and " indicates reverse stoichiometric coefficients. Typically, an elementary reaction contains only three or four species, henceforth the ν_{ki} matrix is fairly sparse for a large set of reactions. For non-elementary reactions, Eq. 3-1 can also represent the reaction expression, however the stoichiometric coefficients possibly will be non-integers.

The net rate of production $\dot{\omega}_k$ of the k th species can be represented as a summation of the rate-of-progress variables for all reactions involving the kth species:

$$\dot{\omega}_k = \sum_{i=1}^{I} \nu_{ki} q_i \ (\mathrm{k}=1,\ldots,\mathrm{K}) \qquad 3\text{-}2$$

where $\nu_{ki} = \nu''_{ki} - \nu'_{ki}$

The rate of progress variable q_i for the ith reaction can be defined by the difference of the forward and reverse rates as

$$q_i = k_{f_i} \prod_{k=1}^{K} [X_k]^{\nu'_{ki}} - k_{r_i} \prod_{k=1}^{K} [X_k]^{\nu''_{ki}} \qquad 3\text{-}3$$

where X_k is the molar concentration of the k th species, k_{f_i} is the forward and k_{r_i} is the reverse rate constant of the ith reaction. As indicated in equation 3-3, the rate-of-progress of a reaction is evaluated, by default, using the concentration of each reactant or product species raised to the power of its stoichiometric coefficient. For instance, the rate-of-progress of a reaction that includes species A with a coefficient of 2 will be second-order with respect to the concentration of A. Equation 3-3 is always valid when mass-action kinetics are obeyed and when the mechanism is written in terms of elementary reactions.

The rate constants for reactions are generally assumed to have Arrhenius form as

$$k_{f_i} = A_i exp^{(\frac{-E_i}{R_c T})} \quad 3\text{-}4$$

where A_i is the pre-exponential factor, T refers to the temperature, E_i is the activation energy of the reaction, R_c is the universal gas constant,. In this formula, the factors affecting collision frequency other than species concentrations are taken into account as for the pre-exponential factor. However, more commonly a modified Arrhenius form of the rate constant is used to take the temperature dependence of the pre-exponential term into consideration as

$$k_{f_i} = A_i T^{\beta_i} exp^{(\frac{-E_i}{R_c T})} \quad 3\text{-}5$$

where β_i is the temperature exponent of the ith reaction. Generally, as properties of the reaction, the values A_i, β_i, and E_i are determined experimentally. This equation also indicates that the reaction rate increases as the temperature increases generally.

For most combustion reactions, the reverse rate constant k_{r_i} can be computed from the forward rate constants through the equilibrium constants by

$$k_{r_i} = \frac{k_{f_i}}{K_{c_i}} \quad 3\text{-}6$$

where K_{c_i} is the equilibrium constant of the ith reaction. However, for certain reactions e.g. those involving electrons or some slow reactions, the use of this equation usually does not apply, then to determine reverse rates constant has to be specified.

Based on the fundamental reaction theory, in order to describe a complex reaction system such as combustion, a chemical kinetic mechanism can be developed, which describes all the reactions present in the combustion process by a compilation of all the species, elementary reactions and reaction rate parameters involved. As proved in previous combustion studies [159, 160], detailed chemical kinetic mechanisms are characteristically used to describe the transformation of reactants into products at the molecular level through a huge number of elementary steps. For instance, the famous GRI 3.0 mechanism is a well-established reaction model for methane combustion produced by the Gas Research Institute [45]. The sets of differential equations describing the rates of formation and destruction of each species are then numerically integrated and the computed concentrations of reactants, intermediates and products are compared to experiments. Furthermore, kinetic modelling describing the reactions, the rate parameters and the thermodynamic and transport properties of species provides the capabilities to be carried out under different environments, e.g. different geometries, temperature and pressure conditions. Such procedure of modelling is widely used in studies of combustion simulation applications [42, 161-163].

3.1.2 Laminar Premixed Flames Modelling

Premixed flame propagation is utilised in many practical combustion systems such as gas turbines and internal combustion engines. Premixed laminar burner-stabilised flame model and freely propagating flame model are both widely used in steady, isobaric, quasi-one-dimensional flame propagation studies [164-166]. Burner-stabilised laminar premixed flames are effectively one-dimensional and can be made quite steady, which enables experimental measurements of temperature and detailed species profiles. Hence such flames are often used to investigate chemical reaction kinetics in combustion research. Besides, laminar flame speed from freely propagating flame is frequently used to describe the combustion of various fuels or determine mixture flammability limits. Consequently, chemical kinetics modelling of laminar burner-stabilised flame and freely propagating flame is essential to interpreting flame experiments and understanding the combustion process.

Representing steady-state, quasi-one-dimensional reacting flows with uniform inlet conditions assumed, both of these two kinds of flames are simulated using a common set of governing conservation equations within a 1D “flow” domain.

Continuity

$$\dot{M} = \rho u A \qquad \text{3-7}$$

Energy

$$\dot{M}\frac{dT}{dx} - \frac{1}{c_p}\frac{d}{dx}\left(\lambda A \frac{dT}{dx}\right) + \frac{A}{c_p}\sum_{k=1}^{K} \dot{\omega}_k h_k W_k = 0 \qquad \text{3-8}$$

Species

$$\dot{M}\frac{dY_k}{dx} - \frac{d}{dx}(\rho A Y_k V_k) - A\dot{\omega}_k W_k = 0 \text{ (k=1,…,K}_g\text{)} \qquad 3\text{-}9$$

Equation of State

$$\rho = \frac{P\overline{W}}{RT} \qquad 3\text{-}10$$

where x is the spatial coordinate; $\dot{M}$ is the mass flow rate (which is independent of x); T is the temperature; Y_k is the mass fraction of the kth species as there are K_g species; P is the pressure; u is the velocity of the fluid mixture; ρ is the mass density; W_k is the molecular weight of the k th species; $\overline{W}$ is the mean molecular weight of the mixture; R is the universal gas constant; λ is the thermal conductivity of the mixture; c_p the constant-pressure heat capacity of the mixture; W_k is the molar rate of production by chemical reaction of the kth species per unit volume; h_k is the specific enthalpy of the kth species; V_k is the diffusion velocity of the kth species; and A is the cross-sectional area of the stream tube encompassing the flame normalised by the burner area.

The net chemical production rate $\dot{\omega}_k$ results from all the chemical reactions involving that species. The reactions are assumed to proceed according to the law of mass action and the forward rate coefficients follow in the modified Arrhenius form as described in previous sections.

The burner-stabilised flame model is quite often used for analysing species profiles to compare flame experiments data with known mass flow rate through burners. Usually the temperature profile is obtained from experiments so only the species transport equations are solved. However, since the chemistry depends strongly on temperature, it is essential to know the temperatures accurately in order to draw conclusions about the chemical kinetics behaviour. If a temperature profile can be measured accurately, it is often better to use this measurement than the temperature profile obtained by solving an energy conservation equation. For cases where the heat losses are known to be negligible, the application can solve a burner-stabilised flame problem in which the temperatures are determined from the energy conservation equation. Comparing these two problem types, the burner-stabilised model may also provide some indication of the heat losses. While the freely propagating flame model is used to determine the laminar flame speed of a gas mixture at certain inlet temperature and pressure conditions. Usually in this model it is assumed to be no heat losses so the temperatures would be obtained from solving the energy equations. Flame speed calculation is related to the transport of heat and thus predicting the temperature distribution is an integral part of the model.

As for the transport properties, a multicomponent diffusion model is used as it is considerably more accurate than the mixture-averaged approach especially when thermal diffusion effects are significant [167, 168].

For the multicomponent formulation, the diffusion velocity is defined as

$$V_k = v_k + w_k \tag{3-11}$$

v_k is the ordinary diffusion velocity and is given as

$$v_k = \frac{1}{X_k \overline{W}} \sum_{j \neq k}^{K} W_j D_{k,j} \boldsymbol{d_j} \tag{3-12}$$

Where X_k is the mole fraction, $\overline{W}$ is the mean molar weight, W_j is the molar mass of species j, $D_{k,j}$ is the ordinary multicomponent diffusion coefficients, for species k diffusing in species j and $\boldsymbol{d_j}$ is defined as

$$\boldsymbol{d_j} = \nabla X_k + (X_k - Y_k) \frac{1}{P} \nabla P \tag{3-13}$$

The thermal diffusion velocity is given as

$$w_k = \frac{{D_k}^T}{\rho Y_k} \frac{1}{T} \nabla T \tag{3-14}$$

where ${D_k}^T$ is the thermal diffusion coefficient for species k.

As for the more details about the matrix of equations, the solution algorithms, and the subsequent determination of the multicomponent diffusion coefficients, thermal diffusion coefficients and thermal conductivities can be referred to literature [169, 170].

Finally, for burner-stabilised premixed flames and freely-propagating premixed laminar flames, the conservation equations governing the two are the same, but the boundary conditions differ. The boundary conditions can be relatively easily implemented: the mass flux fractions and the temperature are specified at the cold boundary. For burner-stabilised flames, as mass flow rate $\dot{M}$ is a known constant, the temperature and mass flux fractions of kth species $\varepsilon_k = Y_k + \rho A \mathrm{Y}_k \mathrm{V}_k / \dot{M}$ are specified at the cold boundary, and vanishing gradients are imposed at the hot boundary. For freely propagating flames $\dot{M}$ is an eigenvalue which will be determined as part of the solution. Therefore, in this study the location of the flame is fixed by specifying the temperature at one point as an additional constraint. In this way it is enough to obtain the solution of the flame speed eigenvalue.

3.1.3 Perfectly Stirred Reactor

Perfectly Stirred Reactor (PSR) is a type of zero-dimensional homogenous open system, which is also referred to as a continuously stirred tank reactor[171]. The contents of a perfect-mixed reactor are assumed to be approximately spatially uniform inside the control volume as a result of high diffusion rates or forced turbulent mixing. This indicates that in PSR the rate of conversion of reactants to products is completely controlled by chemical reaction rates but not by mixing processes. In other words, the reactor is considered as “limited” by reaction kinetics. The essential characteristic of the PSR model is the assumption that the contents of reactor is sufficiently mixed to be described well by spatially averaged or bulk properties. In many practical applications of low-pressure processes, this assumption is valid as a result of the dominance of species diffusion renders. For instance, most reactors under low-pressure or highly diffuse operating conditions.

The major advantage of the PSR model is that such well stirred approximation allows mathematical models to be operated with relatively small computational demands. Thus, such models allow simulation studies to consider and analyse large, detailed chemical reaction mechanisms easily in practical application. Besides sufficiently fast mixing, theoretically the modelling of PSR also requires several assumptions. One is that mass transport to the reactor walls is assumed to be infinitely fast. Another is the flow through the reactor must be characterised by a nominal residence time[172], τ_{res} which can be deduced according to:

$$\tau_{res} = \frac{V\rho}{\dot{m}} \qquad 3\text{-}15$$

where V is the reactor volume, ρ is the density inside the reactor and $\dot{m}$ is the mass flow rate through the reactor. The PSR reactor is assumed to operate at steady state, so no time dependence is included in the equations.

The mass density is calculated from the ideal gas equation of state as

$$\rho = \frac{PW}{RT} \qquad 3\text{-}16$$

where P is the pressure, W the mixture’ s mean molecular mass, R the universal gas constant and T the temperature.

Typically, a PSR consists of a chamber, having inlet and outlet ducts, which may also allow heat loss. Thus, the reactor is uniquely characterised by the residence time and the inlet mixture composition and temperature. As illustrated in Figure 3-1 in the conceptual representation of a generic reactor chamber, a steady flow of well-mixed reactants is introduced to the reactor through the inlet with a given species composition and temperature. Internal mixing is assumed to be infinitely fast and therefore the contents of the reactor are spatially uniform. Consequently, the competition between chemical reaction rate and reactor residence time plays the dominant role in the conversion of reactants to products. The internal state of the reactor is computed by numerically solving the energy and species conservation equations. In this work, as a steady-state implementation of a PSR the governing equations are as follows:

$$\dot{m}(Y_k - Y_k^*) - \dot{\omega}_k W_k V = 0 \qquad 3\text{-}17$$

$$\dot{m}\sum_{k=1}^{K}(Y_k h_k - Y_k^* h_k^*) + Q = 0 \qquad 3\text{-}18$$

where $\dot{m}$ is the mass flow rate, Y_k is the mass fraction of the kth species (total K species), $\dot{\omega}_k$ is the molar rate of production by chemical reaction per unit volume, W_k is the molecular weight of the kth species and V is the reactor volume. h_k is the specific enthalpy of the kth species and Q the reactor heat loss. The superscript (*) indicates the inlet stream qualities.

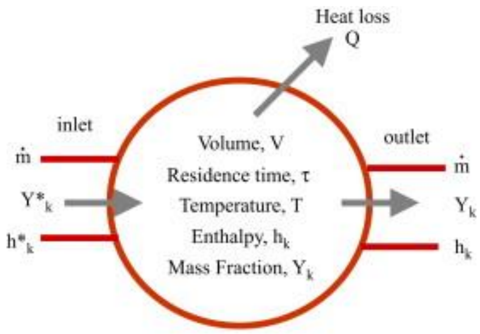


Figure 3-1 Schematic diagram of the perfectly stirred reactor (PSR) [173]

On the base of modelling a single well mixed reactor, a reactor "cluster" composed of many PSR modules connected in series can be used to simulate a practical combustion system. Many successful investigations have been carried out using this methodology where model predictions were in very good agreement with the experimental setup results [174, 175]. The reactor cluster modelling can be realised in several platforms e.g. CHEMKIN [176], which allows the user to build with the possibility of "recycling" streams feeding back to upstream reactors or being directed forward to downstream reactors.

As an illustration, schematic of such a reactor cluster modelling is included as shown in Figure 3-2 with connecting reactors. The symbols R11 , R13, and R32 are examples of recycling streams, defined as fractions of total mass flow out of a reactor [168]. To build the reactor cluster each inlet stream can be assigned its own attributes for flow rates, gas temperature, and composition. Then recycling streams are defined by quantifying the fraction of the outflow from the reactor which will flow into another reactor. When recycling streams are defined, the mass flow from one PSR to the next in series will be one minus the sum of the recycle flows defined from that reactor to all other reactors. As concluded in previous studies [163, 177], this reactor network approach can greatly reduce the amount of computational cost while provide satisfying solutions for a relatively complicated combustion process. However, constructing such a reactor network is rather empirical therefore for different conditions experimental data or more complexed computational fluid dynamics calculation will be needed to determine the PSR cluster's structure with a different number of reactors and connectivity.

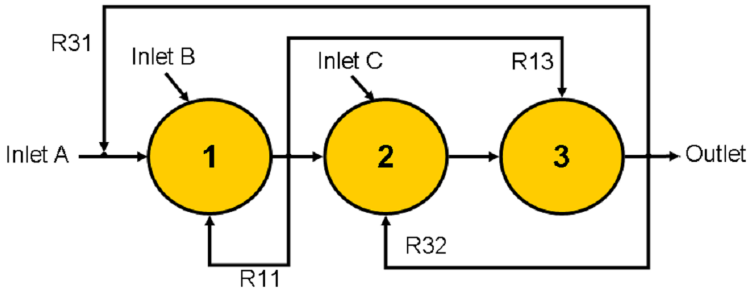


Figure 3-2 Schematic representation of a reactor cluster [168]

3.1.4 Sensitivity Analysis

Sensitivity analysis is a useful tool in interpreting the results of computational simulations. Sensitivity analysis of a problem solution is used to quantitatively understand how the solution depends on certain parameters which appear in a model's definition. In studies of combustion, sensitivity analysis is often an important tool which can be used in analysis of stirred reactor and flame experiments [178].

In this study, e.g. when using CHEMKIN platform, first-order sensitivity coefficients account for the partial derivatives of a dependent variable vector such as the species fractions, gas temperature and, where appropriate, the bulk-phase growth rates, with respect to a parameter vector (e.g. the reaction-rate coefficients) [168]. Using computationally efficient sensitivity analysis methods enables the differential equations to describe the sensitivity coefficients linearly, even if model problem itself is possibly of high non-linearities. Then rate-of-production analysis can directly provide complementary information on the contributions of individual reactions to species net production rates.

Since a lot of mathematical literature can be found on sensitivity analysis and various methods of calculating the sensitivity coefficients from the solution [179, 180], here a brief description of methods used for calculating sensitivity coefficients for steady-state solutions is provided. To compute the sensitivity coefficients for steady-state computations, the vector of governing equations are represented as

$$F(\phi(\alpha);\alpha) = 0 \qquad 3\text{-}19$$

Where F is the residual vector, ϕ is the solution vector, α are model parameters.

The idea is that the equation may depend not only on the solution variables but also on a set of model parameters α. The residual vector F depends on both explicitly and implicitly through the solution vector ϕ. Taking the reaction-rate sensitivity as an example, α is to represent the pre-exponential "A-factors" of the Arrhenius reaction-rate expressions. Differentiated with respect to α, equation (3-19) can be transformed to the matrix equation for the sensitivity coefficients as

$$\frac{\partial F}{\partial \phi}\frac{\partial \phi}{\partial \alpha}|_{F} + \frac{\partial F}{\partial \alpha} = 0 \qquad 3\text{-}20$$

In this equation, the matrix $\frac{\partial \mathrm{F}}{\partial \phi}$ is the solution Jacobian of the original system and $\frac{\partial \mathrm{F}}{\partial \alpha}$ is the matrix of partial derivatives of F with respect to the parameters. The sensitivity coefficients are just defined as $\frac{\partial \mathrm{F}}{\partial \alpha}$. In the matrix, each column indicates the dependence of the residual vector on each parameter. And there are as many columns as there are parameters, which is the number of gas-phase reactions. The sensitivity coefficient matrix $\frac{\partial F}{\partial \alpha}$ contains quantitative information on how each reaction-rate coefficient affects the temperature and species fractions. The sensitivity matrix has a structure similar to that of the matrix $\frac{\partial F}{\partial \alpha}$, in which each column contains the dependence of the solution vector on a particular chemical reaction.

3.1.5 Turbulent Combustion Modelling

In most practical combustion equipment, such as gas turbine, furnace, internal combustion engines, etc., combustion happens in the form of turbulent reacting flows. In contrast to laminar flows in which velocity and scalars can be well-defined in terms of value, turbulent flows are characterised with velocity fluctuation, leading to fluctuations such as temperature, density, composition etc. The fluctuation is generally considered as a result of vortices generated by shear within the flow. As a result, in turbulent flow mixing is greatly enhanced. While in turbulent combustion, turbulence can enhance the chemical reaction or even quench the flame as a consequence of the strong flow accelerations through the flame front induced by heat release. Thus the combination of the subject of turbulence and combustion reactions already reveals the daunting task of turbulent combustion modelling.

As turbulent flame is the main mode in the combustor of gas turbines for power generation, numerical modelling techniques for turbulent combustion are valuable tools for researchers or engineers developing new combustion devices in such area. However, challenge of turbulent combustion process in practical combustors is the presence of a large range of length and chemical time scales spanned by the various processes governing combustion and the degree of coupling between these processes across all scales [172]. In fact, the dynamic range can reach to several orders of magnitude between scales of chemical processes compared with the scales of a real combustor.

In turbulent combustion modelling, both the turbulent fluid flow and the composition of mixture need to be solved. The governing equations for turbulent combustion flow are normally represented as over-all continuity, momentum and additional scalars that can be used to spatially and temporally resolve the mixture's thermodynamic state.

Continuity

$$\frac{\partial \rho}{\partial t} + \nabla \cdot \rho \boldsymbol{u} = 0 \qquad 3\text{-}21$$

Momentum

$$\rho \frac{\partial \boldsymbol{u}}{\partial t} + \rho \boldsymbol{u} \cdot \nabla \boldsymbol{u} = -\nabla p + \nabla \cdot \tau + \rho \sum_{k=1}^{N} Y_k \boldsymbol{f}_k \qquad 3\text{-}22$$

Species continuity

$$\rho \frac{\partial Y_k}{\partial t} + \rho \boldsymbol{u} \cdot \nabla Y_k = \nabla \cdot (-\rho \boldsymbol{V}_k Y_k) + \dot{\omega}_k \ (k = 1, \ldots, N) \qquad 3\text{-}23$$

Energy

$$\rho \frac{\partial e}{\partial t} + \rho \boldsymbol{u} \cdot \nabla e = -\nabla \cdot \boldsymbol{q} - p \nabla \cdot \boldsymbol{u} + \tau : \nabla \boldsymbol{u} + \rho \sum_{k=1}^{N} Y_k \boldsymbol{f}_k \cdot \boldsymbol{V}_k \qquad 3\text{-}24$$

In the governing equations, ρ is the mass density; **u** is the velocity vector; p is the pressure; τ is the viscous stress tensor; $\mathbf{f}_k$ is the body force associated with the k th species per unit mass; $\mathbf{V}_k$ is the diffusive velocity of the kth species, where the velocity of the kth species may be expressed as the sum of the mass-weighted velocity and the diffusive velocity, $\mathbf{u} + \mathbf{V}_k$; $\dot{\omega}_k$ is the kth species production rate; *e* is the mixture internal energy, which may be expressed as $e = \sum_{k=1}^{N} h_k Y_k - p/\rho$; **q** is the heat flux, which represents heat conduction, radiation, and transport through species gradients and the Soret effect.

As it can be seen, a number of terms in the governing equations haven't been explicitly expressed hence constitutive relations, equations of state and other additional auxiliary relations are needed for augmentation. These terms include expressions for the viscous stress, species diffusive velocities, heat flux, body forces, reaction rate of species etc. Constitutive relations is to represent them in continuum models as the bulk of these terms have their origin in the molecular scales. Further description of the constitutive relations, state equations and auxiliary relations can be referred to turbulent combustion literature[172, 181].

In order to solve a turbulent combustion problem as described above, mainly the turbulence modelling, combustion modelling and chemical kinetics modelling need to be considered. Conventionally, three principal strategies have been implemented for modelling the turbulent combustion flow with good adaptivity. They correspond to Direct Numerical Simulation (DNS), Reynolds-Averaged Navier-Stokes (RANS) and Large Eddy Simulation (LES).

DNS is the method in which governing equations are numerically solved without any turbulence model. This means that the whole range of scales in space and time of the turbulence must be accurately resolved. RANS formulation is based on time-averaged equations of mass, momentum and reactive scalars. The idea behind the equations is to decompose instantaneous quantity into its time-averaged and fluctuating quantities (unsteady turbulent motion and its coupling with combustion processes) and then closure models are needed to represent the fluctuating quantities which are unresolved physics. LES is based on spatially filtering the governing equations to capture the contribution of large scale while reduce the computational cost by ignoring the smallest length scales.

RANS is commonly used in engineering applications for gas turbine development [182, 183]. However, since the filter scale of RANS is large, accuracy is compromised. To accurately model the turbulent combustion, it requires resolving a very wide range of time and length scales, all of which affect the flow field. And this can be achieved by DNS. However, DNS is not practical for engineering applications as a result of the extremely computationally expensive required resources [184, 185]. Between RANS and DNS sits LES, which is increasingly becoming a reliable tool for practical apparatus e.g. gas turbines [186-188].

Compared with the conventional RANS method, LES captures large scale information in both the momentum and scalar fields corresponding to the role of large flow structures on mixing and combustion. It is very crucial capturing these flow structure interacting with combustion chemistry in a wide-ranging practical applications. For instance, swirling flows in gas turbine engines serve to stabilise the flame and enhance the volumetric rate of heat release. Since closure in LES aims mainly at subgrid scale physics, a higher degree of universality in statistics can be achieved while the contribution from geometry-dependent large scales are eliminated from consideration. These advantages indicate LES to be considered as promising in the turbulent combustion simulation area.

The implementation of Large Eddy Simulation for turbulent combustion firstly needs a filtering operation applied to the conservation equations. In this way the conservation equations are spatially filtered so as to separate eddies to large scales and small scales. Usually, based on density-weighted filtering, the well-established Favre-filtered conservation equations can be described as follows [181, 189].

Continuity

$$\frac{\partial\bar{\rho}}{\partial t}+\nabla\cdot\bar{\rho}\widetilde{\boldsymbol{u}}=0 \qquad 3\text{-}25$$

Momentum

$$\bar{\rho}\frac{\partial\widetilde{\boldsymbol{u}}}{\partial t}+\bar{\rho}\widetilde{\boldsymbol{u}}\cdot\nabla\widetilde{\boldsymbol{u}}=-\nabla\bar{p}+\nabla\cdot\bar{\tau}+\bar{\rho}\sum_{k=1}^{N}\widetilde{Y_k\boldsymbol{f}_k}+\nabla\cdot(\bar{\rho}\widetilde{\boldsymbol{u}}\widetilde{\boldsymbol{u}}-\bar{\rho}\widetilde{\boldsymbol{u}\boldsymbol{u}}) \qquad 3\text{-}26$$

Energy

$$\bar{\rho}\frac{\partial\tilde{e}}{\partial t}+\bar{\rho}\widetilde{\boldsymbol{u}}\cdot\nabla\tilde{e}=-\nabla\cdot\tilde{q}-\overline{p\nabla\cdot\boldsymbol{u}}+\overline{\tau:\nabla\boldsymbol{u}}+\bar{\rho}\sum_{k=1}^{N}Y_k\widetilde{\boldsymbol{f}_k\cdot}\boldsymbol{V}_k+\nabla\cdot(\bar{\rho}\widetilde{\boldsymbol{u}}\tilde{e}-\bar{\rho}\widetilde{\boldsymbol{u}e}) \qquad 3\text{-}27$$

Species

$$\bar{\rho}\frac{\partial\widetilde{Y_k}}{\partial t}+\bar{\rho}\widetilde{\boldsymbol{u}}\cdot\nabla\widetilde{Y_k}=\nabla\cdot\left(-\bar{\rho}\widetilde{\boldsymbol{V}_kY_k}\right)+\overline{\omega_k}+\nabla\cdot\left(\bar{\rho}\widetilde{\boldsymbol{u}}\widetilde{Y_k}-\bar{\rho}\widetilde{\boldsymbol{u}Y_k}\right) \qquad 3\text{-}28$$

Here in these equations the overbar corresponds to a process of unweighted spatial filtering and the ‘ ~ ’ corresponds to a density-weighted spatial filtering. In the filtered equations, several additional terms are present corresponding to subgrid scale stresses $\bar{\rho}\widetilde{\boldsymbol{u}}\widetilde{\boldsymbol{u}}-\bar{\rho}\widetilde{\boldsymbol{u}\boldsymbol{u}}$ and scalar fluxes such as $\bar{\rho}\widetilde{\boldsymbol{u}}\widetilde{Y_k}-\bar{\rho}\widetilde{\boldsymbol{u}Y_k}$ and $\bar{\rho}\widetilde{\boldsymbol{u}}\tilde{e}-\bar{\rho}\widetilde{\boldsymbol{u}e}$. These unclosed terms require modelling. The molecular diffusion term $\nabla\cdot\left(-\bar{\rho}\widetilde{\mathbf{V}_kY_k}\right)$, may be insignificant in the governing equation relative to the scalar flux on the LES resolution. In fact, as turbulent diffusion term is usually assumed to be much larger than the molecular diffusion term, the molecular diffusion term is often dropped from the above governing equations.

3.1.5.1 Turbulence Modelling

The filter and average process inevitably introduces extra terms related to the sub grid eddies which are unclosed, so sub-grid scale (SGS) models are needed to solve those terms. The SGS stress tensor $\bar{\rho}\widetilde{\boldsymbol{u}}\widetilde{\boldsymbol{u}}-\bar{\rho}\widetilde{\boldsymbol{u}\boldsymbol{u}}$ usually can be addressed using various models, for which more detailed discussions can be referred to [190, 191]. One of the most commonly used is the Smagorinsky model [192]. In the typical form of constant coefficient Smagorinsky SGS model, the Reynolds stress part $\tau_{ij} = \widetilde{u_i}\widetilde{u_j} - \widetilde{u_i u_j}$ is decomposed into two parts, of which the traceless component τ_{ij}^d is defined as

$$\tau_{ij}^d = \tau_{ij} - \frac{1}{3}\tau_{kk}\delta_{ij} \qquad 3\text{-}29$$

Then τ_{ij}^d is modelled by a so called eddy viscosity model as

$$\tau_{ij}^d = -2\nu_t \cdot \tilde{S}_{ij} = -2(C_s\Delta)^2|\tilde{S}|\tilde{S}_{ij} \qquad 3\text{-}30$$

where $\tilde{S}_{ij}$ is the filtered strain rate tensor and $|\tilde{S}| = \sqrt{2\tilde{S}_{ij}\tilde{S}_{ij}}$ is its norm. Δ is the filter width (typically grid size), C_s is the Smagorinsky constant, of which the value is important in obtaining accurate predictions. The advantage of this model is its simplicity, which makes it very popular. On the basis of this, more models are also developed to improve the performance of Smagorinsky model [193].

3.1.5.2 Combustion Model

To use LES for turbulent combustion modelling, one main difficulty lies in the fact that the reaction layer is usually thinner than the grid size and therefore hard to be resolved. Consequently, the most critical closure arises from modelling the filtered reaction rates $\bar{\omega}_k$ as the reaction source term in the governing equations. Several formulations have been proposed in the literature [194-196]. It should be remarked that LES of turbulent combustion is a relatively recent field of research. There is a variety of models that are valid in different regimes. The modelling approach employed in this study is the Partially Stirred Reactor (PaSR) which can account for the turbulence/chemistry interaction. The PaSR concept is proved effective in turbulent combustion simulation applications [197, 198]. Besides, since it can offer complex chemistry treatment, it is suitable for the simulation of combustion in this study.

The main idea is to deal with the chemical kinetics coupled with micromixing by representing combustion in a Partially Stirred Reactor of a computational cell size, in which reactions are assumed to occur in fraction of its volume. Thus under the PaSR framework, a computational cell is split into the reacting and non-reacting zones. In reacting zones, each species is assumed to be homogeneously mixed with each other that is in perfectly stirred reactor (PSR) conditions. While in the non-reacting zones, it is assumed no reaction occurs. Therefore, the composition changes due to mass exchange with the reacting zone. In this way any fluctuations are neglected when calculating the chemical source terms. In the method, three average concentrations are distinguished in the reactor as shown in Figure 3-3, the mean mixture concentration of the feed c_0, the mixture concentration in the reaction zone c, and the mixture concentration at the exit c1.

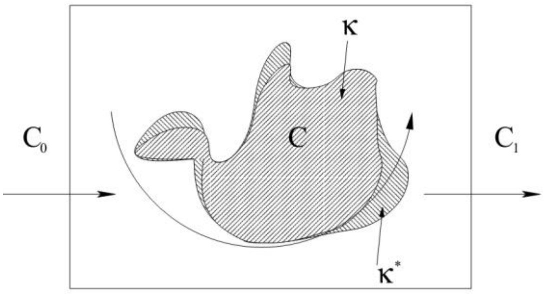


Figure 3-3 Conceptual diagram of PaSR reactor [199]

In the combustion process of the cell, initial concentration in the reaction zone firstly changes from c0 to c as it reacts and then reaction mixture c is mixed with the no reaction mixture c0 by turbulence, resulting in the averaged concentration c1. The reaction rate of this computational cell is determined by the fraction of the reactor in this cell. Thus, the key issue to apply the PaSR concept is to figure out the mass fraction of the reacting zones. The mass fraction of κ is expressed as follow.

$$\kappa = \frac{\tau_c}{\tau_c + \tau_{mix}} \tag{3-31}$$

where τ_c is the chemical time scale and $\tau_{mix}$is the characteristic time for turbulence.

The chemical time scale τ_c can be obtained from the calculation of the multi-step reaction equations which reflect the evolution process of each species, while the turbulence time scale τ_{mix} accounts for the exchange between fresh gases and burnt mixture. To describe different scales in turbulent flows, the τ_{mix} can be expressed as follow [198].

$$\tau_{mix} = C_{mix}\sqrt{\frac{\nu}{\varepsilon}} \tag{3-32}$$

where C_{mix} is a constant of which the value can vary between 0.001-0.3, ν is kinematic viscosity, ε is the dissipation rate of turbulent kinetic energy. More discussion about the mixing time for turbulence can be referred to [198].

Based on the PaSR theory above, the SGS chemical source term in the governing equation can be settled. The filtered chemical reaction rate $\overline{\omega}_k$ in LES is described as follow.

$$\overline{\omega}_k = \kappa \dot{\omega}_k \qquad 3\text{-}33$$

where $\dot{\omega}_k$ can be calculated by the mass action principle based on the density-weighted species concentrations and temperature as described in previous section.

3.2 Experimental Methodology

3.2.1 Generic Swirl Burner Testing

The test facilities for generic swirl burner experiments are at the Gas Turbine Research Centre (GTRC) of Cardiff University [200]. The GTRC enables novel research studies to be conducted into the functionality of new Gas Turbine (GT) combustion systems, components and fuels under elevated conditions of temperature and pressure as would be experienced within a gas turbine engine during operation. An extensive suite of test rigs is available for the characterisation of fuel sprays, nozzles, and combustion systems using traditional fuels as well as alternative and renewable fuels. Non-intrusive measurement techniques enable a better understanding of the fundamental phenomena occurring within the combustion system without influencing what is being measured.

Figure 3-4 Photograph of high pressure combustor rig

The High Pressure Combustor Rig is a multi-purpose combustion facility for combustor fundamentals research and development work as in Figure 3-5. The facility consists of inlet/premixer, combustor, and exhaust sections. An extensive range of state-of-the-art measurement sections are available, some unique, each with different capabilities, all of which are predominately non-intrusive. Exhaust gas samples are collected and transmitted to a comprehensive on-line gas analysis suite. Various fuels may be fired including kerosene, diesel, bio-diesels, natural gas, methane, ammonia and a range of simulated synthesis gases. Measurements can be made with the following maximum throughputs: Combustion Air Flow Rate <5 kg/s; Combustion Pressure <16 bar abs; Combustion Air Pre-Heat Temperature: <900 K. The optical combustion measurement section can be used with this facility as shown in Figure 3-5. There are also several measurement sections available with this facility such as the combustion instability measurement section, the auto-ignition measurement section, the wall cooling measurement section, the hot end simulator.

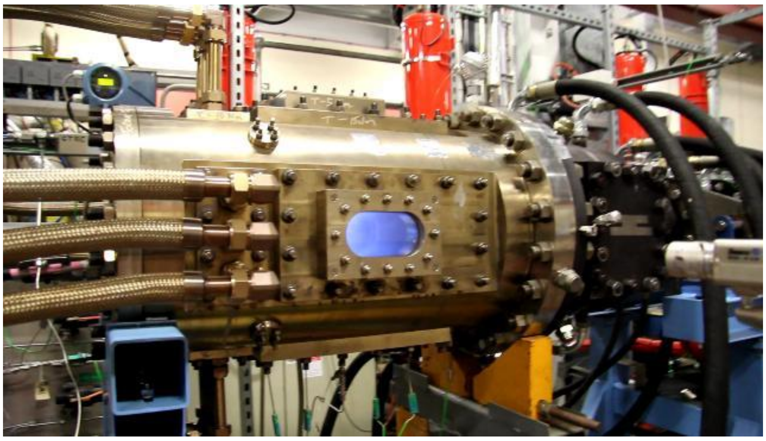


Figure 3-5 The optical combustion measurement section: high pressure optical pressure casing

3.2.2 Chemiluminescence

Chemiluminescence describes the emission of light (luminescence) produced by a chemical reaction. As it has been demonstrated to be closely related to flame properties [201, 202], chemiluminescence has been the basis of many combustion diagnostic techniques: Certain radical species such as CH* and OH* will give off radiation at specific wavelengths and the heat release rate can be calculated by measuring the amount of light radiated from a flame at those wavelengths. Thus, with the detection of chemiluminescent emission associated to a specific excited radical much relevant information can be extracted about the combustion process. Furthermore, chemiluminescence map [203] can be more revealing than point data as it is able to give description of the flame structure or heat release patterns.

In the previous studies of gas turbine relevant combustion from GTRC, chemiluminescence emission, e.g. from OH*, has often been used and analysed as an indicator of flame behaviour for a variety kinds of fuels [204, 205]. In fact as a type of optical sensor technology it is found to have advantages in our gas turbine combustion research. Using only an intensified charge-coupled device camera fitted with a filter at the selected wave-length e.g. OH around 310 nm, photons emission of the desired species can be detected. In addition, as the source of the chemiluminescence is spread throughout the domain, the intensity can be used as an indication of flame location or heat release rate, and whereby the intensity of the chemiluminescence is the integrated value over the line of sight of the camera. Moreover, with respect to other techniques like laser diagnostics, chemiluminescence imaging is simple to perform, since it only needs optical access in one direction, and is relatively cheap as well. Specifically, in this study of ammonia combustion in swirl combustor, a Dantec Dynamics Hi Sense Mk II CCD camera with a 1.3 megapixel resolution was coupled to a Hamamatsu C9546-03L image intensifier, so transient flame structures can be obtained efficiently with high speed imaging of OH* chemiluminescence. More details of the specific setup will be described in the chapter of experimental test work of gas turbine combustor.

CHAPTER 4

Numerical Study of Co-firing Ammonia with Methane

Chapter 4

A potential combustion enhancer for ammonia is methane, as it is the main fuel of gas turbines for power generation. Potentially, an ammonia/methane blend could be used not only from green ammonia sources, but also from by-product ammonia obtained from industrial processes. Ammonia addition could support peak-hour energy consumption requirements with fuel cost reduction. For instance, an immediate beneficiary of this blend could be steelworks companies that produce ammonia as a by-product of coke oven gas cleaning [206, 207]. More recently, a new research programme "Power to Ammonia" has initiated in the Netherlands looking into potentially turning gas-fired power plants into 'super batteries' [208]. Initial tests will focus on co-firing ammonia with methane in order to determine fuel blends that cause the lowest impact on gas turbine systems in order to reduce retrofitting costs in currently running facilities. Therefore, in this chapter research appraises ammonia/methane as the fuel to be studied for the purpose of potential applications e.g. in gas turbine combustion for large scale power generation in those energy intensive industries [35, 37, 54, 209, 210].

4.1 Chemical Kinetics Modelling Reduction of Ammonia/Methane Combustion

It is a practice to develop a computational fluid dynamics (CFD) based methodology alongside complex chemistry for ammonia combustion application, since it can help to capture more accurate information for the prediction of NO_x emissions, turbulent reacting flows, combustion dynamics, autoignition, etc. Thus, to utilise ammonia/methane effectively in a gas turbine, CFD simulation can serve as a powerful tool for analysing and designing ammonia combustion systems. However, the large number of species and reactions in detailed mechanisms makes it almost impossible to conduct CFD simulations with detailed chemistry for practical complex combustion systems such as a gas turbine combustor. For instance, the mechanism used in the present work, the Konnov's mechanism [33], has over 100 species and 1,200 reactions. Using a reduced reaction mechanism instead of a detailed one can substantially decrease the computational time and memory requirement, thus making feasible large scale calculations for practical gas turbine combustors with complex chemistry. However, there are very few studies [40, 62] concerning the use of reduced mechanisms for ammonia combustion under gas turbine conditions. These reduced mechanisms are developed based on a single fuel composition not including the presence of CH_4. Furthermore, no research concerning ammonia combustion mechanism reduction has been tested with multi-dimensional CFD simulation. Thus, there is a need to reduce detailed ammonia/methane combustion mechanisms in order to apply them to CFD simulation for practical gas turbine combustion research.

Due to the breadth of previous validation studies for Konnov's mechanism, it was an obvious choice for the simulation of ammonia/methane combustion in the present work. Kumar et al. [35] showed that Konnov's mechanism is the most adept at predicting ammonia based combustion for fuel mixtures in a jet flame for the four mechanisms considered. Duynslaegher et al. [40] improved Konnov's kinetic mechanism and then reduced it for use in a SI engine numerical simulation. Nozari [62] conducted a numerical study of laminar flame speed and NO_x emission for NH_3/H_2 mixtures at elevated pressure conditions using a validated Konnov mechanism. Duynslaegher et al. [31] studied the laminar flame speed, flame temperature and species concentrations using Konnov's mechanism at elevated pressures and temperatures. Duynslaegher and Jeanmart [34] simulated an ammonia/oxygen/hydrogen/argon premixed flat flame using Konnov's mechanism. Across the four mechanisms used in that study, Konnov's mechanism demonstrated the best performance for prediction of species mole fraction profiles across the flame. In sum, Konnov's kinetic scheme has shown great performance for the combustion of ammonia-based fuel amongst the range of mechanisms tested in various studies.

Therefore, Konnov's mechanism was initially employed to start understanding the various mechanisms involved in the combustion of ammonia-based fuels. In the present work reduced variations of the Konnov mechanism are compared to existing experimental data to appraise the suitability of ammonia/methane combustion kinetics under conditions of typical gas turbine combustion. The aim is to find a reduced mechanism to represent the kinetics of ammonia/methane combustion with sufficient accuracy under elevated pressure and temperature conditions. Considering the strong turbulence and interactions between turbulence and chemistry in gas turbines, the differences between the reduced mechanisms can potentially lead to significant deviation in final results for CFD simulations. Therefore in the present work not only ignition-delay times and laminar flames of NH_3/CH_4 are validated with the reduced mechanisms, but also turbulent combustion has been investigated to validate the performance of the proposed reduced mechanisms in more practical environments. Thus a comprehensive comparison in different dimensional levels (0D, 1D, 2D) was performed to generate and assess reduced kinetic mechanism models of ammonia/methane combustion under gas turbine conditions.

The full Konnov model comprises 129 species participating in 1231 reactions. This model has been reduced with the path flux analysis methodology described by Sun et al. [211] and Gou et al. [212] and implemented in their Chem-RC software [213]. In the mechanism reduction process [214], the path flux analysis methodology ranks the importance of the chemical reactions and their participating species based on the magnitude of the reacting flux through each species as determined for a series of baseline simulations of the detailed model. For this study, the detailed model was evaluated with homogeneous (ignition delay) simulations and with extinction curves generated by perfectly stirred reactor (PSR) simulations. For each case, mixture mole fractions of $NH_3/CH_4/O_2/N_2$ 0.088/0.0565/0.1795/0.675 corresponding to stoichiometric fuel-in-air conditions for a NH_3/CH_4 molar ratio of 61/39, which is the same ratio as that utilised in a generic swirl burner experimental campaign in [209]. For the constant volume ignition delay type calculations temperatures of 1000 K, 1200 K, 1500 K and 1800 K are used with pressures of 1 atm, 5 atm 12.5 atm. For the perfectly stirred reactor calculations an initial temperature of 300 K and maximum residence time of 33 seconds are selected, with simulations executed again at 1 atm, 5 atm 12.5 atm.

In assessing the importance of each reaction, the analysis considers the magnitude of the flux through both the "first generation" species participating in each (initial) reaction and the "second generation" species which result from the participation of the product species of the initial reaction in the other reactions described by the model. The importance of each species is then quantified by an interaction coefficient index. A series of reduced models are produced (of 31, 48, 61, 77 and 84 species) by exercising a threshold index (of 0.6, 0.3, 0.215, 0.15, and 0.05 respectively) where only species with an interaction coefficient index greater than the selected threshold index are included in each particular reduced model.

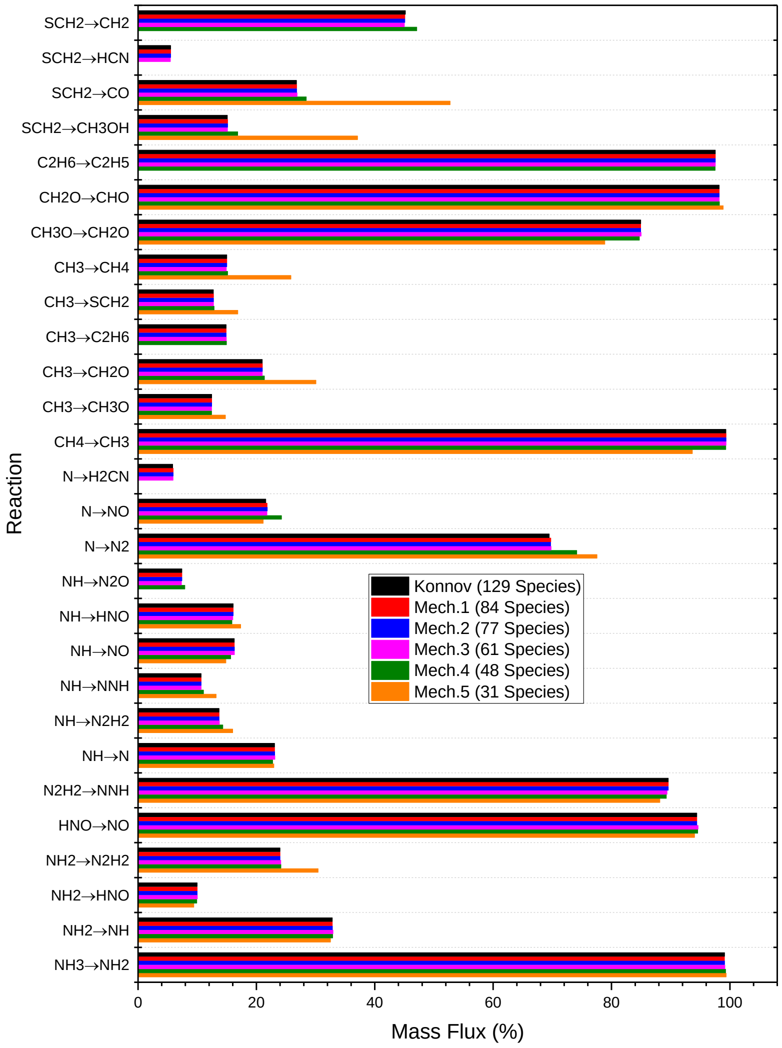


Figure 4-1 Species mass flux simulated with the Konnov and each of the reduced models in a constant volume perfectly stirred reactor for a fuel mixture of NH_3/CH_4: 61/39 at E.R.=1, 17 atm and 1550 K.

To compare the validity of each of the reduced models, chemical flux and sensitivity analyses of a stoichiometric fuel in air mixture of NH_3/CH_4 (61/39) were performed under constant volume, homogenous and constant internal energy conditions of 1550 K and 17 atm. The results are presented in Figure 4-1 and Figure 4-2 respectively. The flux analysis clearly shows how well the reduced models Mech.1-4 capture the flux behaviour of the original Konnov model. It is only when the species number is reduced to <40, as is the case with Mech.5 that a significant digression from the behaviour of the Konnov model is noted. For example, as ethane (C_2H_6) was excluded as a species from Mech.5, CH_3 may not be consumed by recombination to C_2H_6, as is the case in the others models, therefore the model over predicts the mass flux to other avenues such as $CH_3 \rightarrow CH_4$, $CH_3 \rightarrow SCH_2$, $CH_3 \rightarrow CH_2O$ and $CH_3 \rightarrow CH_3O$. This pathway allows the rate of radical propagation/branching to be increased relative to the detailed model where methyl recombination to ethane is an important reactivity slowing the radical chain termination step.

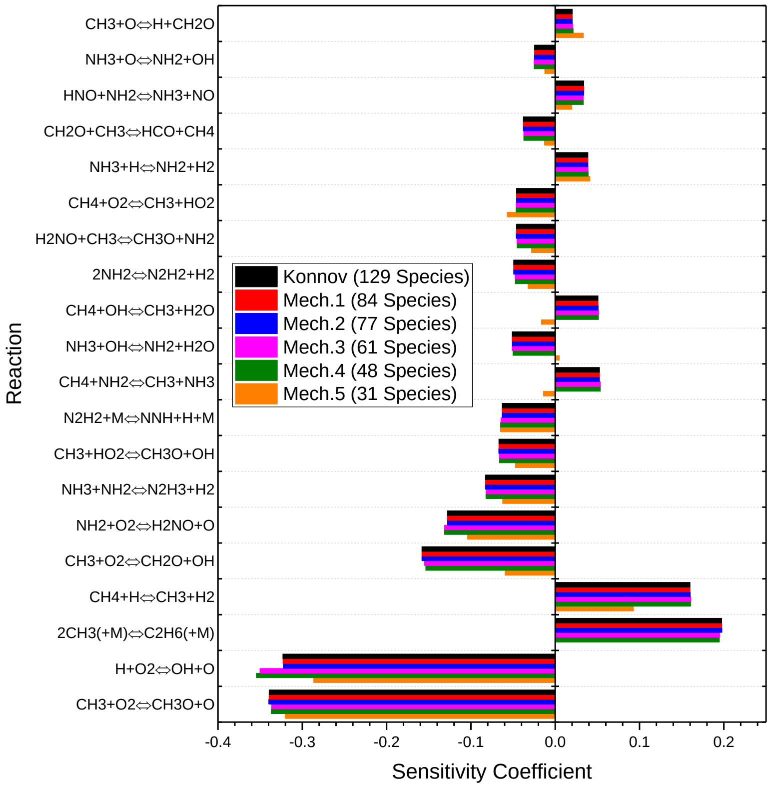


Figure 4-2 Sensitivity analysis of major reactions to ignition delay time for Konnov and each of the reduced models in a constant volume perfectly stirred reactor for a fuel mixture of NH_3/CH_4: 61/39 at E.R.=1, 17 atm and 1550 K.

Figure 4-2 shows a comparison of sensitivity analysis of the reactions affecting the ignition delay time for each reduced model. A negative value indicates that a reaction reduces the ignition delay time. For most models the $CH_3 + O_2 = CH_3O + O$ reaction was the most sensitive. However, for Mech.3 and Mech.4 the most sensitive reaction was the $H + O_2 = O + OH$. This shows an important degrading in the fidelity of the oxidation description, as the major radical chain branching reaction switches between a methyl radical dominated system, to one dominated by the hydrogen atom in Mech. 3 and 4. As expected, Mech.5 shows the largest deviation from the Konnov model and even opposing behaviour for the reactions of $CH_4 + OH = CH_3 + H_2O$ and $CH_4 + NH_2 = CH_3 + NH_3$. The third most sensitive reaction for all models was the $2CH_3 (+M) = C_2H_6 (+M)$, however for Mech.5 the species C_2H_6 was excluded thus this reaction does not take place in the model. These omissions probably invalidate this reduced model as an accurate representation of the ammonia/methane oxidation mechanism. Mech. 1 and 2, show very close important similarity to the detailed model, and are therefore recommended for use. In addition, the more severely reduced Mech. 3 and 4 also bare close resemblance to the detailed description, but do show of modes degradation in fidelity. This analysis highlights the limitations of such reduced models in their ability to capture the reactivity of the original Konnov model.

Table 4-1 Full Konnov and Reduced Mechanisms

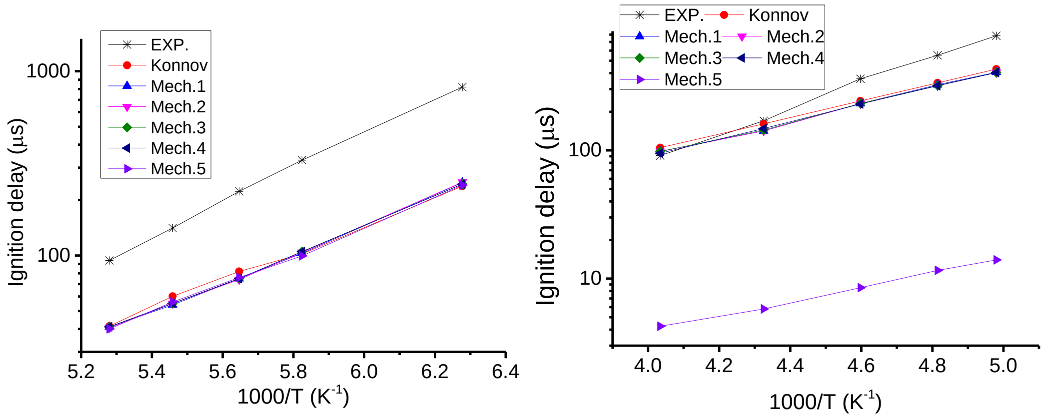
Name	No. Species	No. Elementary Reactions
Konnov [33]	129	1231
Mech.1	84	940
Mech.2	77	874
Mech.3	61	687
Mech.4	48	500
Mech.5	31	243

The fewer species and reactions there are in a reduced mechanism, the more computational cost can be saved. However, it is still needed to retain a balance between the accuracy and efficiency for the use of the reduced mechanisms in simulation studies. Therefore, based on the calculated results, five reduced mechanisms were obtained as choices for their application in computational simulations as shown in Table 4-1. The five reduced mechanisms are available in "Appendix A".

4.2 Performance Assessment of the Chemical Kinetics Models

4.2.1 Ignition Delay Times Calculation

Ignition delay times validation studies were conducted using Konnov's mechanism and the five different reduced mechanisms for several ammonia mixtures under different pressures. Figure 4-3 presents validation study results using ammonia-oxygen-argon mixtures. In Figure 4-3a, it can be seen that the prediction by the full Konnov mechanism and the reduced mechanisms present a considerable deviation from the experimental data, with average relative error around 63%. However, except for Mech. 5, accuracy is much better (average relative error around 27%.) at lower pressure, Figure 4-3b. Since the Konnov mechanism was developed under low pressure conditions, the results emphasise the necessity to optimise the detailed mechanism for ammonia combustion under higher pressure conditions. Nevertheless, it is noted that there is good correlation between the full and the reduced mechanisms. The validation for NH_3 is not so satisfying under high pressure conditions, this indicates improvements for ignition chemistry of pure NH_3 fuel are still needed.



a b

Figure 4-3 Ignition delay times of NH_3 mixtures (0.4%NH_3/0.6%O_2/99%Ar). a) 30.0 atm; b) 1.4 atm. Experiments from [44]

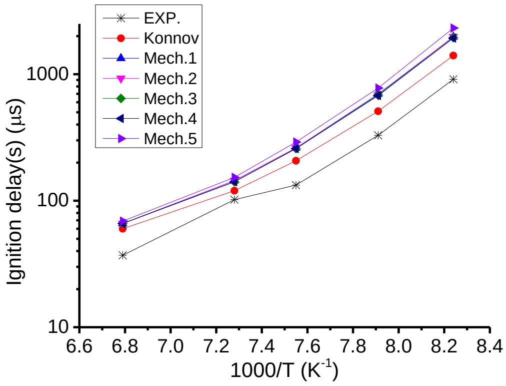


Figure 4-4 Ignition delay times of NH_3/CH_4 contained mixtures (0.02%NH_3/0.089%CH_4/0.297%H_2/0.297%CO/0.21%H_2O/0.157%CO_2/0.950%O_2/97.98%Ar) 12.0 atm, Experiments from [215].

Figure 4-4 shows the comparison between ignition-delay times of NH_3 and CH_4 containing syngas mixture against predictions from Konnov's mechanism and the reduced mechanisms. Under the high pressure condition, the full and reduced mechanisms predict relatively longer ignition delay times compared to experimental data. Although Konnov's mechanism presents the shortest ignition delay time predictions, thus showing better prediction to the experimental data, the reduced mechanisms are close to Konnov's mechanism with relative deviation around 26.6%. These results suggest that the full and reduced mechanisms can have better performance in predicting ignition delay times of ammonia/methane combustion under gas turbine conditions than pure ammonia. The possible cause for the discrepancies can be either that the isothermal boundary conditions are not exactly the same or the idealization of homogeneity in the numerical calculation.

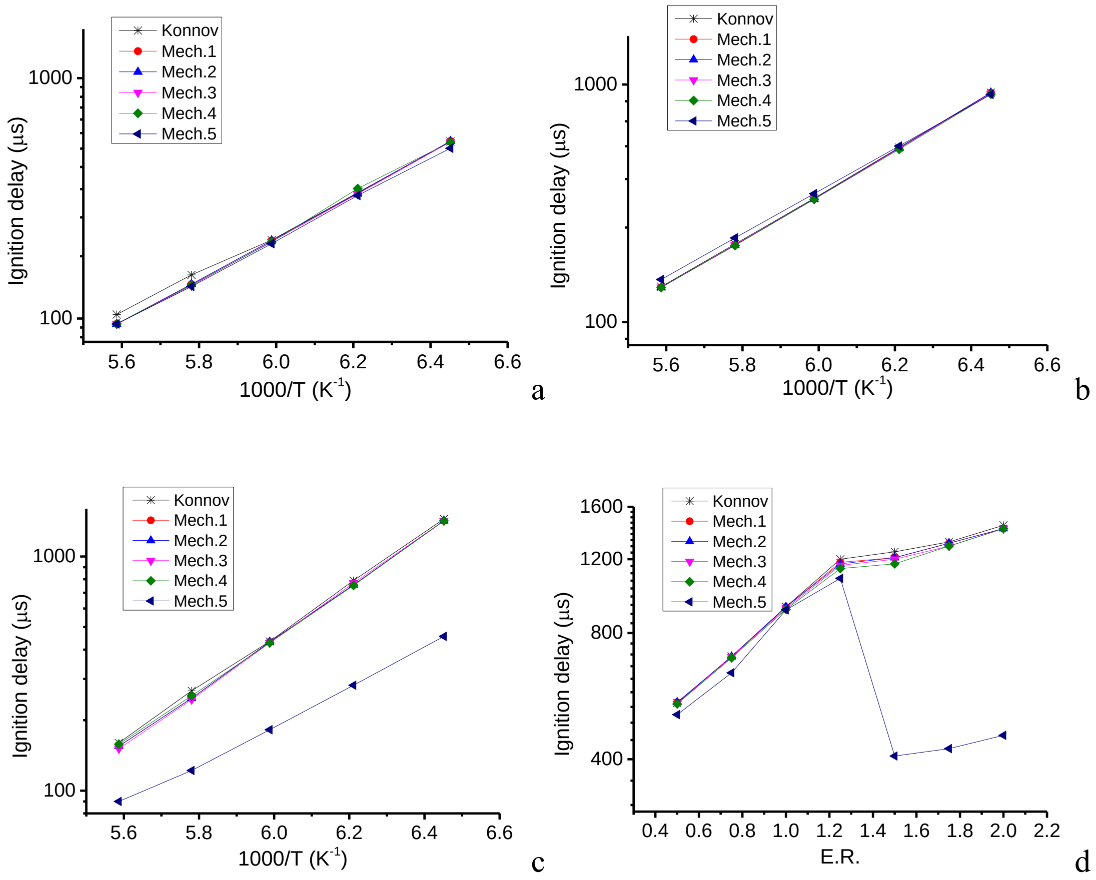


Figure 4-5 Ignition delay times prediction of NH_3/CH_4 mixtures under gas turbine conditions (17atm) a) E.R.=0.5; b) E.R.=1; c) E.R.=2; d) E.R.=0.5-2, T=1550K.

To assess the consistency of the reduced mechanisms with full Konnov's mechanism further, ignition delay time predictions of ammonia/methane mixtures were performed under the pressure of 17 atm to re-produce a typical ambient pressure inside a land-based gas turbine engine, as shown in Figure 4-5. In the simulation, ammonia/methane mixtures were diluted in 99% Ar under different equivalence ratios at a pressure of 17 atm. The mole fraction of ammonia and methane was set at 61% and 39%, respectively. This is the same ratio as that utilised in a generic swirl burner experimental campaign in [209]. As observed in Figure 4-5, in most cases, reduced mechanisms show good agreement to the full Konnov mechanism. However, Mech. 5 largely under-predicts the ignition delay times at an equivalence ratio of 2.0, Figure 4-5c. It is also observed that the equivalence ratio has a significant effect on the ignition delay time for ammonia/methane combustion blends. Figure 6d shows how ignition delay times increase with equivalence ratio. Except for Mech.5, all the other reduced mechanisms show good agreement with full Konnov's mechanism within the studied range of equivalence ratios between 0.5-2. The equivalence ratio effect on ignition delay times for NH_3/CH_4 mixture is obvious under high pressure conditions. For instance, the factor between ignition delay times obtained at E.R. of 1 and E.R. of 0.5 is about 1.7 at 1670K whilst a larger factor of 1.9 was found between E.R. of 2 and E.R. of 1. There is very little previous research concerning ignition delay times of NH_3/CH_4 mixtures under high pressure conditions and experimental measurements in particular are required.

4.2.2 Validation of Major Species Predictions in Laminar Flames

To validate the performance of the reduced mechanism models for NH_3/CH_4 combustion, major product concentrations were predicted against experimental data from burner-stabilised premixed flames of ammonia/methane mixture investigated by Tian [41], Figure 4-6~Figure 4-11. In these figures, R refers to the mole ratio of NH_3/CH_4. All the experimental and modelling work by Tian, studied premixed $NH_3/CH_4/O_2/Ar$ flames at low pressure of 4.0 kPa under stoichiometric conditions, the same combustion conditions are simulated in the present work.

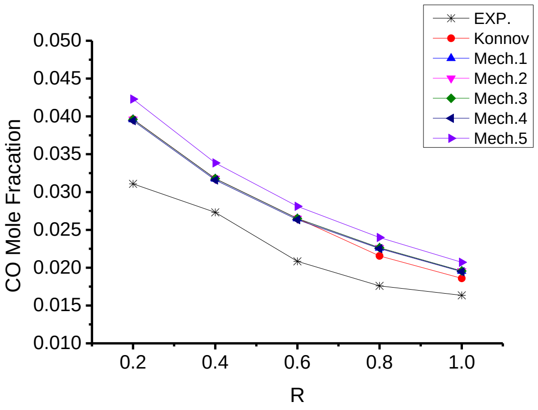


Figure 4-6 Final mole fraction of CO with different R

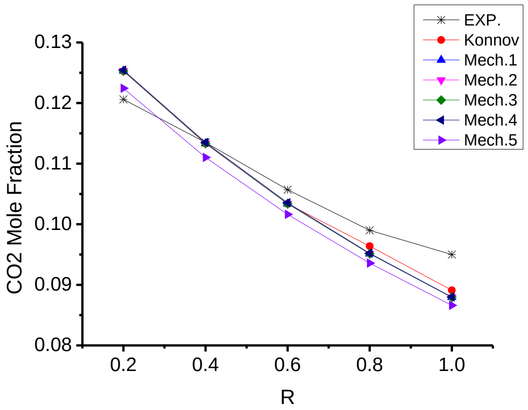


Figure 4-7 Final mole fraction of CO_2 with different R

As observed in Figure 4-6 and Figure 4-7, the concentration of CO and CO_2 decreases when R increases, as expected, the decreasing trend resulting primarily from the reduced methane component in the NH_3/CH_4 mixture. The predicted and experimental data for CO and CO_2 show satisfactory agreement in general, with the larger discrepancy between experimental CO concentration and its predictions. The average relative errors for CO and CO_2 are about 21% and 4% respectively for all the mechanisms considered.

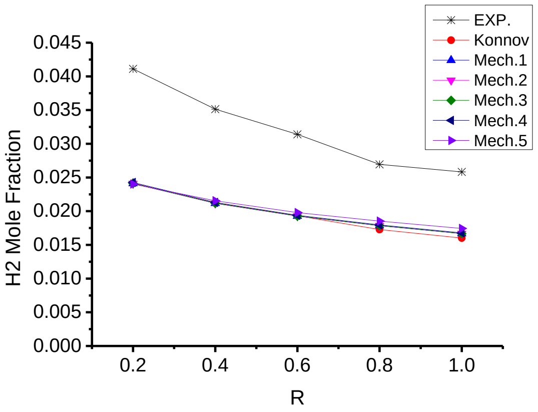


Figure 4-8 Final mole fraction of H_2 with different R

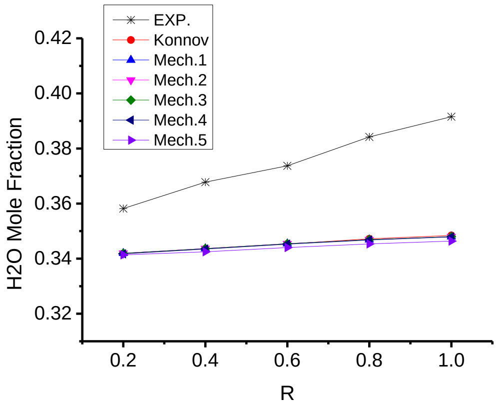


Figure 4-9 Final mole fraction of H_2O with different R

The concentration of major hydrogenous products shown in Figure 4-8 and Figure 4-9, shows relative errors for H_2 and H_2O of around 41% and 45% respectively, emphasising that the hydrogen chemistry still requires optimisation. It can also be seen that R has a similar effect on H_2 as that on CO, whilst the concentration of H_2O increases with increasing R. Figure 4-10 and Figure 4-11 show that Konnov's mechanism and most of the reduced mechanisms perform well in predicting the concentration of the two nitrous products. For the prediction of NO, the best performance is achieved by Mech.1 with relative error of 2.8% while Mech.5 overpredicted the NO concentration about 22%. It is clear that the quantities of N_2 and NO increase while augmenting R, as expected. To utilise ammonia and methane in gas turbine combustors, the emission of CO and NO will of course be an essential environmental concern.

Although the above results are obtained under low pressure conditions and clearly some species predictions still need to be improved, nevertheless, the results still provide important information in assessing qualitatively the performance of NH_3/CH_4 combustion. Now that the concentrations of major products corresponding to different mole ratios (R) of NH_3/CH_4 have been simulated, Konnov's mechanism and the reduced mechanisms can provide some insight into the NH_3/CH_4 combustion kinetics analysis to assist in optimising the fuel mixture ratio for the study on gas turbine utilisation.

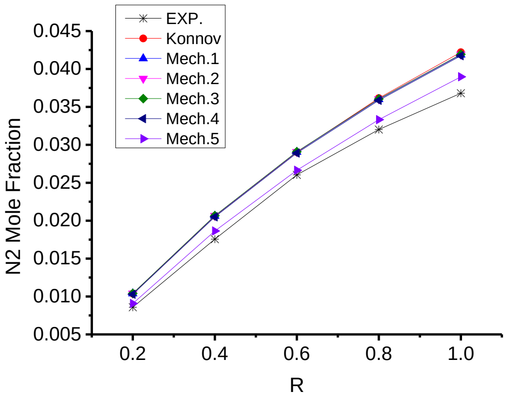


Figure 4-10 Final mole fraction of N_2 with different R

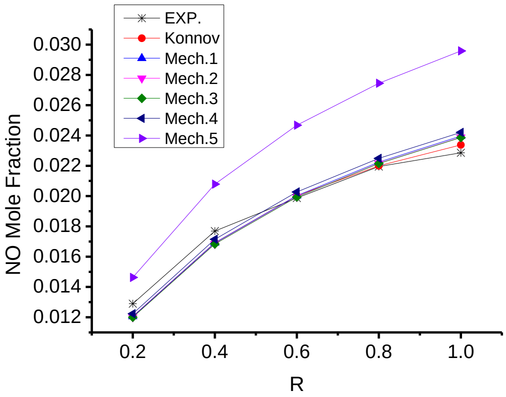


Figure 4-11 Final mole fraction of NO with different R

4.2.3 2D Turbulent Combustion under Gas Turbine Conditions

To verify the performance of the reduced mechanisms further for the use in CFD simulations, a 2D model for turbulent flame combustion was built. The geometry of the burner consists of an inlet tube and a combustion chamber, Figure 4-12. The flame is stabilised down the dump in a recirculation zone by its sudden expansion. The burner is meshed with a structured grid of 13,575 cells. The modelling work is performed with Large Eddy Simulation (LES) coupled with complex chemistry. The CFD solver used for LES is from OpenFOAM toolbox [216, 217]. The case studied has a fuel mixture of 39% CH_4 and 61% NH_3 premixed with air at an equivalence ratio of 1. The Reynolds number is ~2.8×10^4. To explore the performance of the reduced mechanisms under gas turbine conditions, an inlet temperature of 600 °C and pressure of 17 atm was specified.

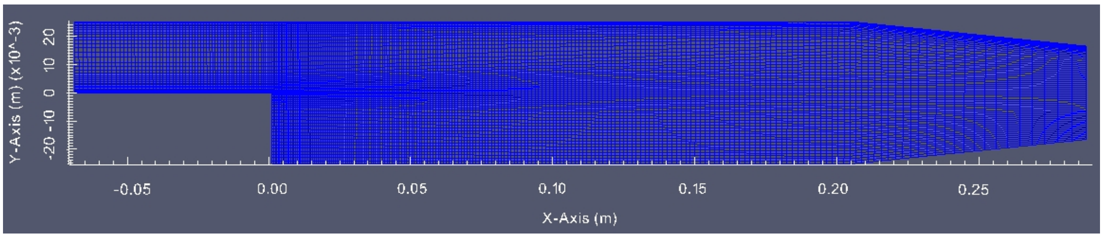


Figure 4-12 The geometry of the burner for turbulent combustion

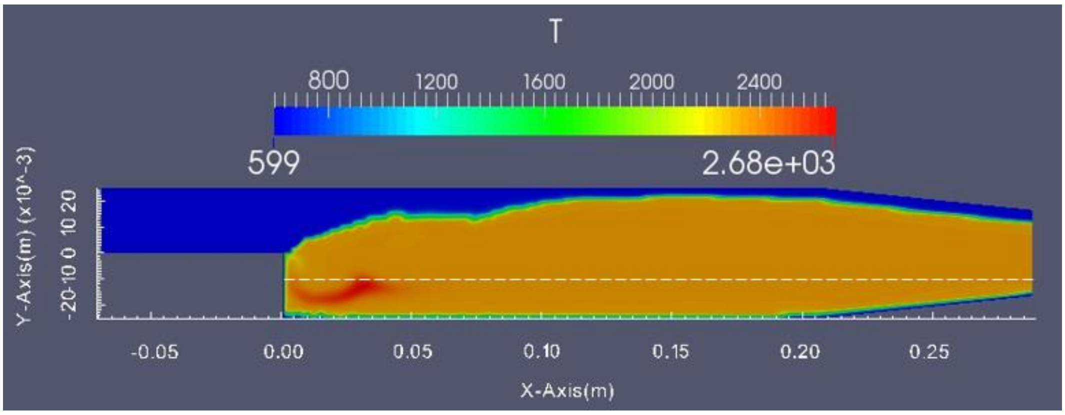


Figure 4-13 Temperature distribution calculation with the Konnov mechanism

When assessing the applicability of the reduced mechanisms, CFD turbulent combustion simulations were performed with parallel computing technology, in which 64 cores were used during the calculation process with different reduced mechanisms. In terms of the processing time from ignition to steady state combustion, the shortest computational time was achieved with Mech. 5 taking 6.05h whilst Konnov's mechanism and Mech. 1-4 took 56.32h, 46.94h, 37.75h, 30.28h and 19.79h respectively. Figure 4-13 shows the temperature field for the turbulent flame simulation using full Konnov's mechanism. Along the dashed line (y=-10^{-2} m), different parameters using the reduced mechanisms are compared in Figure 4-13~Figure 4-17.

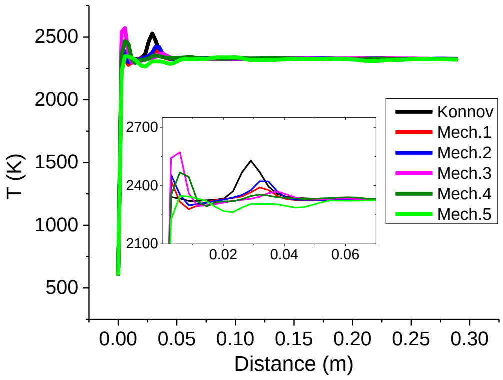


Figure 4-14 Computed profiles of temperature

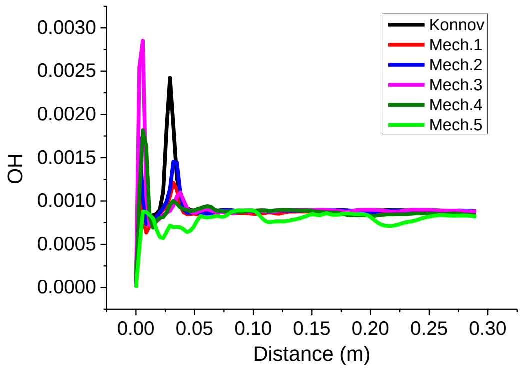


Figure 4-15 Computed profiles of OH mass fraction

Temperature profiles using the reduced mechanisms agree with Konnov's mechanism achieving ~2500 K in the post flame zone, Figure 4-14. In Figure 4-15, most mechanisms predict good results for OH species concentration, but at small distances, Mech. 3 clearly predicts higher OH concentration than the Konnov mechanism, whilst Mech. 5 predicts a relatively lower OH concentration. Different magnitude and location of the OH peak indicate that flame fronts emerge at different locations, also accounting for differences in temperatures between simulations. Since the OH radical is a significant molecule through the combustion process of ammonia/methane fuels, these mechanisms can be used to carry out preliminary performance predictions towards combustion characterisation of such blends. However, it must be emphasised from the previous section that there is still work to do on new reaction mechanism to completely and accurately capture the reaction mechanism of ammonia/methane combustion.

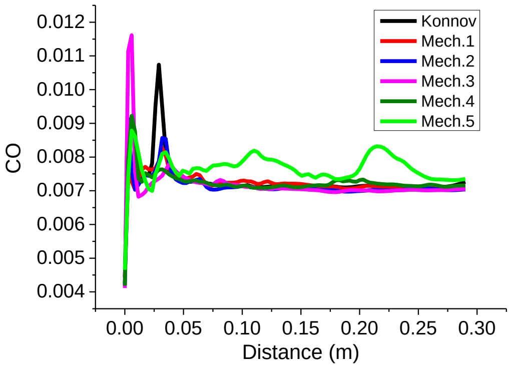


Figure 4-16 Computed profiles of CO mass fraction

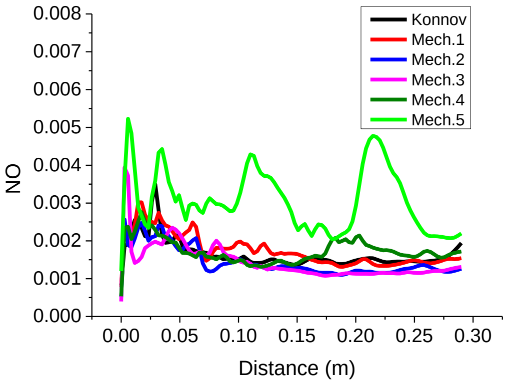


Figure 4-17 Computed profiles of NO mass fraction

Figure 4-16 and Figure 4-17 show emission prediction profiles using different mechanisms. As shown in Figure 4-16, in terms of exit CO emission concentration the five reduced mechanisms produce good agreement with the full Konnov's mechanism. At smaller distances, Mech. 3 shows higher peak value of CO emission than the Konnov mechanism, whilst other reduced mechanisms generate lower predictions. Moreover, Mech. 5 gives considerably higher predictions from distance 0.07 to 0.25. These trends suggest that the reduced mechanisms are adequate in predicting exhaust CO emissions. To capture CO formation within the flame structure, the reduced mechanisms can cause some deviation from the full Konnov mechanism, especially Mech. 5. For NO emission, Mech.1-4 have predicted almost identical concentration profiles as the Konnov mechanism. Since NO is highly temperature sensitive, the reduced mechanisms show good potential for simulation using the complex chemistry coupled with turbulence.

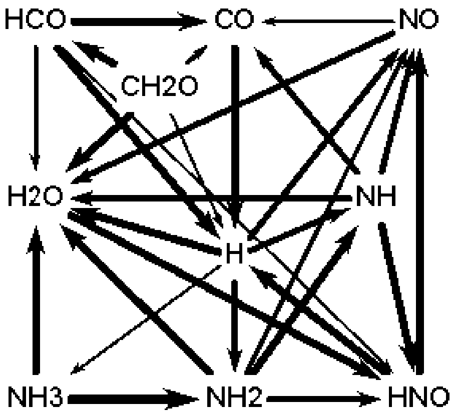


Figure 4-18 Reaction path of NO formation

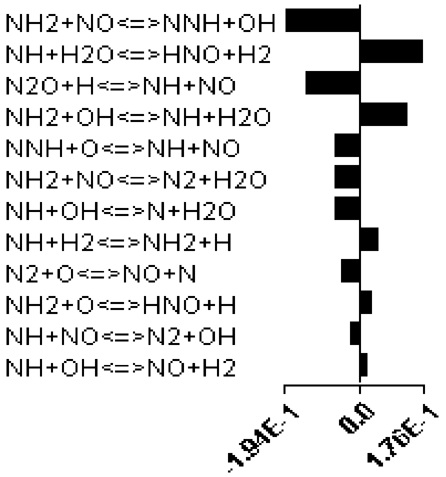


Figure 4-19 Normalized sensitivity of NO using Konnov’s mechanism

Since NO emission is a major concern when utilising ammonia combustion, pathway analyses and sensitivity analyses of NO formation were also conducted using Konnov’s mechanism for this specific blend. As shown in Figure 4-18 and Figure 4-19, the most enhancing radical for NO formation is HNO, followed by NH and NH_2 radicals. Therefore, the profiles of the HNO radical were extracted using all the reduced mechanisms utilised. As expected, Mech.1-4 provide results comparable to Konnov’s mechanism, while Mech.5 shows by far the largest discrepancy of more than 90%. The different fates of these amine species, as predicted by the reduced mechanisms, give rise to the different NO emission results, Figure 4-20.

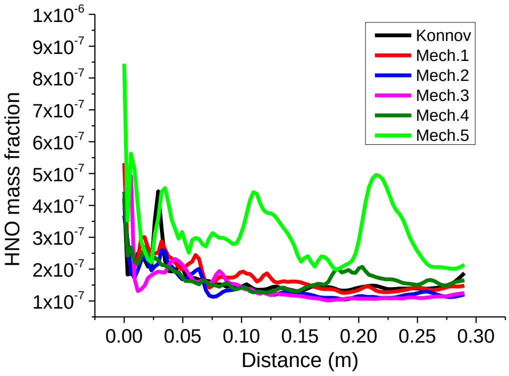


Figure 4-20 Computed profiles of HNO mass fraction

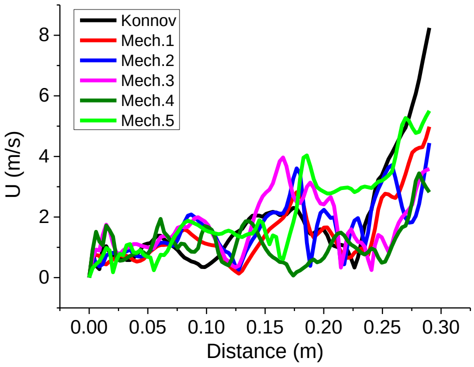


Figure 4-21 Computed profiles of velocity magnitude

Figure 4-21 shows velocity magnitude profiles along the dashed line. As chemical reactions interact with turbulence in the flame, the flow field will also be an essential indication for the performance of the mechanisms and the overall simulation. It can be seen that the predicted velocity magnitude fluctuates along the burner. Generally, all reduced mechanisms have given acceptable predictions compared to Konnov's mechanism. In this simulation of turbulent combustion, where turbulence and recirculation are take into account in the combustion process, all reduced mechanisms but Mech.5 show good performance under gas turbine conditions.

In general, most of the reduced mechanisms except Mech. 5 computed acceptable results compared with full Konnov's mechanism. This indicates that the reduced mechanisms Mech. 1-4 are qualified for the study of temperature field, exhaust emissions, flow field of the NH_3/CH_4 flame with 2D CFD modelling. From this study, overall Mech. 4 is recommended for future use in 3D CFD simulation, due to its relatively short computational time and reasonable accuracy.

4.3 Combustion Characteristics of Ammonia/Methane Mixtures

4.3.1 Ignition Delay

Auto-ignition is one of common problems that occur in real industrial facilities e.g. gas turbine engines. It can happen in the premixer which leads to overheating and subsequent damage to the fuel injector [215] . It is therefore essential to understand the influence of NH_3 on the ignition characteristics of the NH_3/CH_4 fuel blends system. Figure 4-22 shows ignition delay time calculation results with a variation of NH_3 mole fraction in NH_3/CH_4 fuel blends at temperatures ~2000 K based on modified Konnov methaniam. A clear increase of ignition delay times can be found with more NH_3. It is generally the same trend as shown in the work of Mathieu [44] for ammonia ignition under different equivalence ratios. It can be seen that same as Mathieu's work, equivalence ratio seems to have a moderate effect compared with the effect of ammonia content. It is shown that the values of ignition delay times are below the averaged values estimated by mole proportions of NH_3 to CH_4, which indicates a strong non-linear influence of ammonia substitution effect of CH_4 on chemical kinetics. When the NH_3 mole fraction is more than 50% in the fuel blend, the increased rate of ignition delay time augments, meaning that ammonia dominates the process of ignition delay. For instance, for stoichiometric mixtures a factor ~3.4 can be found between ignition delay times obtained at a NH_3 mole fraction of 100% and 50%, whist a smaller factor of 1.6 is found between NH_3 mole fractions of 50% and 0%.

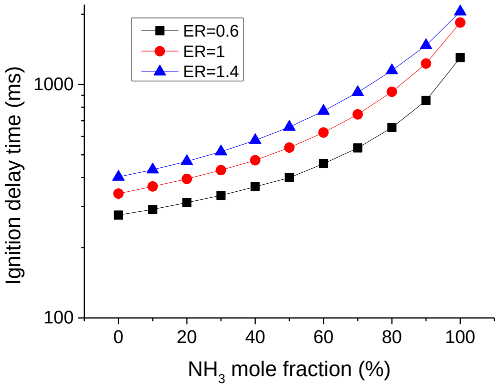


Figure 4-22 Ignition delay times as a function of ammonia fraction in the fuel blend

The ignition delay time prediction was also performed under different equivalence ratio conditions as shown in Figure 4-22. It can be observed that for a certain NH_3/CH_4 fuel mixture with the increase of equivalence ratio ignition delay times will also increase. Actually, in practical applications auto-ignition becomes a more common issue especially when using conventional fuels at higher pressure ratios as those used in modern gas turbines. From the results above, it can be identified that since ammonia substituting methane will lead to an obvious increase in the ignition delay times, using NH_3/CH_4 as fuel can help reduce the risk of auto-ignition in premixed gas turbine chambers.

4.3.2 Laminar Flame Speed Characteristics

Numerical simulation results of characteristics for NH_3/CH_4 flame propagation are illustrated in Figure 4-23 and Figure 4-24. In Figure 4-23, unstretched laminar flame speed is plotted as a function of NH_3 fraction at three different equivalence ratios (E.R.=0.6, 1.0, 1.4). It can be seen that from pure methane (NH_3%=0) to pure ammonia (NH_3%=100%) laminar flame speed decreases almost linearly with the increase of NH_3 fraction in the fuel blend. These results have shown the same tendency of flame speed with ammonia addition with the work of Nozari and Karabeyoglu [62] in which ammonia is combusted with hydrogen. For different equivalence ratios, the flame speed exhibits a significant sensitivity to ammonia substitution, in which near stoichiometric conditions a more significant change in gradient can be observed. Under stoichiometric conditions, the flame speed decreases about 30 mm/s with each 10 percentage increase of NH_3 fraction whilst the decrease rate drops to about 8 mm/s for equivalence ratios of 0.6 and 1.4. The reason of this phenomenon is mainly due to the relatively lower reactivity and flame speed of ammonia than that of methane. As flame speed is a key parameter for a fuel in real combustion development, this suggests that the low flame speed of high NH_3 mixtures can limit their application in practical energy devices.

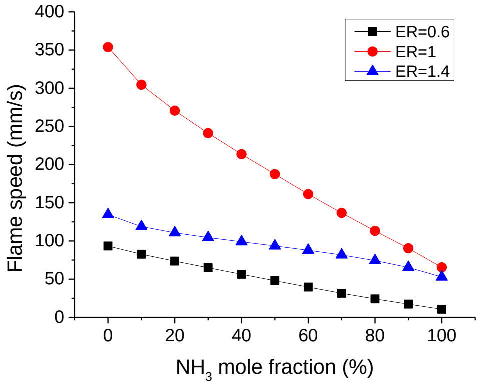


Figure 4-23 Flame speed as a function of ammonia fraction in the fuel

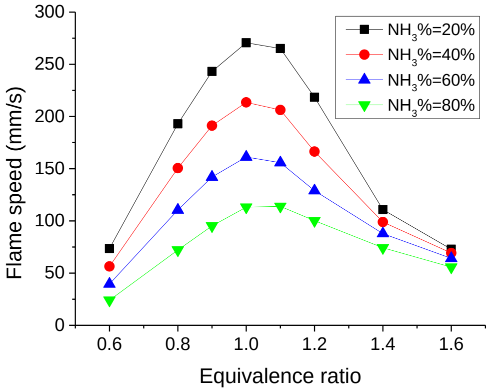


Figure 4-24 Laminar flame speed as a function of E.R.(equivalence ratio)

Figure 4-24 shows the unstretched laminar flame speed against equivalence ratios ranging from 0.6 to 1.6 at different ammonia fractions. For all the cases of NH_3/CH_4 combustion studied, laminar flame speed of fuel-lean mixtures increases with the equivalence ratio up to stoichiometric conditions and then decreases under fuel-rich regimes. The maximum value of the flame speed is presented at the equivalence ratio of 1.0. For a certain equivalence ratio the flame speed increases with the decrease of ammonia fraction and the increase becomes more remarkable for NH_3/CH_4 flames near stoichiometric conditions. Passing stoichiometry, hot, unreacted ammonia in the fuel-air mixture will start recombining with NO present in the flue gases, thus promoting two effects: reduction of NO_x [59] and an increase of flame speed compared to lean fuel conditions. Similar results have also been reported in previous ammonia combustion related research where the flame speed and NO_x emission of ammonia combustion were studied in relation to the effect of equivalence ratio [31]. This indicates that in practical application using ammonia to substitute methane, equivalence ratios near stoichiometric condition are more favourable for better flame propagation properties, with rich fuel conditions more favourable than lean environments.

4.3.3 Emission Characteristics

NO_x emissions are an essential concern when using ammonia as a fuel [16, 27, 205]. In the present work, NO concentrations in the final flame exhaust gas were investigated to gain a deep insight into characteristics of the main NO_x product with a wide range of NH_3 fractions and equivalence ratios as shown in Figure 4-25 and Figure 4-26. It must be remembered that ammonia based flames not only produce high temperature, Zeldovich NO_x, but also fuel bound emissions due to the intrinsic characteristics of ammonia. Figure 4-25 shows the NO emission fractions in the burnt gas as a function of NH_3 fraction under different equivalence ratios. It can be observed that the NO emission curves show the same pattern, increasing first and then dropping with the increase of NH_3 fraction. However, the peaks of NO emission are quite different for different equivalence ratios. For instance, for an equivalence ratio of 1.4, the maximum value is presented at NH_3 fractions of ~20% whilst it is at about NH_3 fraction of 60% for an equivalence ratio of 1.0. This indicates how the influence of equivalence ratio on NO_x emissions production is critical as illustrated in Figure 4-26. From Figure 4-25 it can also be observed that ammonia substituting methane in a large proportion can have the same level of NO_x emissions as high-methane proportion fuel blends (low content ammonia cases), which suggests the feasibility of using ammonia as primary fuel.

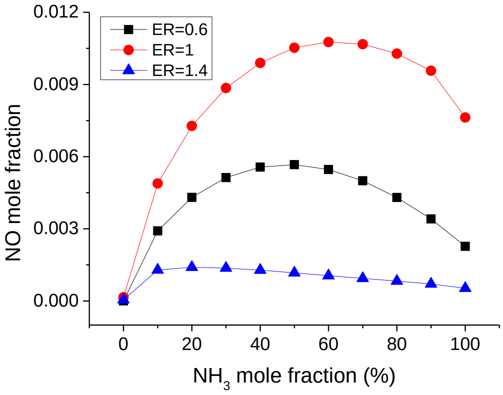


Figure 4-25 NO mole fraction in burnt gas as a function of ammonia fraction in fuel blends

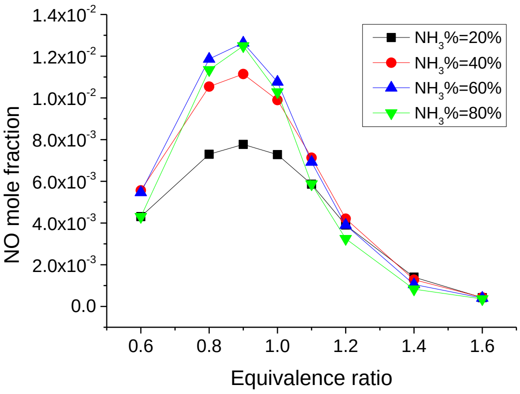


Figure 4-26 NO mole fraction in burnt gas as a function of E.R.

Furthermore, the characteristics of NO_x emission in Figure 4-25 indicate the variation of NO_x formation in NH_3/CH_4 combustion with different fuel blends. To understand the phenomenon, the adiabatic flame temperature was plotted against NH_3 fraction in Figure 4-27, in which flame temperature is decreased with the increase of NH_3 fraction in fuel blends as NH_3 has a lower adiabatic temperature than CH_4. Comparing Figure 4-25 with Figure 4-27, it can be noticed that NO_x emissions vary with the same trend as the adiabatic flame temperature only at high NH_3 fraction regions. For instance, under stoichiometric condition when NH_3 mole fraction is more than 60%, the adiabatic flame temperature and NO_x emission decrease with the increase of NH_3 mole fraction, whilst NO_x emissions increase with more CH_4 being substituted by NH_3 within the region where NH_3 is less than 60%. Actually, the trend of temperature and NO emission within the range of ammonia mole fraction less than 50% is the same as in Tian's work [41], which can be a good demonstration for the results of the present study. Moreover, reference [62] also shows some NO_x emission results with the effect of ammonia added in hydrogen: The NO_x formation level increases with ammonia content in the fuel mixture decreasing when energy fraction of ammonia in the fuel mixture is less than 20%, and then NO_x emission drops with the ammonia percentage increasing after the ammonia fraction is more than 20%.

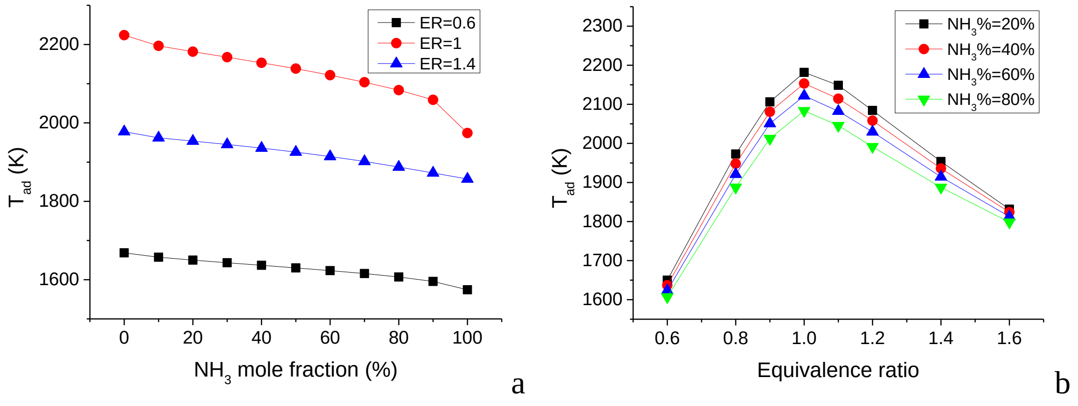


Figure 4-27 Adiabatic flame temperature (T_{ad}) as a function of ammonia fraction in fuel blends (a) and equivalence ratio (b)

In low NH_3 content regions where thermal NO_x have more contribution to the total NO_x production, the result seems contradictory to the general understanding of thermal NO_x and fuel bond NO_x, as a first glance would expect a decrease in total NO_x production with increasing NH_3 fraction in fuel blends. A detailed sensitivity analysis in the present study shows that reactions $NH+H_2=NH_2+H$, $NH_2+O=HNO+H$ and

$NH+H_2O=HNO+H_2$ play the most significant role in promoting reactions in NO_x formation in a wide range of fuel blends and equivalence ratios. Thus when ammonia begins to be added to the methane, more NH and NH_2 are available to promote fuel bound NO formation. It can be determined that the fuel-bond NO_x is more sensitive than thermal NO_x to the increase of total NO_x emission in low NH_3 content blends regions, although in such regions thermal NO_x is the dominating mechanism in the total NO_x emission. Therefore the NO_x emission trend is still a result of fuel bond versus thermal NO_x production: when NH_3 mole fraction is low in the fuel blends, the increase of fuel bond NO_x formation is more sensitive and plays a more prominent role in NO_x emission increase. Consequently, with more ammonia and oxygen, e.g. lean conditions, in the fuel mixtures NO_x emissions increase due to abundant fuel-bound nitrogen in ammonia. In high NH_3 mole fraction regions, the recombination of ammonia with NO_x produces a decay of the pollutant, thus consuming not only thermal NO_x but also those produced during fuel-bonding reactions.

Figure 4-26 shows the effect of equivalence ratio ranging from 0.6 to 1.6 on NO formation for different NH_3/CH_4 mixture compositions. It is obvious that equivalence ratio conditions have significant impact on NO emission level in the exhaust. Also, there is no variation with NH_3/CH_4 fuel blends composition observed on the position of NO peak emissions: under fuel lean conditions (ER<1.0), NO emissions increase with the increase of equivalence ratio and reaches the maximum point at equivalence ratio of around 0.9 for all curves. After the peak value, NO emissions drop with increase of equivalence ratio.

When comparing Figure 4-26 with Figure 4-24, one interesting phenomenon that can be observed is that the flame speed is higher with E.R.=1.4 than E.R.=0.6, which indicates rapid combustion with E.R.=1.4 resulting in higher combustion temperatures (Figure 4-27b) and therefore one will expect a higher NO emission formation. However the simulation results presented in Figure 4-26 shows NO emissions with E.R.=1.4 are lower than E.R.=0.6. Taking a detailed look into the NO_x calculation results in Figure 4-26, it can be seen that the NO_x emission drops quickly in the fuel rich region with the increase of equivalence ratio. Actually, the reason why NO emission at E.R. of 1.4 is lower than E.R. of 0.6 is mainly due to the excess unreacted ammonia for high equivalence ratio conditions, as previously stated. Under the E.R.

of 1.4 there are much more unreacted ammonia in the fuel-air mixture, thus the ammonia can play an important role in the deNO$_x$ process as NO is removed by further reactions with NH$_2$ generated from ammonia [59]. Similar phenomena as the ammonia/methane flames in the present work have already been reported in previous ammonia combustion study [31], in which the flame speed and NO$_x$ emission of ammonia combustion were studied in relation to the effect of equivalence ratio. Also, similar conclusions can also be found in [28, 62] for ammonia/hydrogen mixtures, which demonstrates the consistent characters of ammonia-based fuel combustion. Moreover, as tested in real engine applications of ammonia/hydrocarbon studies in [113, 205], relatively much lower NO$_x$ emissions are observed under fuel rich conditions for ammonia-based fuels.

Another phenomenon that can be observed is that for a certain equivalence ratio NO emissions increase with the increase of ammonia fraction but the variation becomes slight for fuel rich conditions. On the other hand from the stoichiometric region to fuel rich conditions, the increase of NO emissions as a result of more CH$_4$ being replaced by NH$_3$ becomes much smaller in comparison to the fuel lean region, e.g. NO emissions with 40%NH$_3$ and 80%NH$_3$ are quite close. The results also show that for all the flames with different NH$_3$/CH$_4$ mixture compositions, the NO emissions in the fuel-rich region are relatively lower than under fuel-lean conditions. These results imply the necessity and importance of optimal control of the stoichiometry using ammonia-based fuels. Specifically, operating NH$_3$/CH$_4$ in fuel rich conditions can be a choice to reduce NO emissions in practical combustion applications.

As an essential parameter influencing the NO$_x$ emissions, the effect of equivalence ratio were studied on adiabatic flame temperature at different NH$_3$ fractions as illustrated in Figure 4-27b. The curves show a peak value at about equivalence ratio of 1.0 as the same phenomena observed in laminar flame speed calculation shown in Figure 4-24, which represents the maximum net heat release considering the endothermic procedure of NH$_3$ decomposition. Comparing with Figure 4-26, it can be observed that the peak of adiabatic flame temperature is at the higher equivalence ratio than NO$_x$ emission at equivalence ratio of ~0.9. When E.R.<0.9, the adiabatic temperature increases with the increase of equivalence ratio. As expected, the increasing trend of adiabatic temperature leads to higher NO$_x$ emission production due to more thermal NO_x formation. However, in the region of 0.9<E.R.<1.0, although the adiabatic temperature increases with the increase of equivalence ratio, NO_x emission begins to decline, which indicates thermal NO_x formation is less dominant in relation to fuel bond NO_x formation under such conditions. When E.R.>1.0, NO_x emission levels drop quickly due to both surplus NH_3 functioning on NO_x reduction and decrease of the adiabatic temperature leading to less thermal NO_x emissions.

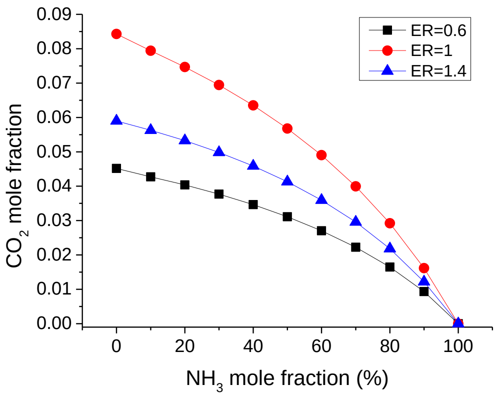


Figure 4-28 CO_2 mole fraction in burnt gas as a function of ammonia fraction in fuel blends

Figure 4-28~Figure 4-30 show the main carbonous products concentration in burnt gas at different NH_3 mole fractions and equivalence ratios. In Figure 4-28, as expected with more fraction of CH_4 substituted by NH_3, CO_2 emissions drop accordingly as less carbon is available in the fuel blends. It also can be seen that stoichiometric conditions have more CO_2 products than fuel lean and fuel rich conditions. This is mainly due to the better combustion efficiency. As expected, blends with >60% NH_3 produce half CO_2 than pure methane. Figure 4-29 and Figure 4-30 give the CO emission characteristics at different NH_3 mole fractions and equivalence ratios, respectively. In Figure 4-29, CO emission levels drop as the NH_3 mole fraction increases. Specifically, CO emissions drop faster as the NH_3 fraction increases under high equivalence ratio conditions, e.g. E.R.=1.4. The trend of two major carbonous products CO and CO_2 with different NH_3 fractions in the fuel blends agrees with the conclusions of NH_3/CH_4 combustion in the work of Tian et. al. [41]. These decreasing trends result primarily from the reduced methane component in the NH_3/CH_4 mixture. The results of the present work not only give satisfactory agreement with the experimental data in [41], but also expand the knowledge on high ammonia content fuels and different equivalence ratio conditions which have not been studied before. Figure 4-30 shows

CO fraction in burnt gas as a function of equivalence ratio ranging from 0.6 to 1.6. The results clearly show an increasing trend of CO emission with the increase of equivalence ratio. As shown in Figure 4-31 it is possible to identify three regimes in the NH_3/CH_4 flames depending on the equivalence ratio. In the cases of equivalence ratio less than 0.9, CO emission production grows slightly with equivalence ratio. In the cases of 0.9<E.R.<1.1, CO emission increases almost exponentially with the increase of equivalence ratio. Finally when equivalence ratio is larger than 1.1 the increase of CO emissions becomes relatively slow as the equivalence ratio increases. Thus in this situation, to control the CO emission level in the exhaust for practical use, it is better to conduct the combustion of NH_3/CH_4 mixture in the fuel lean regime. However, from previous analyses it has been shown that NO_x emissions are noticeably high under fuel lean conditions. Thus the contradiction between NO_x and CO emissions reduction suggests an optimisation needs to be carefully settled in terms of stoichiometry design. To meet the stringent emission standard of industrial application nowadays, other possible solutions can also be considered including selective catalytic reduction (SCR) of NO_x, reburning techniques, oxygen-enhanced combustion etc., which are out of the scope of this study.

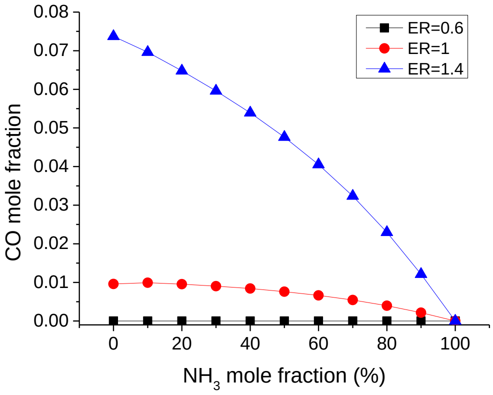


Figure 4-29 CO mole fraction in burnt gas as a function of ammonia fraction in fuel blends

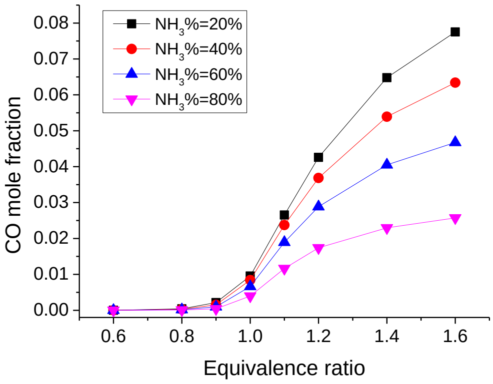


Figure 4-30 CO mole fraction in burnt gas as a function of E.R.

4.3.4 Flame Structure Analysis

To gain a deep insight into the flames of NH_3 substituting CH_4 for premixed combustion application, studies of detailed flame structure were also performed for NH_3/CH_4 flames. As shown in Figure 4-31, some major radicals in structures of freely propagating NH_3/CH_4 flames are illustrated for different NH_3 fractions in fuel blends under stoichiometric conditions. Figure 4-31a-c show the concentration of OH, H and O radicals as a function of distance through the flames. The peaks of these radicals are all presented at the position of about 11 mm above the burner. Comparison of the figures shows that in stoichiometric NH_3/CH_4 flames OH radical has the largest maximum concentrations among these radicals while the peak concentrations of O radical is much lower compared to OH and H. For all the three radicals, it is obviously observed that with more mole fraction of NH_3 in fuel blends, peak concentrations of the radicals are decreased indicating decreasing reaction rates and thus laminar flame speed. This is due to the relatively less reactivity of ammonia compared to methane leading to weaker flames. On the contrary, as shown in Figure 4-31d NH_2 originated from ammonia shows a different trend in the flames' reaction zone with more NH_3 substituting CH_4. The peak value of NH_2 keeps increasing with the increase of NH_3 in the fuel blends. The trend observed has been demonstrated to be consistent with the unstretched laminar flame speed calculation results in Figure 4-23, which shows that with an increase of NH_3 fraction in the fuel blends the laminar flame speed tends to decrease. Quantitatively, as demonstrated in previous studies [28, 63, 218], certain key radicals have a strong correlation with laminar flame speed for premixed flames. In the present study, calculations of NH_3/CH_4 flame speed show that the peak value of OH, H, O and NH_2 are of the highest relevance. In Figure 4-32, laminar flame speed of NH_3/CH_4 fuel blends under stoichiometric conditions are plotted as the function of $(OH+H+O+NH_2)_{max}$. Results suggest a quasi-linear relation between the NH_3/CH_4 flame speed and the maximum mole fraction of $OH+H+O+NH_2$ in the flames.

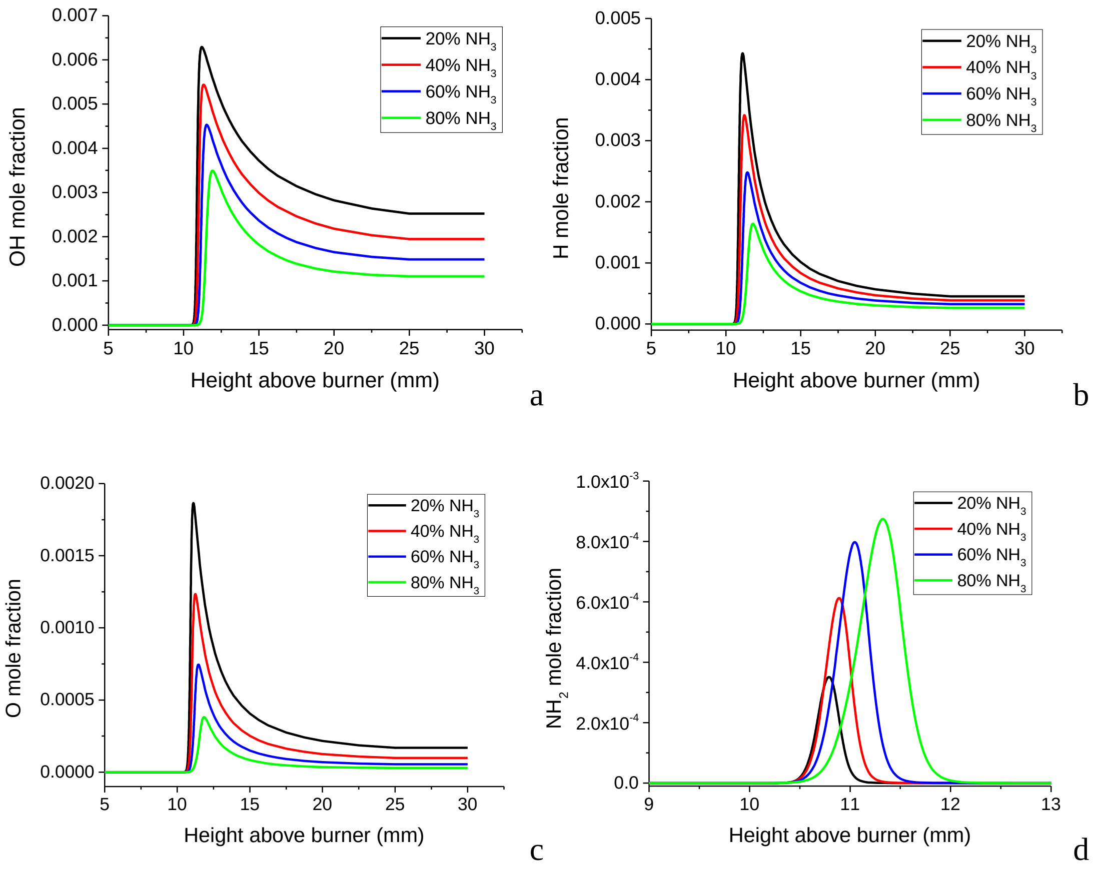


Figure 4-31 Predicted OH, H, O and NH_2 radicals in premixed ammonia/methane flames (E.R.=1)

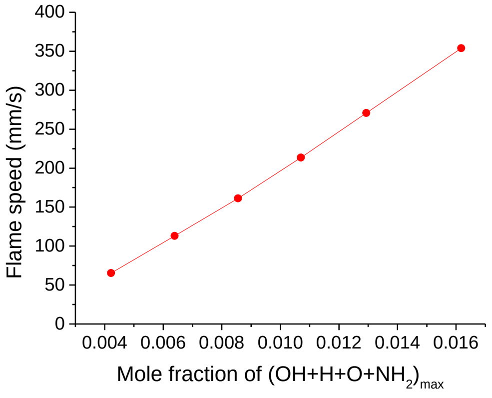


Figure 4-32 Laminar flame speed as a function of maximum mole fraction of $OH+H+O+NH_2$ radicals

Figure 4-33 shows the concentration of NO and CO as a function of distance through the flames. For CO profiles, it is shown that the peak value of CO concentration declines when increasing ammonia fraction in fuel blends, which is the same decreasing trend as CO concentration in the exhaust. The maximum value of NO concentration in the flame shows the same trend of NO concentration in the burnt gas that is NO emission of 60% NH_3 fuel mixture is higher than other fuel blends, e.g. 40% NH_3 and 80% NH_3 cases. Comparing with Figure 4-31, it can be observed that the maximum concentration of CO and NO is presented at the same position of the OH, H, O radical peaks in the reaction zone. This indicates emissions are mainly generated in the flame front as these extremely active radicals play essential roles in branching chain reactions. Furthermore, the formation of the CO and NO emission can be characterised by some important precursors. Through production rate and sensitivity analysis, HNO and HCO are the predominate promotors for NO and CO formation, respectively. For instance, most sensible reactions of the NO formation is from the reactions HNO + H = NO + H_2 and HNO + OH = NO + H_2O in NH_3/CH_4 combustion. Therefore, the profiles of HNO and HCO radicals in stoichiometric premixed flames are described as shown in Figure 4-34. As expected, the maximum peaks of HNO and HCO radical concentration with different NH_3 concentration in fuel blends are the same as for NO and CO.

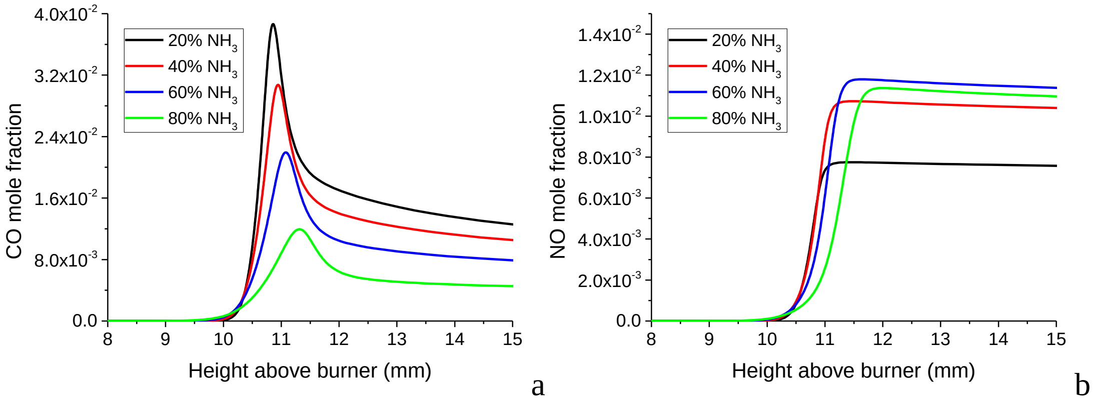


Figure 4-33 Predicted CO (a) and NO (b) species in premixed ammonia/methane flames (E.R. =1)

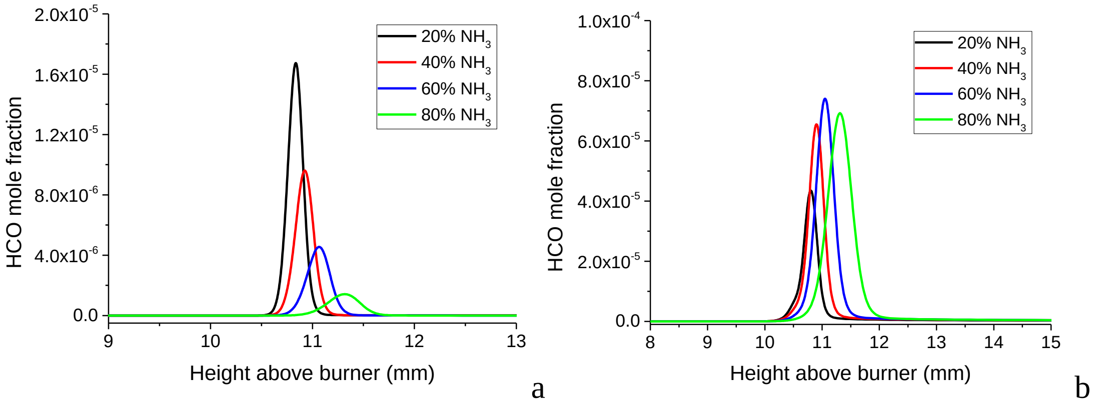


Figure 4-34 Predicted HCO (a) and HNO (b) radicals in premixed ammonia/methane flames (E.R. =1)

4.3.5 Effect of Pressure and Temperature

To explore the feasibility of utilising ammonia/methane blends as fuel for practical application, it is essential to investigate the combustion characteristics under elevated pressure and temperature conditions, which is usually encountered in industrial power. For instance, for a typical heavy-duty industrial gas turbine with compression ratio of 17, an isentropic compression process in the compressor will lead to an initial temperature of unburnt air/ammonia/methane mixture rising to about 680 K and a pressure of 17 atm before it is ignited in the combustor. Unfortunately, up to now there is no data on realistic industrial operational conditions for NH_3/CH_4 combustion which can be used to help analyse or optimise gas turbine applications. Therefore, it is necessary to investigate the effects of pressure and temperature for NH_3/CH_4 combustion. In Figure 4-35~Figure 4-40, premixed flames of 60%NH_3/40%CH_4 fuel blends, which were proved to be a potential composition choice for practical gas turbine engine use [205], were numerically studied under stoichiometric conditions to obtain typical combustion properties such as laminar flame speed and emissions concentration.

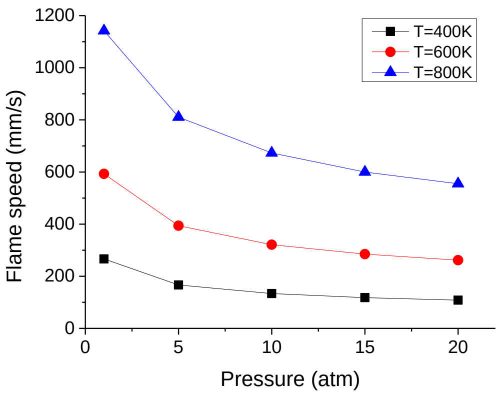


Figure 4-35 Flame speed as a function of pressure

Figure 4-35 shows the effect of pressure on laminar flame speed at different initial temperature conditions. It can be observed that the increase of pressure has a negative effect on the flame propagation. However with the increase of pressure, the negative effect on laminar flame speed tends to be much smaller when it comes to high pressure conditions. The results also indicate that under relative high temperature conditions, the effect of pressure tends to have more impact on the laminar flame speed. For instance, under the initial temperature of 800K the laminar flame speed of NH_3/CH_4 shows an obvious decrease with the increase of pressure whilst quite slight decrease of laminar flame speed can be observed when the initial temperature is 400K. This suggests that under practical industrial conditions (e.g. gas turbine), pressure conditions will be an essential factor for the design and optimisation of performance of NH_3/CH_4 combustion applications.

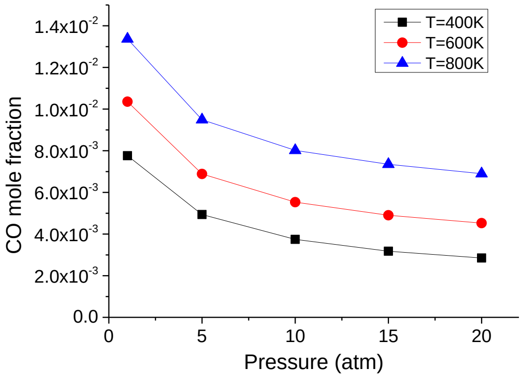


Figure 4-36 CO mole fraction in burnt gas as a function of pressure

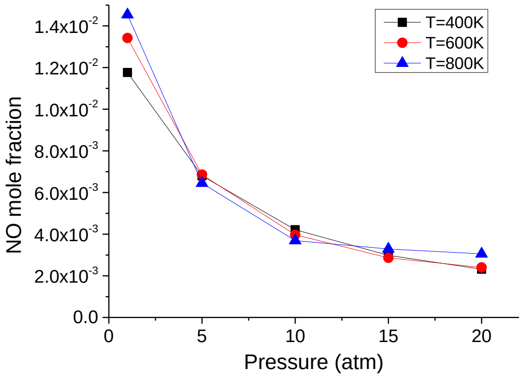


Figure 4-37 NO mole fraction in burnt gas as a function of pressure

Figure 4-36 and Figure 4-37 illustrate the CO and NO emission concentrations in the burnt gas as a function of pressure at different initial temperature conditions. With the increase of pressure, reduction of both CO and NO emissions is obtained. For instance, a significant reduction in NO is observed with the increase of pressure. The NO concentration in the burnt gas under 20 atm is only about 20% of that under atmospheric conditions. From the figures, NO emissions are more sensitive to pressure than CO as a greater NO reduction is obtained from 1atm to 20 atm. Furthermore, a difference on the profiles of CO emissions can also be observed at different inlet temperature. As the pressure increases, the adiabatic temperature tends to increase slightly as shown in Figure 4-38, which will lead to a little more thermal NO_x formation in the flame. Therefore, the decrease of total NO emission with the increase of pressure suggests that pressure is a more important factor which affects the kinetics of fuel-bond NO formation more significantly than for thermal NO. These results agree with similar emission trends of the pressure effect on ammonia-based fuel reported in previous experimental and numerical work [31, 62, 205]. Especially as an important concern in ammonia combustion, the significant NO reduction effect shown in the simulation can suggest a quite good potential using ammonia-based fuel under elevated conditions in practice.

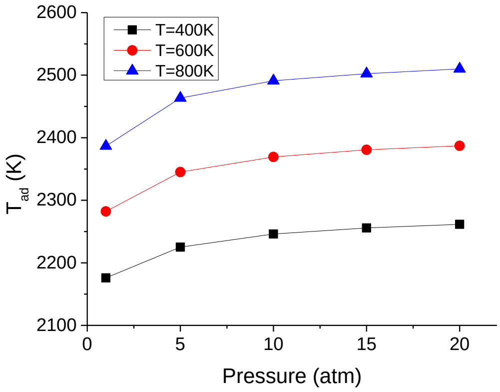


Figure 4-38 Adiabatic flame temperature as a function of pressure

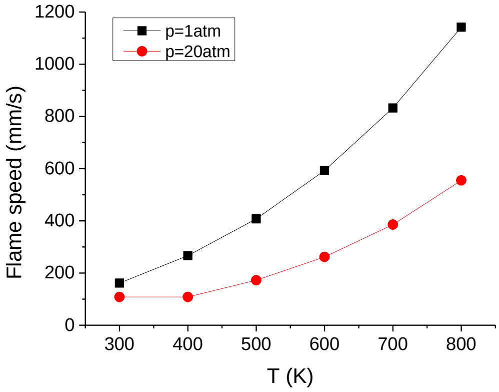


Figure 4-39 Effect of unburnt gas temperature on flame speed

Figure 4-39 and Figure 4-40 show the effect of initial temperature on different properties of NH_3/CH_4 premixed combustion under stoichiometric condition. In Figure 4-39, laminar flame speed increases with the increase of initial temperature due to augmentation of flame temperature and therefore higher reaction rates. The promoting effect of initial temperature on flame propagation is smaller under high pressure conditions than low pressure conditions, which indicates that the augmentation of pressure has an inhibiting effect on the flame speed enhancement. In Figure 4-40a, CO emissions increase with the increase of initial temperature at both atmospheric and high pressure conditions, while in Figure 4-40b NO emissions also increase with initial temperature but much slower than the CO profile. The results suggest that the combined effect of elevated pressure and initial temperature can eventually lead to a decrease in NO_x and CO emissions. Specifically, under high pressure conditions (20 atm), it can be observed the effect of initial temperature condition on NO emission is extremely small, which means pressure is the main factor influencing the NO formation in practical engine operational conditions.

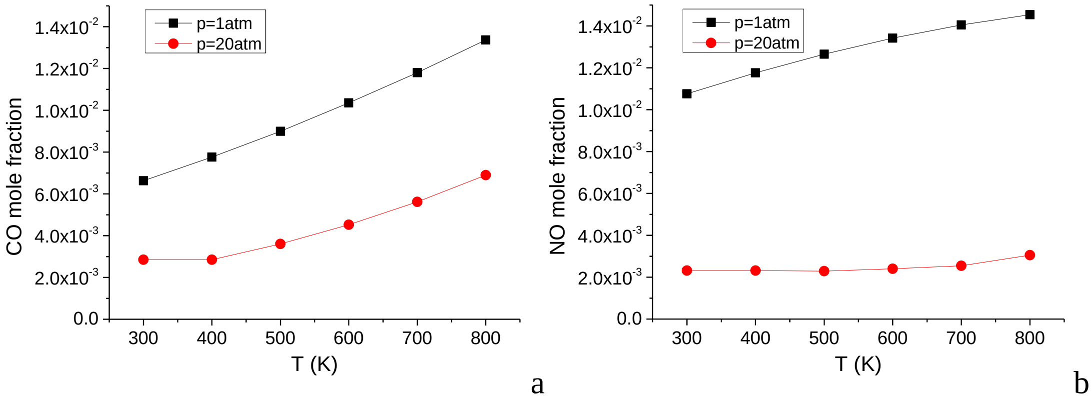


Figure 4-40 Effect of unburnt gas temperature on CO and NO emission in exhaust

4.4 Summary

In this chapter, Konnov’s mechanism and five reduced chemical kinetic mechanisms based on it have been appraised with the aim of investigating NH_3/CH_4 combustion in practical systems. The reduced mechanisms were examined using 0D, 1D and 2D models, under high temperature and pressure conditions, indicative of gas turbine combustors.

Ignition delay time calculations with reduced mechanisms for highly diluted ammonia under high pressure showed relatively larger deviations from the shock tube experimental data published previously, compared to low pressure conditions. Ignition delay time predictions for ammonia/methane contained blends showed that the reduced mechanisms provide reasonable agreement with experiment data. Furthermore, under high pressure (17 atm) and different equivalence ratio conditions, ignition delay times predictions for ammonia/methane using Mech.1-4 demonstrated good performance against the full Konnov mechanism, while Mech.5 worked well for equivalence ratios in the range of 0.5 to 1.25 only. Also, combustion product calculations for NH_3/CH_4 in a burner-stabilised premixed flame showed good accuracy for all reduced mechanisms and the full Konnov’s mechanism, which validates the capability of species concentration prediction. Finally, to assess the performance for use in practical CFD analyses, temperature profiles, OH radicals, CO, NO emissions and velocity magnitudes in a turbulent flame were predicted with reduced mechanisms under gas turbine conditions, all showing good agreement with those obtained through the full Konnov's mechanism apart from Mech.5.

In an overall assessment of the predictive capability of the reduced mechanisms for future CFD analysis, the model proposed for future ammonia/methane research is Mech.4, providing a good compromise between predictive capability compared to the full Konnov model and computational run-time.

Moreover, to explore the potential of utilising ammonia as a fuel for low carbon future energy systems, numerical simulation of co-firing ammonia with methane were performed. The detailed chemical-kinetics mechanism model was used for high ammonia content or pure ammonia combustion.

The ignition delay time calculations show that both the ammonia fraction in fuel blends and equivalence ratio have important impact on the ignition delay time of ammonia/methane fuel blends. Significant higher ignition delay time using NH_3/CH_4 fuel blends were observed compared to those using pure methane.

Laminar flame speed calculation results show that NH_3 fraction in the fuel blends has a significant negative effect on flame speed. As with the increase of ammonia fraction, ammonia/methane flame propagation is weakened, suggesting the need of developing new techniques to promote stable operational conditions using these blends. However, fuel-rich conditions show greater values to lean conditions as a consequence of further ammonia reaction.

Emission characteristic results show that when using ammonia as primary fuel in the blends, CO emission will be lower. Ammonia substituting methane in a large proportion can have the same level of NO_x emissions as low content ammonia cases, which suggests the feasibility of using ammonia as primary fuel, with the advantage of going richer in equivalence ratio to ensure recombination of unburned ammonia with NO_x, thus lowering the latter.

Flame structure analyses show that decrease in chemical reactivity with more ammonia fraction leading to the reduction of flame speed, phenomenon illustrated by the decrease of H, O and OH radical mole fractions in the flame. Also, NO and CO emissions have strong correlations with maximum radical concentrations like HNO and HCO in the reaction zone at different NH_3 fractions.

The study of the effects of engine-relevant conditions show that the elevated pressure will decrease the NO and CO emissions whilst increased initial temperature will lead to the augmentation of emissions. However, simulation results show that pressure is a more prominent factor which affects the kinetics in practical engine operational conditions than temperature, which indicates a good potential of using ammonia-based fuels under gas turbine industrial conditions.

CHAPTER 5

Chemical Kinetics Study of Ammonia/Hydrogen Combustion

Chapter 5

Hydrogen is a carbon neutral fuel, and an excellent combustion promotor for ammonia, on the other hand ammonia is also a hydrogen carrier and can be cracked to produce hydrogen, therefore ammonia/hydrogen blends can be seen as flexible fuel sources. Practically, there is a potential that ammonia/hydrogen can be used as an alternative fuel for the purpose of applications in industrial systems e.g. gas turbine of the future [135]. To utilise ammonia/hydrogen effectively, it is essential to understand better the reaction mechanisms using detailed chemical kinetic models. In addition, conducting computational fluid dynamics (CFD) simulations coupled with detailed ammonia combustion chemistry can serve as a more practical and powerful tool for analysing and designing ammonia combustion systems. The challenging conditions in practical combustion systems (e.g. gas turbine combustors) require a more specific study on the chemical progression of ammonia/hydrogen species, which is still immature for development of large scale industrial systems. Some previous studies [35, 40, 44, 62] have developed detailed chemical mechanisms of ammonia combustion and provided agreement between measurements and simulations, e.g. Hayakawa et al. [32], Kumar and Meyer [35] , Duynslaegher et al. [40], etc. However, in most studies limited chemical mechanism models, initial conditions and combustion characteristic parameters have been investigated. Therefore, mechanism studies are still not enough for more practical use, e.g. 3D CFD simulation of gas turbine conditions.

Therefore, there is a need to comprehensively compare the performance of different detailed ammonia combustion mechanisms in order to define the most suitable at present, simultaneously identifying the strengths and weaknesses of the mechanisms for further research. This can be resolved using numerical models to distinguish which one is capable of providing a better correlation to ammonia combustion kinetics especially under typical industrial conditions. Without any previous study in the field, it is clear that there is a great opportunity in the area to develop new mechanisms, CFD simulations, experimental setups and industrial designs. As a fundamentally important aspect, it is essential to develop a detailed kinetic mechanism in order to predict phenomena such as auto-ignition, flashback, and emission characteristics under gas turbine operational conditions for future developments. To achieve this goal, in this chapter, the present work develops a kinetic mechanism by improving Mathieu's model to validate comprehensively the combustion properties such as ignition delay times, flame speed, NO_x emissions, etc. The improved mechanism is prepared for use in CFD calculations for prediction of the turbulent reacting flow field inside a gas turbine combustor for ammonia/hydrogen utilisation. Furthermore, the mechanism was reduced to represent the kinetics of ammonia/hydrogen combustion with 'sufficient' accuracy, but including fewer species and reactions. In this way, the reduced mechanism is rendered more suitable for application in 3D CFD simulation studies of practical gas turbines.

5.1 Chemical Kinetic Mechanism Evaluation for Premixed Combustion of Ammonia/Hydrogen Fuels

One aim of the present study is to compare the performance of different detailed ammonia (NH_3) combustion mechanisms and distinguish which is most capable of representing ammonia-based fuels combustion kinetics especially under industrial conditions such as gas turbine combustors. Therefore 12 recently published or tested ammonia mechanisms in literature were employed to investigate their performance on modelling ammonia-based fuel combustion. For instance, Konnov mechanism provides full implementation of kinetic data for NO formation, which has been validated by many combustion studies [35, 39]. Other mechanisms tested in this study include the Tian mechanism [41], the Mathieu mechanism [44], the Duynslaegher mechanism [40], the Klippenstein mechanism[219], the Dagaut mechanism [220], the Miller mechanism [221], the Lindstedt mechanism [29], the ÅA mechanism [48], the Mendiara mechanism [43], the Mével mechanism [222] and the GRI 3.0 mechanism [45]. In fact, among these detailed chemical mechanism models developed for ammonia combustion most of them were developed based on low pressure conditions. Only the model of Mathieu and Petersen was examined under pressure up to 30 atm based on shock tube experiments. The rest of the mechanisms were built up using atmospheric or low pressure conditions. Although they were not developed for conditions inside gas turbine combustors, it is meaningful to validate and expand their application range and compare the accuracy of these mechanisms for their application in gas turbines running on ammonia/hydrogen fuel blends. To comprehensively evaluate the accuracy of each detailed kinetic mechanism, unstretched flame speed, ignition delay times and NO_x emissions are studied for premixed ammonia-based fuel combustion.

5.1.1 Flame Propagation

To examine the performance of existing NH_3 combustion mechanisms for unstretched laminar flame speed calculation of premixed NH_3/H_2 flames, different initial NH_3 concentrations(40%~61.5%) in the fuel gas and different equivalence ratios (0.80-1.25) were simulated to compare them with results produced by Li et al. [60]. In the experimental work, ammonia/hydrogen/air flame at normal temperature and pressure (NTP) using the Bunsen burner method were performed. The purity of fuel gas is 99.999% and mass flow controllers with an accuracy ±1.0% were used. The computational code of a premixed flame from Cantera [223] was employed in the present study. This modelling approach [32, 62] can in principle provide analysis of unstretched flame speed, reaction rates, radical concentrations, sensitivity analyses, etc. In the model, flame speed is defined as the flame front velocity relative to the flow into the unburnt mixture. The flame speed calculation model is used to determine the characteristic flame speed of the gas mixture at specified pressure and inlet temperature. The flame speed prediction model in Cantera is stabilised in an axisymmetric stagnation flow, and computed along the stagnation streamline using a similarity solution to reduce the three-dimensional governing equations to a single dimension.

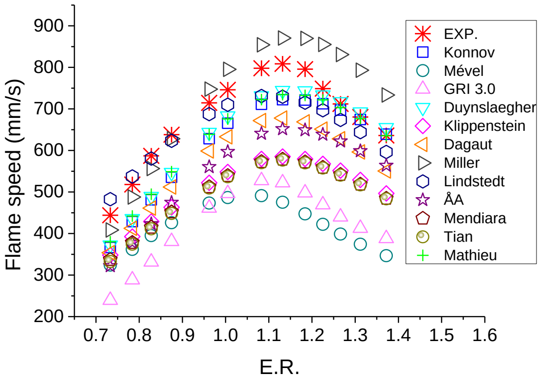


Figure 5-1 Flame speed calculation of 40% NH_3 flame at normal temperature and pressure. Experiments as in [60]

Figure 5-1~Figure 5-3 show flame speed calculation results of different NH_3/H_2 mixtures using different chemical mechanisms. All the three NH_3/H_2 combustion results have shown that the flame speed will increase first and then decrease with the increase of equivalence ratio. Almost all the mechanisms have predicted the same trend of the flame speed with experimental data. The maximum flame speed is achieved around equivalence ratio of 1.1.

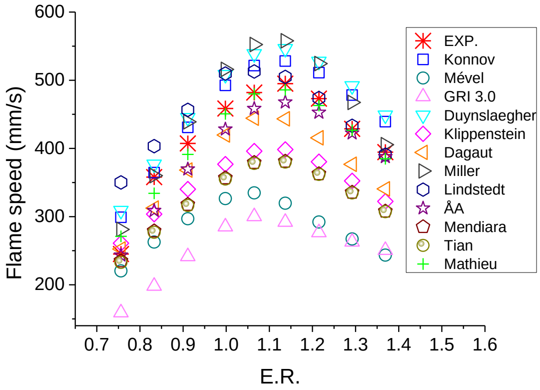


Figure 5-2 Flame speed calculation of 50% NH_3 flame at normal temperature and pressure. Experiments as in [60]

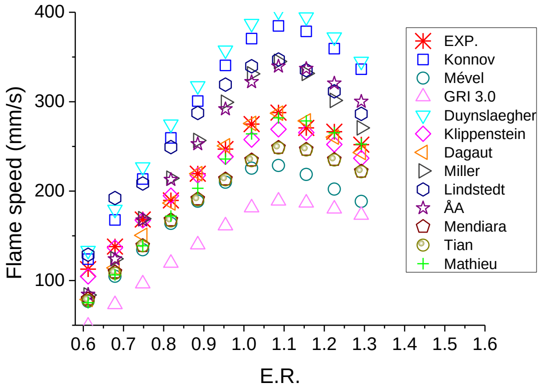


Figure 5-3 Flame speed calculation of 61.5% NH_3 flame at normal temperature and pressure. Experiments as in [60]

In Figure 5-1, the 40%NH_3/60%H_2 blend is simulated for the unstretched laminar flame speed investigation. From the results, it can be seen that most of the mechanisms have predicted slower flame speed compared to experimental data. The best predictions are obtained by the Lindstedt mechanism, the Miller mechanism, the Mathieu mechanism, the Duynslaegher mechanism and the Konnov mechanism with average relative errors of 3.99%, 5.96%, 8.53%, 8.61% and 10.08% respectively. A more detailed analysis of the results shows that in different equivalence ratio conditions the accuracy of different mechanisms varies. Near stoichiometric conditions (0.90<ER<1.20), the deviations of all the mechanisms are relatively larger, which indicates mechanisms for this range of equivalence ratio still need to be studied. Under fuel lean conditions (E.R.<0.90), the best predictions are obtained by the Miller mechanism with an average relative error of 1.72% while the Mathieu mechanism has given the best prediction under fuel rich condition(E.R.>1.20) with an average relative error of 1.38%. These results indicate that chemical reaction kinetics of this mixture are affected by equivalence ratio.

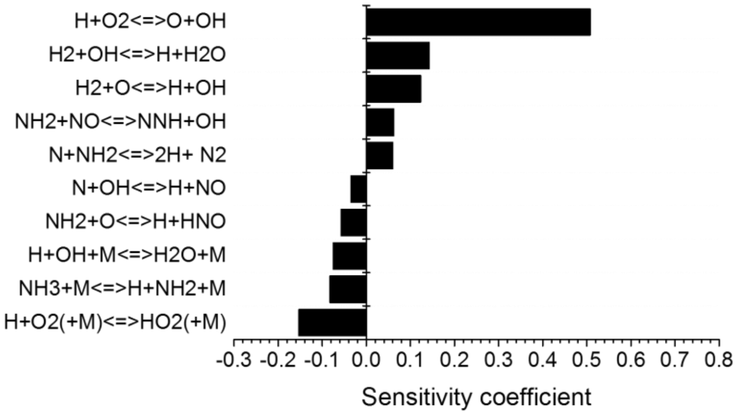


Figure 5-4 Sensitivity analysis of flame speed by Mathieu mechanism (40.0%NH_3, E.R.=0.83)

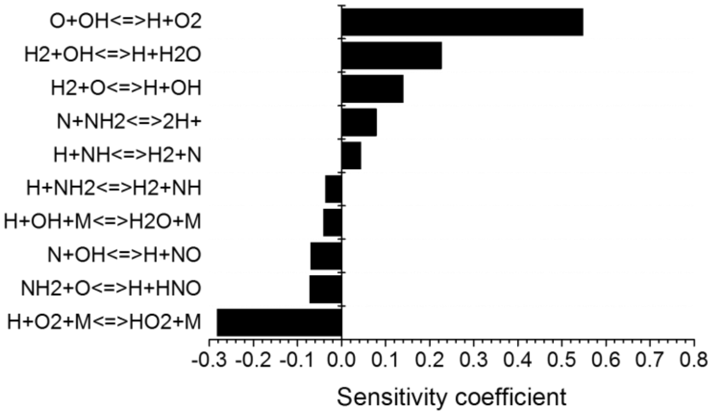


Figure 5-5 Sensitivity analysis of flame speed by Miller mechanism (40.0%NH_3, E.R.=0.83)

Under rich conditions, for the combustion of 40.0% NH_3 concentration in fuel, to illustrate the difference between different mechanisms, sensitivity analyses were conducted. As shown in Figure 5-4~Figure 5-7, most-sensitive reactions for the flame speed calculation of Mathieu mechanism and Miller mechanism are compared, as they produced the most accurate prediction under fuel lean and fuel rich conditions respectively. For fuel lean conditions, it can be seen from Figure 5-4 and Figure 5-5 that the reactions $H+O_2=O+OH$ and $H+O_2(+M) =HO_2(+M)$ have the largest impacts on the predictions of flame speed in both mechanisms. The difference between them is that these reactions play a more prominent role in the Miller mechanism than in the Mathieu mechanism. Even further, in both mechanisms the reaction H_2+OH=H+H_2O is the second most promoting reaction for flame speed. For fuel rich conditions, Figure 5-6 and Figure 5-7 show that the promoting reaction H+O_2=O+OH has the largest impacts on the predictions of flame speed in both mechanisms while the most inhibiting reactions in the two mechanisms are different, N+OH=H+NO in Mathieu mechanism and H+O_2(+M)=H+O_2(+M) in Miller mechanism. In fact, differences between rate constants of some key reactions produce also a great impact on flame speed calculation. For instance, concerning the most inhibiting reaction H+O_2(+M) =HO_2(+M), the rate constant is $k=4.65\times10^{12}\cdot T^{0.44}$ in Mathieu mechanism while in Miller mechanism the value is $k=3.67\times10^{17}\cdot T^{-0.72}$. This case shows how these differences can alter the performance when predicting laminar flame speed.

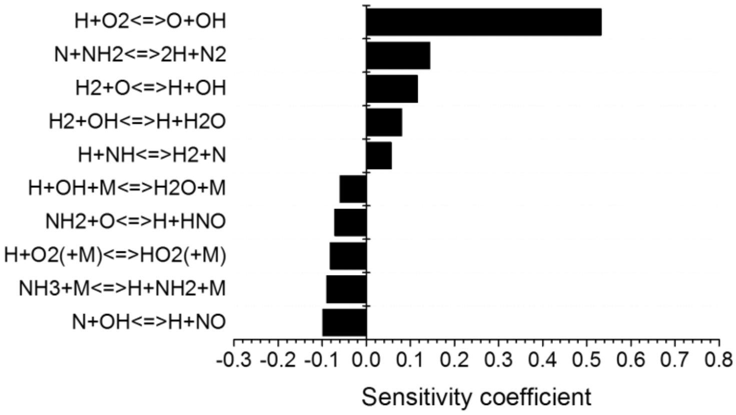


Figure 5-6 Sensitivity analysis of flame speed by Mathieu mechanism (40.0%NH_3, E.R.=1.23)

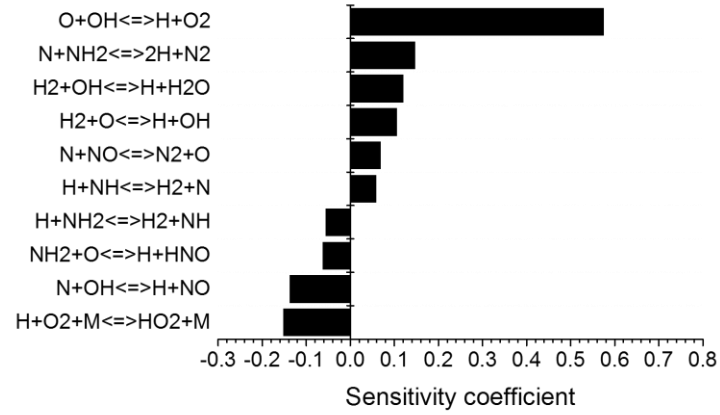


Figure 5-7 Sensitivity analysis of flame speed by Miller mechanism (40.0%NH_3, E.R.=1.23)

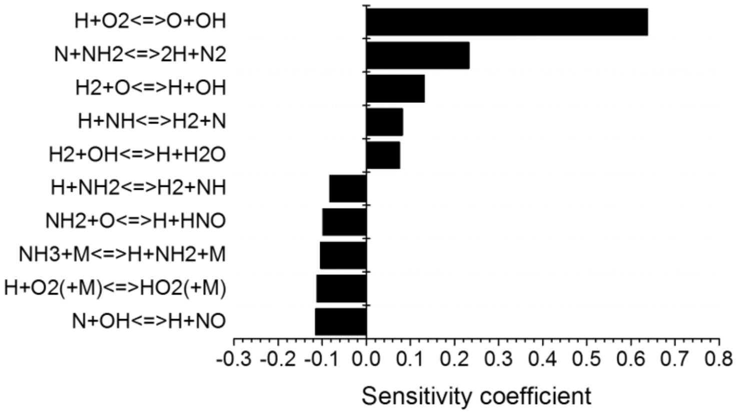


Figure 5-8 Sensitivity analysis of flame speed by Mathieu mechanism (50.0%NH_3, E.R.=1.23)

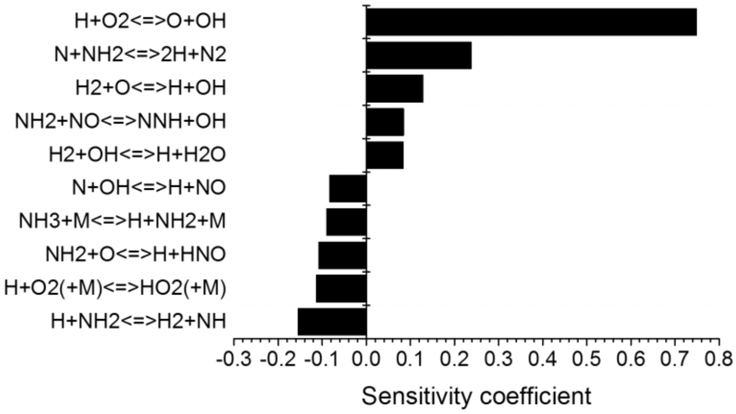


Figure 5-9 Sensitivity analysis of flame speed by Mathieu mechanism (61.5%NH_3, E.R.=1.23)

Figure 5-2 and Figure 5-3 show the flame speed calculation results for 50.0% and 61.5% of initial NH_3 concentration in the fuel blend respectively. In Figure 5-2, the best predictions are obtained by Mathieu mechanism, ÅA mechanism, , Miller mechanism, Lindstedt mechanism and Dagaut mechanism with average relative errors of 3.36%, 5.38%, 9.51%, 9.72%, 9.99% respectively. In Figure 5-3, the most accurate calculations are obtained by Klippenstein mechanism, Dagaut mechanism and Mathieu mechanism with average relative errors of 3.81%, 6.37%, 9.50% respectively. The simulation results from Figure 5-1~Figure 5-3 have shown that the Mathieu mechanism has the best performance (all average relative errors <10%) within the range of this study, which indicates the Mathieu mechanism is capable to produce a good prediction for flame speed prediction for different ratios of NH_3/H_2 fuel mixtures. Thus, sensitivity analysis using the Mathieu mechanism were performed for the combustion of 50.0% and 61.5% of initial NH_3 to illustrate the difference between combustion kinetics of different fuel mixtures, as shown in Figure 5-8 and Figure 5-9.

The results show that both $H+O_2=O+OH$ and $N+NH_2=2H+N_2$ are the most promoting reactions while the most inhibiting reactions are different for the two different fuel mixtures. Furthermore, comparing Figure 5-8 and Figure 5-9 with Figure 5-6, it is observed that the sensitivity of the sensitive reactions continuously change according to the proportion of NH_3 in the fuel mixture. For instance, the most sensitive reaction $H+O_2=O+OH$ plays a more prominent role with the increase of NH_3 concentration in the fuel mixture while $H+NH_2=H_2+NH$ plays the most inhibiting role in combustion kinetics of high NH_3 concentration mixtures.

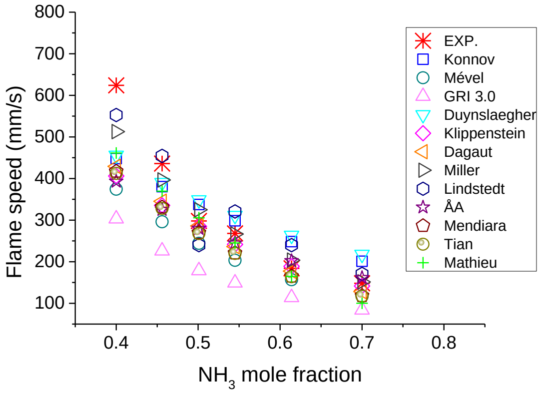


Figure 5-10 Flame speed calculation of fuel lean condition (E.R.=0.80) at normal temperature and pressure. Experiments as in [60]

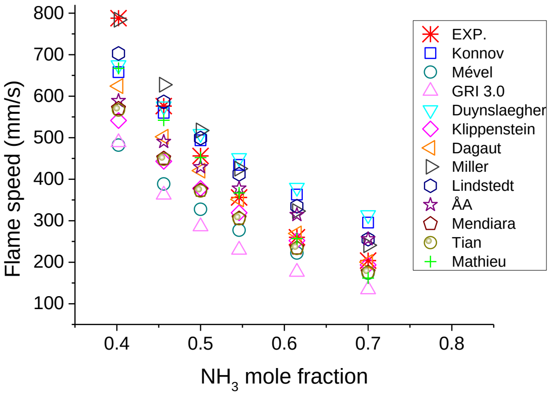


Figure 5-11 Flame speed calculation of stoichiometric condition (E.R.=1.00) at normal temperature and pressure. Experiments as in [60]

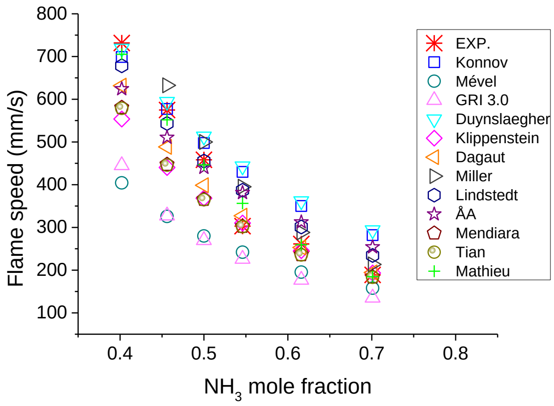


Figure 5-12 Flame speed calculation of fuel rich condition (E.R.=1.25) at normal temperature and pressure. Experiments as in [60]

Figure 5-10~Figure 5-12 show flame speed calculation results under different equivalence ratio conditions with detailed chemical mechanisms. As shown in the figures, the flame speed of the NH_3/H_2 mixtures decreases with the increase of NH_3 concentration due to smaller amount of hydrogen atoms in the flame as the H_2 addition decreases. For stoichiometric condition, the five mechanisms of the best performance are obtained by the Mathieu mechanism, Dagaut mechanism, Miller mechanism, Klippenstein mechanism and Lindstedt mechanism. For fuel rich conditions, the best agreement with experimental data was obtained by the Mathieu mechanism, Dagaut mechanism, Mendiara mechanism, Tian mechanism and Klippenstein mechanism. The results show the Mathieu mechanism performs with the best accuracy for flame speed prediction under stoichiometric and fuel rich cases with average relative error of 7.85% and 5.14% respectively. Meanwhile, the performance of the mechanisms used in this study for fuel lean condition is relatively poorer, in which the best predictions are obtained by Klippenstein mechanism, Dagaut mechanism, Miller mechanism, Lindstedt mechanism and Mathieu mechanism with average relative errors of 13.21%, 14.12%, 14.15%, 15.29%, 15.90% respectively. This indicates that fuel lean combustion chemistry for NH_3/H_2 still needs to be better optimised. However, generally for all the equivalence ratio conditions in this study the Mathieu mechanism shows the best and satisfying accuracy among the detailed chemical mechanisms tested.

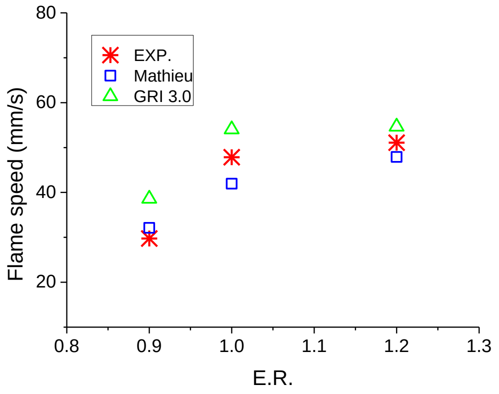


Figure 5-13 Flame speed calculation of ammonia (p=0.3MPa). Experiments as in [32]

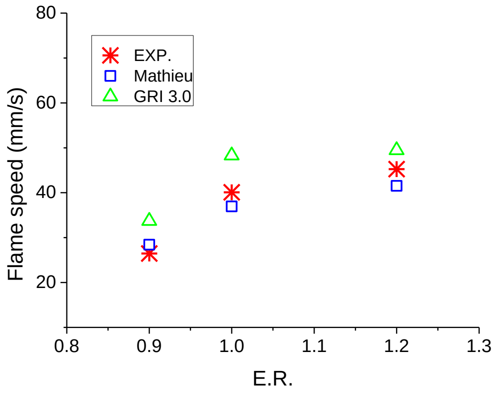


Figure 5-14 Flame speed calculation of ammonia (p=0.5MPa). Experiments as in [32]

To further study ammonia’s combustion chemistry for future practical applications, elevated pressure conditions are of great significance as usually met in gas turbine operation processes. Recently Hayakawa et al. [32] studied the unstretched laminar flame speed of premixed ammonia flames at various pressures up to 0.5 MPa experimentally. Since the study of Hayakawa et al. has already compared several detailed chemical mechanisms and indicates that GRI 3.0 mechanism shows the best performance for flame speed prediction under elevated pressure conditions, here in this study the Mathieu mechanism was tested and compared with GRI 3.0 mechanism under elevated pressure conditions, as shown in Figure 5-13 and Figure 5-14. From the results it can be seen that flame speed decreases with the increase of pressure. Although both the Mathieu and GRI 3.0 mechanisms have shown good accuracy for flame speed calculation under elevated conditions, the Mathieu mechanism has a better performance. Actually, although NH_3 related reactions are present in the GRI

3.0 mechanism, the ammonia chemistry in this mechanism is still not fully developed, as also mentioned in the study of Hayakawa et al. Since GRI 3.0 is still very popular in the gas turbine industry, it is necessary to notice that GRI 3.0 is not a model suitable for NH_3 combustion modelling. The Mathieu mechanism has already shown the best capability for simulating ammonia/hydrogen fuel under various conditions. Thus, Mathieu mechanism is recommended for ammonia/hydrogen fuels' flame speed simulations of this study.

5.1.2 Emission Analysis

To validate the performance of the existing chemical mechanisms for NH_3/H_2 combustion, NO_x emissions and some major species concentrations were predicted against experimental data from burner-stabilised premixed flames investigated by Duynslaegher et al. [39, 40], Figure 5-15~Figure 5-18. In the experimental work of Duynslaegher et al., molecular beam mass spectrometer system were used to determine the structure of the laminar premixed flames burning at low pressure conditions. Eight ammonia containing flames with different initial operating conditions were studied. In these flame structure studies at low pressure conditions, random errors for hydrogen and amidogen radicals are around 5% and 3% for ammonia and nitrogen monoxide. The initial conditions represented by point numbers are illustrated in Table 5-1.

Table 5-1 Flame inlet composition and initial conditions (from [39])

No.	NH_3	H_2	O_2	Ar	E.R.	p(mbar)
1	0.25	0.05	0.21	0.48	1	60
2	0.24	0.07	0.21	0.47	1	50
3	0.22	0.1	0.21	0.46	1	50
4	0.21	0.13	0.21	0.45	1	50
5	0.22	0.1	0.24	0.43	0.9	50
6	0.22	0.1	0.2	0.48	1.1	50
7	0.25	0.05	0.21	0.48	1	90
8	0.25	0.05	0.21	0.48	1	120

As shown in Figure 5-15, prediction of N_2 is quite satisfying with all the mechanisms of which the relative errors are all less than 5%. For the calculation of H_2, the predictions by most mechanisms are acceptable with relative errors about 10%. For N_2O emissions, Figure 5-17 shows the prediction results using different mechanisms. It can be seen that only Duynslaegher and GRI 3.0 mechanisms give best agreement with experimental data. This is because in Duynslaegher mechanism the N_2O chemistry is specifically optimised to have better accuracy. It indicates that the N_2O chemistry still needs to be improved for most of the ammonia combustion mechanisms. However, since the final concentration of N_2O in exhaust is rather low, NO_x will be regarded as the main pollutant for NH_3/H_2 flames. For exhaust NO emissions, all the chemical mechanisms tested give acceptable predictions except GRI 3.0 mechanism as shown in Figure 5-18.

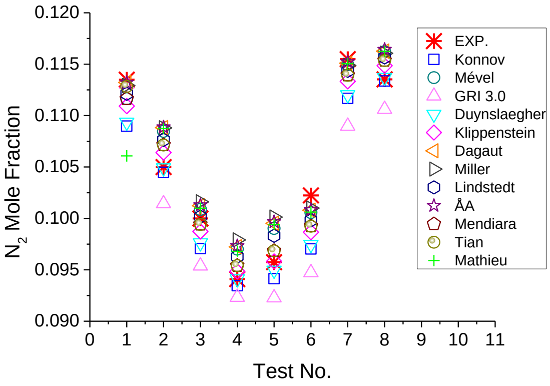


Figure 5-15 Mole fraction of N_2 in burnt gas. Experiments as in [39]

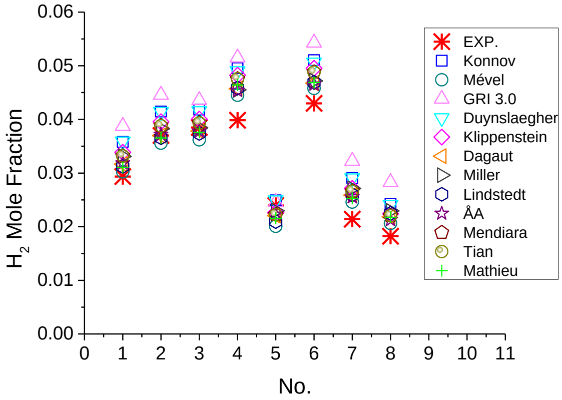


Figure 5-16 Mole fraction of H_2 in burnt gas. Experiments as in [39]

To develop ammonia as an alternative fuel, NO_x emissions are one of the essential concerns. Comparing flame test numbers 2, 3 and 4, it can be seen that increase of NH_3 concentration in initial fuel leads to higher NO concentration in the burnt gas, which is mainly due to the increase of fuel-bond NO_x emissions. From flame test numbers 3, 5 and 6, it is observed a strong impact of equivalence ratio on NO yield. From fuel lean condition to fuel rich condition, a large drop in the NO concentration can be observed from E.R.=0.90 to E.R.=1.10. This indicates the fuel rich combustion can be preferred for practical industrial use of ammonia/hydrogen fuels. A comparison of flame test numbers 1, 7 and 8 reveal the effect of pressure on the formation of NO emission. From 60-120 mbar, an obvious decrease of NO concentration can be observed. It should be noticed that the initial conditions in the study of Duynslaegher et al. [40] are still different from the high pressure operational conditions of practical gas turbine. As mentioned in the study of Duynslaegher et al. [40], the aim was to analyse the ammonia/hydrogen combustion chemistry for practical spark ignition engines. Nevertheless, the different pressure conditions studied by Duynslaegher have relevance to draw some of the effects of pressure that have not been studied in other related studies for NH_3/H_2 combustion. Since there is still no experimental study for ammonia/hydrogen emissions under elevated pressure conditions, this comparison can still provide essential information for NO_x emission predictions.

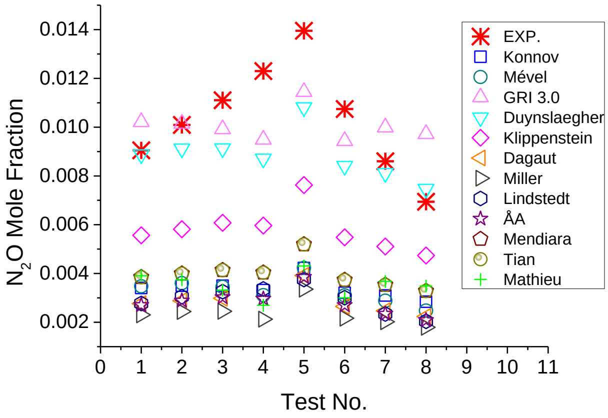


Figure 5-17 Mole fraction of highest N_2O in burnt gas. Experiments as in [39]

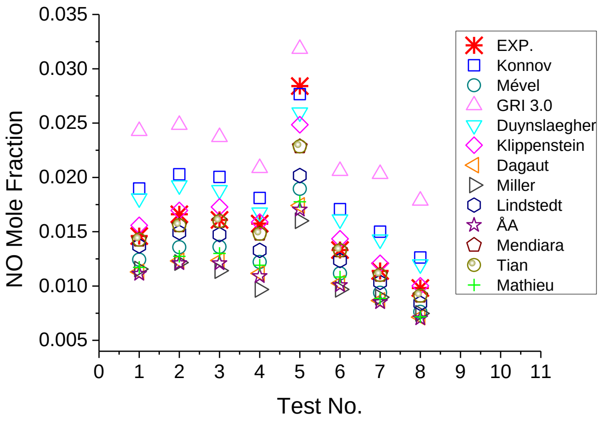


Figure 5-18 Mole fraction of NO in burnt gas. Experiments as in [39]

For NO_x emission predictions, among the mechanisms tested, Tian mechanism, Klippenstein mechanism and Mendiara mechanism have performed the best accuracy with average relative errors of 5.68%, 5.69% and 5.72% respectively, while the relative error of the Mathieu mechanism, which shows the best performance in flame speed calculation, shows a prediction of 23.98%. Also, relatively old mechanisms such as Miller mechanism and Lindstedt mechanism show rather big deviations for NO_x emission predictions although they have shown fair performance for flame speed calculations. Actually, in previous literature there are studies reporting discrepancies between experimental results and these old mechanisms. For instance, Um et al. [27] over-estimated flame temperatures and NO_x emissions for non-premixed NH_3/H_2 flames, while Lee et al.[26] also claimed discrepancies among the predictions and measurements for laminar premixed NH_3/H_2 combustion using Miller mechanism and Lindstedt mechanism. This indicates that these mechanism models are not suited for future ammonia combustion studies as a great deal of improvements have already been made in chemical mechanism developments. More recent mechanisms (e.g. Tian mechanism [41] and Mendiara mechanism [43]) have been updated with much more extensive reactions for NH_3 chemistry.

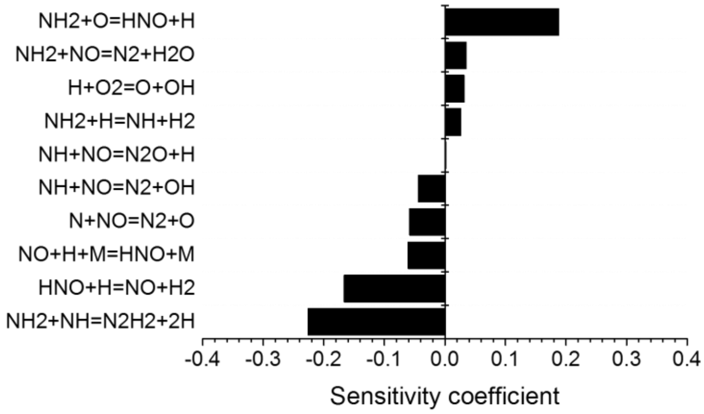


Figure 5-19 Sensitivity analysis of NO by Tian mechanism (flame 1)

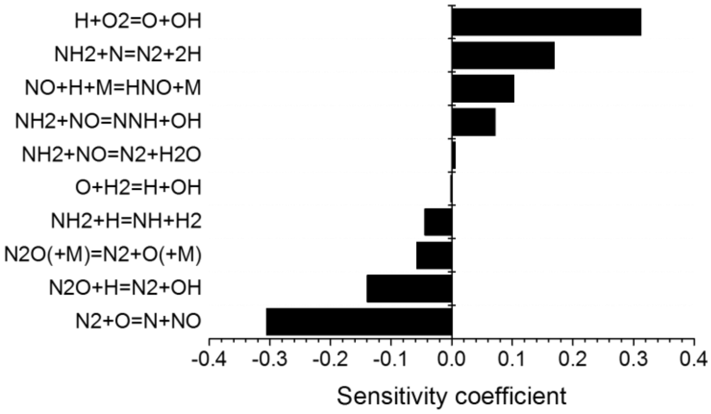


Figure 5-20 Sensitivity analysis of NO by Mathieu mechanism (flame 1)

To illustrate the difference between mechanisms in NO_x emission calculation, sensitivity analyses were conducted. For instance, sensitive reactions of the Tian and Mathieu mechanisms for flame 1 are identified as shown in Figure 5-19 and Figure 5-20. It can be seen that there is an obvious difference between the two models. In the Tian mechanism, the most promoting reaction is $NH_2+O=HNO+H$ while $H+O_2=OH+O$ and $NH_2+N=N_2+2H$ are the most promoting reactions in the Mathieu mechanism. In the Mathieu mechanism the role of N_2O species is quite important for the NO formation but not quite noticeable for Tian mechanism. These differences shown in the sensitivity analysis are mainly responsible for the discrepancy between the NO_x prediction performances of the two mechanism models. A pathway analysis of NO formation with Tian mechanism is illustrated in Figure 5-21. The major source of the NO formation comes from oxidation of HNO. As the sensitivity analysis shows, the reaction $NH_2+O=HNO+H$ plays the key role in the NO formation process. When ammonia is consumed initially with O/OH, NH_2 is produced. Then the NH_2 is mainly converted into HNO and NH. The conversion from HNO and NH to NO is mainly through the reactions $HNO+H=NO+H_2$ and $NH+O=NO+H$.

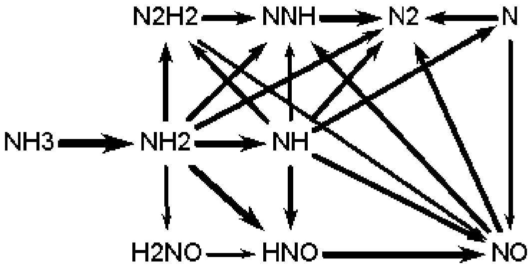


Figure 5-21 Pathway of NO formation

5.1.3 Ignition Delay

To comprehensively study the performance of different chemical mechanisms for premixed combustion, ignition delay times validation studies were also conducted to compare with the experimental data by Mathieu and Petersen [44]. The ignition delay time was measured using the chemiluminescence emission of the excited-state hydroxyl radical . Experiments were performed at three different pressure conditions (around 1.4, 11, and 30 atm), and three equivalence ratios (0.5, 1.0, and 2.0).The total uncertainty in the experimental study was estimated to be 10%. In [44], several up-to-date mechanisms have been tested for ignition delay time calculations of ammonia. From these studies, the Mathieu mechanism has been proved to have the best accuracy under different pressure conditions.

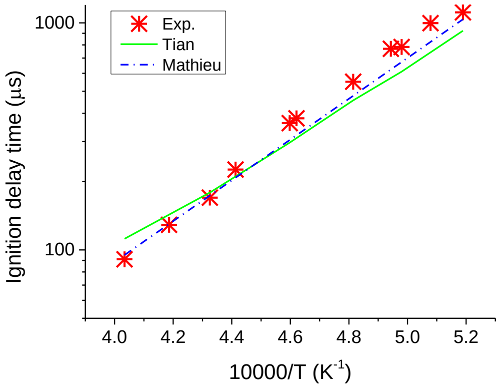


Figure 5-22 Ignition delay times of NH_3 mixtures (0.4%NH_3/0.6%O_2/99%Ar). 1.4 atm. Experiments from [44]

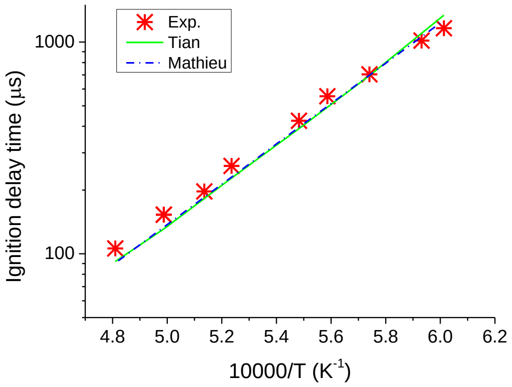


Figure 5-23 Ignition delay times of NH_3 mixtures (0.5715%NH3/0.4285%O2/99%Ar). 11 atm. Experiments from [44]

Thus, considering Tian mechanism showed the best performance for NO_x emission prediction in the previous section and it was not tested in [44], ignition delay time calculations using Tian mechanism were also compared with Mathieu mechanism as shown in Figure 5-22~Figure 5-24. Generally, under all the pressure conditions studied, both Tian mechanism and Mathieu mechanism have shown quite good accuracy for ignition delay times prediction though Mathieu mechanism performs slightly better. Specifically, under low and medium pressure conditions (1.4 and 11 atm), these two mechanisms show quite close results with each other while under high pressure condition (30 atm) Mathieu mechanism shows a better performance than Tian mechanism. This indicates that Mathieu mechanism can perform better for ignition delay time calculations under high pressure conditions.

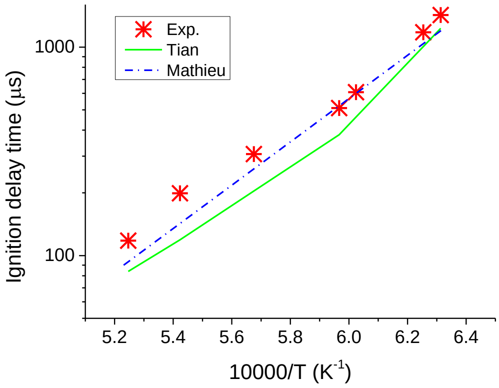


Figure 5-24 Ignition delay times of NH_3 mixtures (0.7273%NH3/0.2727%O2/99%Ar). 30 atm. Experiments from [44]

To illustrate the difference between the chemical mechanisms for ignition chemistry, sensitivity analyses were also conducted as shown in Figure 5-25 and Figure 5-26. Under the condition of 30 atm, equivalence ratio of 2, it can be seen that the most inhibiting reaction NH_3+OH=NH_2+H_2O is the same in both mechanisms. Also, promoting reactions H+O_2=O+OH and 2NH_2=NH_3+NH play a prominent role in both mechanisms. A noticeable difference is that in Tian mechanism, H+O_2=O+OH plays as the most promoting reaction while NH+O_2=HNO+O is the most promoting reaction in Mathieu mechanism. Another difference is that the N_2H_2 species plays an important role in Tian mechanism. Moreover, several differences are visible between Tian mechanism and Mathieu mechanism, with the role of the N_2H_2 species being very important in Tian mechanism. These differences account for the deviation from experimental data.

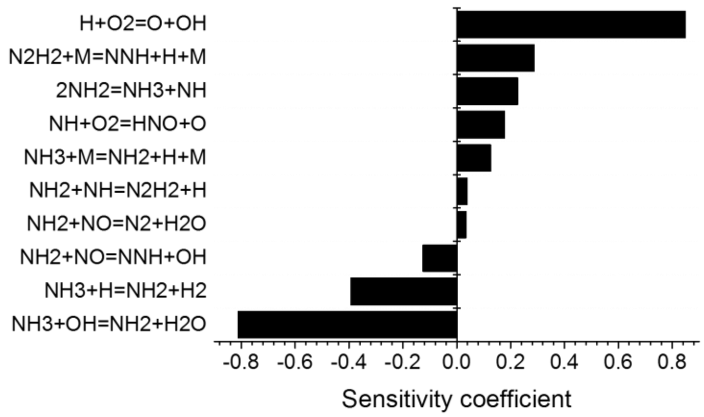


Figure 5-25 Sensitivity analysis of OH by Tian mechanism ($0.4\%NH_3/0.6\%O_2/99\%Ar$). 30 atm

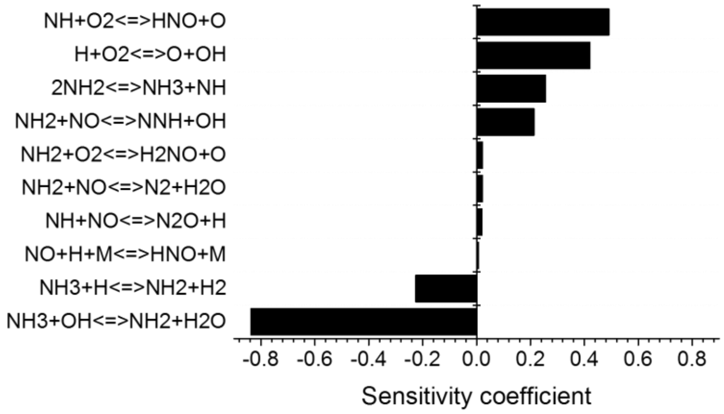


Figure 5-26 Sensitivity analysis of OH by Mathieu mechanism ($0.4\%NH_3/0.6\%O_2/99\%Ar$). 30 atm

5.2 Establishing a New Chemical Mechanism for Ammonia/Hydrogen Fuel Blends under Gas Turbine Conditions

To study ammonia/hydrogen combustion in gas turbines, it is necessary to develop a detailed chemical-kinetics mechanism which can validate comprehensively the combustion properties under high pressure conditions. Mathieu’s mechanism was built for shock-tube experiments of ammonia ignition delay time measurements under pressure conditions of up to 30 atm. Therefore, the chemical kinetic model proposed in the present work was mostly based on recent work performed by Mathieu under high-pressure conditions [44]. To improve the performance of the mechanism concerning NO_x emissions and flame speed prediction, several reactions are modified according to the kinetic analysis of the main reactions as shown in Table 5-2. The mechanism developed involves 55 species and 276 elementary reactions, and is available in Appendix B.

Table 5-2 Modified reactions compared with the Mathieu mechanism

Reactions	A	n	Ea	Ref.
$N+NO=N_2+O$	2.10E+13	0	0	[43]
$NO+H+M=HNO+M$	1.50E+15	-0.4	0	[41]
$HNO+H=NO+H_2$	4.40E+11	0.7	650	[41]
$N_2O+H=NH+NO$	6.70E+22	-2.16	37155	[33]
$N_2O+H=N_2+OH$	5.00E+13	0	15200	[40]

The modifications of rate constants were performed based on contribution rate calculations and sensitivity analysis. To develop a kinetic mechanism which can comprehensively validate different combustion properties of NH_3/H_2 fuel blends, NO_x emission, laminar flame speed and ignition delay times are all taken into consideration in the present study. Therefore, the sensitive reactions were firstly extracted for modification. Then, through modifications of rate constants of the most sensitive reactions for a particular combustion property, the performance of such properties can be systematically improved. After simulation predictions, various choices can be made to effect a balance between the accuracy of different combustion properties. According to this procedure, five reactions were modified. Taking the reaction NO+H+M=HNO+M for instance, the modification of the kinetic data set in the present work slowed down this reaction, which gives rise to higher NO_x emission predictions to overcome the problem of underestimating NO_x associated with Mathieu's mechanism.

In order to use the detailed chemical kinetics mechanism for future practical application and design of gas turbine combustor research, it is necessary to reduce the scale of the ammonia/hydrogen mechanism. Actually it was found in this study that the CFD calculation takes a long time for NH_3/H_2 combustion in a simple burner, which is mainly due to the fact that the mechanism developed in the present study is still too large. Hence it is desirable to reduce the improved chemical-kinetics mechanism so that it can be implemented in full scale 3D CFD numerical simulations in future. Therefore, a preliminary mechanism reduction was performed for the improved mechanism using the Directed Relation Graph (DRG) method, which has been described in detail by Bendtsen et al. [224], and implemented in the Chemked II software programme [225]. In the present study the detailed chemical-kinetics mechanism was evaluated with homogeneous (ignition delay) simulations generated by perfectly stirred reactor (PSR) simulations at constant pressure. The computation was conducted for initial temperatures at 2000 K and a constant pressure of 17 atm. The mixture with mole fractions of $NH_3/H_2/O_2/N_2$ 0.088/0.0565/0.1795/0.675 was chosen, corresponding to stoichiometric fuel-in-air conditions for a NH_3/H_2 molar ratio of 60/40, which is the same ratio as that utilised in a recent experimental study within a generic swirl burner. After this case of reaction chemistry is calculated under such particular initial conditions, the results were prepared for the reduction of the mechanism model. The formation process using the DRG method starts with specifying several important species. Then, with all these initial targeted species the generation of a reactions graph is undertaken. A subset of reactions that are important for the targeted species is selected to be included in the list of important reactions. Simultaneously, new species appearing in these reactions are added into the important species list. The next step selects reactions that are important for the new species. The procedure is repeated until no new species appear. Finally, a reactions graph is produced with the important species to be considered in the reduced model. Thus, the final list forms a particular reduced reaction mechanism for the specific initial conditions. In the reduction procedure, three reduced kinetic models were generated by exercising different control indexes, which are related to the accuracy of the reactions selected. In the following study, the three reduced mechanisms with 108 reactions, 91 reactions and 74 reactions are specified by ‘Mech. 6’, ‘Mech. 7’ and ‘Mech. 8’ as shown in Table 5-3, which are available in “Appendix B”.

Table 5-3 Full mechanism of present study and reduced mechanisms

Name	No. Species	No. Elementary Reactions
The full mechanism	55	276
Mech. 6	24	108
Mech. 7	24	91
Mech. 8	23	74

5.3 Verification of the Chemical Kinetic Model

5.3.1 NO_x Emission Prediction

To develop ammonia as an alternative fuel, NO_x emission is a primary concern. A burner-stabilised premixed flame model was employed to validate the performance of the NH_3/H_2 combustion mechanism developed for NO_x emission predictions. In the model, simulation of this kind of flame can effectively provide data of the chemical kinetics of the NH_3/H_2 combustion process and help to interpret flame experiments. The simulation was carried out under low pressure conditions with various ammonia/hydrogen ratios and equivalence ratios to simulate the experimental results of premixed ammonia/hydrogen combustion provided by Duynslaegher et al. [39] as shown in Table 5-1.

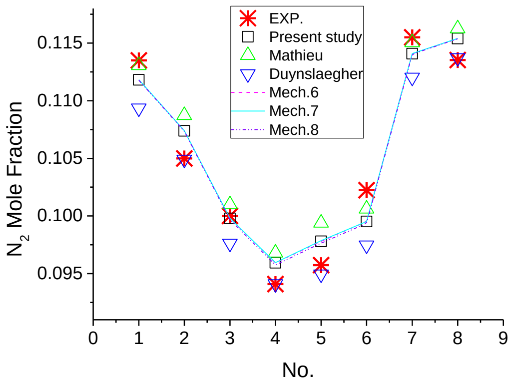


Figure 5-27 Mole fraction of N_2 in burnt gas. Experiments corresponding to [39]

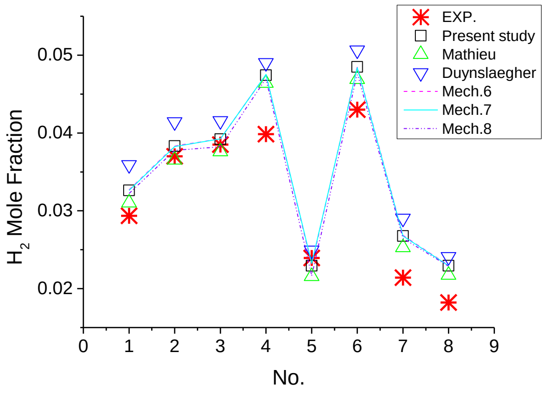


Figure 5-28 Mole fraction of H_2 in burnt gas. Experiments corresponding to [39]

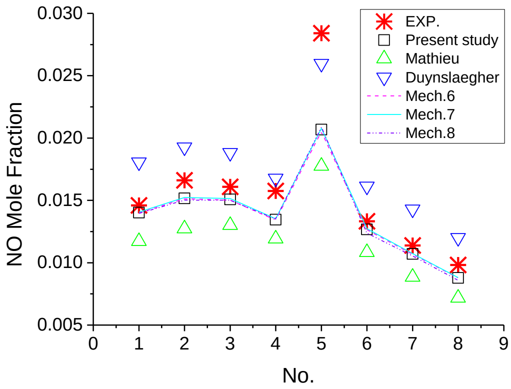


Figure 5-29 Mole fraction of NO in burnt gas. Experiments corresponding to [39]

As shown in Figure 5-27~Figure 5-29, NO_x emissions and some major species of $NH_3/H_2/O_2/Ar$ combustion were properly predicted with the reaction kinetics model developed in the present study against experimental data from burner-stabilised premixed flames investigated by Duynslaegher et al. To provide a comprehensive evaluation of the chemical-kinetics mechanism model of the present study, the up-to-date ammonia mechanisms the Mathieu and Duynslaegher mechanisms were also used in the calculation for reference. The experimental conditions were replicated in the simulation, which represent different conditions, such as different initial NH_3 concentrations (flame 2-4), different equivalence ratios (flames 3,5,6), different pressures (flames 1,7,8), etc. As shown in Figure 5-27, prediction of N_2 using different mechanisms varies with the initial conditions. The Mathieu mechanism and the present mechanism show better performance for test No. 1,3,6,7, while the Duynslaegher mechanism shows better prediction of N_2 for other test points. Generally, all the mechanisms tested have shown acceptable performance with average relative errors of 17.04%, 20.03%, 18.49%, 17.09%, 16.91% and 16.68% respectively using the present mechanism, the Mathieu mechanism, the Duynslaegher mechanism, the reduced mechanisms Mech. 6, Mech. 7 and Mech. 8. Figure 5-29 shows the calculation results of H_2, in which the predictions by most mechanisms are quite near to each other. At some test points such as No.4 the deviation from the experiment is higher, which indicates the prediction of H_2 needs to be improved when using high hydrogen concentration in NH_3/H_2 mixtures. The average relative errors of the present mechanism, the Mathieu mechanism and the reduced mechanisms are around 10% while the average relative error for the Duynslaegher mechanism is higher than others with 19.37%. From the predictions in Figure 5-29, it can be seen that the Mathieu mechanism under-predicts NO_x emissions, whilst the Duynslaegher mechanism over-predicts them in most cases. Generally, the chemical-kinetics mechanism model developed in the present study shows the best performance among the three mechanisms used for comparison with the average relative error of 10.26%. The largest discrepancy occurs during test No.5, which is the only condition using fuel lean mixtures. This indicates that further development of reaction mechanism is needed for fuel lean combustion conditions. Moreover, the reduced mechanisms have also shown good agreement with the full mechanism of the present study with relative errors of around 10% against experimental data.

The simulation results show that all the mechanisms correctly capture the trend of NO_x emission under different experimental conditions. Comparing flame 2, 3 and 4, it can be seen that increase of NH_3 concentration in the fuel leads to higher NO concentration in the burnt gas, which is mainly due to the increase of 'fuel-bond' NO_x emissions. Flames 3, 5 and 6 demonstrate a strong dependence of equivalence ratio on NO yield. From fuel lean condition to fuel rich condition, a large drop in the NO concentration is observed from E.R.= 0.9 to E.R.=1.1. This indicates the fuel rich combustion is preferential for practical, industrial use of ammonia/hydrogen fuel. A comparison of flame 1, 7 and 8 reveals the effect of pressure on the formation of NO emissions. From 60-120 mbar, an obvious decrease of NO concentration can be observed.

To illustrate NO formation processes in the NH_3/H_2 flame, the main reaction pathways of NO formation were analysed (Figure 5-30), using the chemical-kinetic mechanism developed in the present study. It shows that the major source of the NO formation comes from oxidation of HNO, N and NH. When ammonia is consumed initially with O/OH, NH_2 is produced. NH_2 is then converted mainly into HNO and NH. Through production rate analyses, it was found the reaction $HNO+H=NO+H_2$ gives rise to the biggest contribution in the NO formation process. The conversion from N and NH to NO is mainly through the reactions $N+O_2=NO+O$ and $NH+O=NO+H$, but with smaller net contribution to NO formation in comparison with HNO.

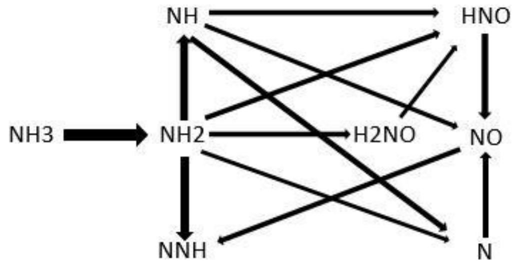


Figure 5-30 Pathway analysis of the NO formation

To investigate the potential of utilising NH_3/H_2 fuels in gas turbine power generation sets, the effects of elevated pressure conditions were appraised with the improved chemical-kinetic mechanism. Take the fuel mixture of flame No. 1 as example, as shown in Figure 5-31, NO_x emissions decrease with the increase of pressure with considerable decreases observed from 'medium' pressure to 'high' pressure. Quantitatively, the results show that NO_x emission levels can be less than 5ppm when the pressure condition is more than 10 atm, and less than 1 ppm when pressure is higher than 20 atm. This significant result indicates that the deployment of NH_3/H_2 blends in gas turbines is very promising as NO_x emissions are likely to be reduced under real operating conditions.

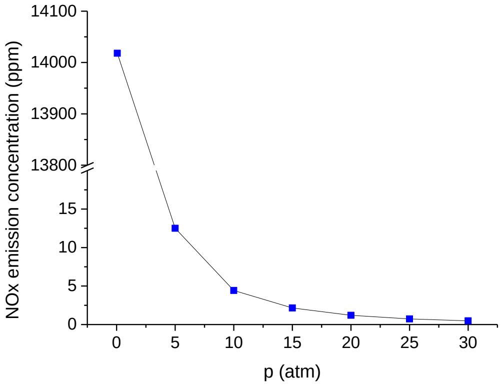


Figure 5-31 NO_x emission as a function of pressure

To evaluate the performance of the kinetic model for gas turbines further, pressurised conditions need to be investigated. However, there are still scarce experimental data of NO_x emission available in the literature for validation of ammonia combustion simulation. Figure 5-32~Figure 5-34 show the NO sub-mechanism validation under 10 atm conditions using the experimental data by Dayma and Dagaut [226], where $H_2/O_2/NO$ mixtures in N_2 were measured in a jet stirred reactor. Under fuel-lean conditions, the mechanism advocated in the present study and the Mathieu mechanism shows good agreement with the NO profile under 10 atm, especially for temperatures higher than 900 K, whilst the Duynslaegher mechanism largely under-predicts NO emissions. Below 900 K, the improved mechanism and the Mathieu mechanism slightly over-predicts NO emissions, but the transition point around 790 K is successfully captured, whereas the Duynslaegher mechanism shows temperatures 60 K higher than experimental results. For stoichiometric conditions, the improved mechanism and the Mathieu mechanism successfully capture the trend for NO emission predictions, whilst considerable discrepancies can be observed between the results of the Duynslaegher mechanism and the experiments. For fuel rich conditions, the improved mechanism and Mathieu's mechanism slightly over-predicted NO emissions at high temperature ranges but still with acceptable values, whilst the Duynslaegher mechanism fails to capture the profile of NO emission. In all the equivalence ratio conditions, the reduced mechanisms have shown good agreement with the full mechanism as shown in the figures. Generally, the improved mechanism and Mathieu's mechanism perform very similarly under elevated conditions. This indicates that the new mechanism proposed has good potential for NO_x emission predictions for gas turbine operational conditions.

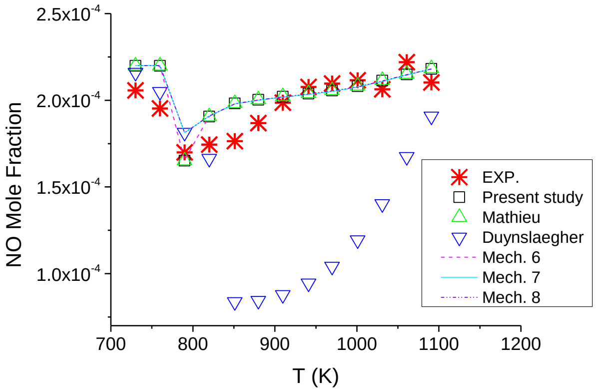


Figure 5-32 NO prediction of hydrogen-oxygen-nitrogen and 220ppm NO mixtures in a jet stirred reactor at 10 atm, E.R.=0.5. Experiments as in [226]

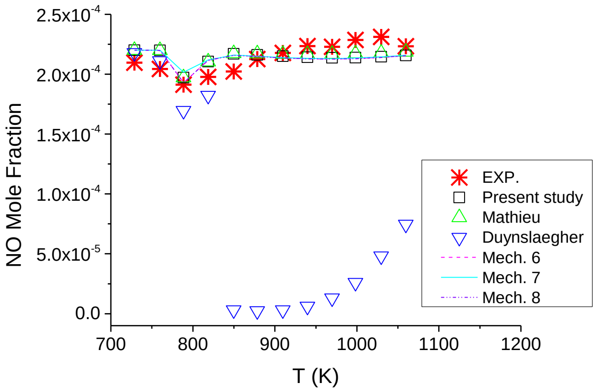


Figure 5-33 NO prediction of hydrogen-oxygen-nitrogen and 220ppm NO mixtures in a jet stirred reactor at 10 atm, E.R.=1. Experiments as in [226]

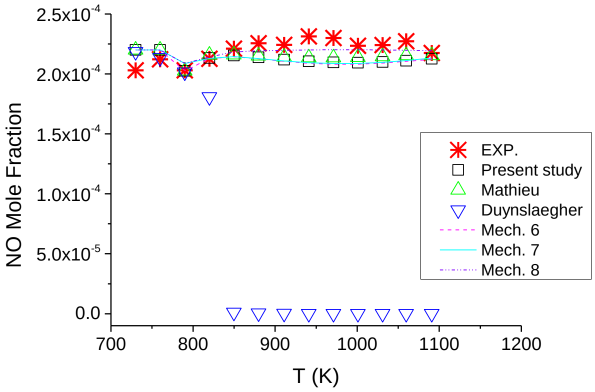


Figure 5-34 NO prediction of hydrogen-oxygen-nitrogen and 220ppm NO mixtures in a jet stirred reactor at 10 atm, E.R.=1.5. Experiments as in [226]

5.3.2 Laminar Flame Speed

As mentioned before, flame speed is one of the most important properties of premixed combustion flames. It is also used as an essential parameter for verification of detailed chemical mechanisms. Therefore, numerical simulations were performed by modelling one dimensional premixed freely propagating laminar flames of ammonia/hydrogen mixtures. To validate the performance of the improved mechanism comprehensively, numerical simulations were undertaken under conditions corresponding to the experiments of Li [60] and Hayakawa [32] to enable the comparison of unstretched laminar flame speed values, in which different ammonia/hydrogen ratios, equivalence ratios and pressure conditions were studied.

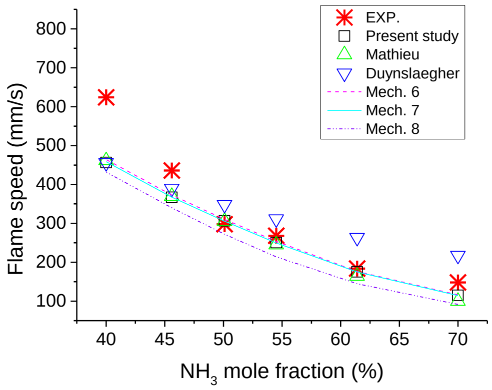


Figure 5-35 Flame speed calculation of different NH_3 fractions in NH_3/H_2 fuel blends under fuel lean condition (E.R.=0.8). Experiments as in [60]

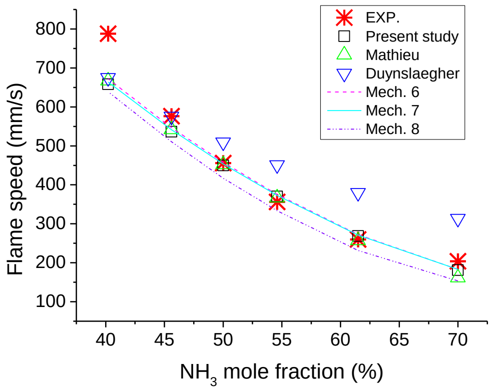


Figure 5-36 Flame speed calculation of different NH_3 fractions in NH_3/H_2 fuel blends under stoichiometric condition (E.R.=1). Experiments as in [60]

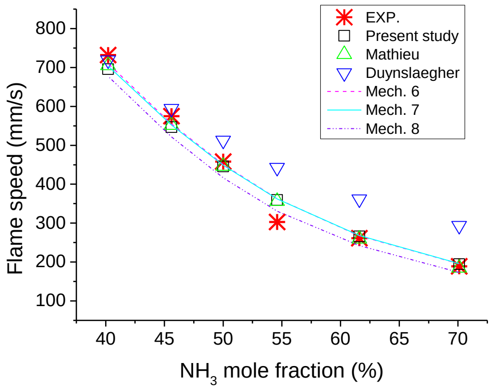


Figure 5-37 Flame speed calculation of different NH_3 fractions in NH_3/H_2 fuel blends under fuel rich condition (E.R.=1.25). Experiments as in [60]

In Figure 5-35~Figure 5-37, the simulation results show a decrease in flame speed of the NH_3/H_2 mixtures with the increase of NH_3 concentration due to less amount of free hydrogen atoms in the flame as the H_2 addition decreases. Generally, under all the equivalence ratio conditions the improved mechanism and Mathieu's mechanism perform almost similarly with reasonable accuracy in predicting flame speed of NH_3/H_2 blends, while the performance of the Duynslaegher mechanism is consistently relatively poorer. For fuel lean conditions, the deviation between simulation results and experimental results is greater when the ammonia fraction is low (<50%). For stoichiometric and fuel rich conditions, reasonable agreement with experimental data was obtained by using the improved mechanism and Mathieu's mechanism. Therefore, the improved chemical-kinetics mechanism performs well for flame speed predictions under lean, stoichiometric and fuel rich cases with average relative errors of 13.21%, 7.18% and 6.01% respectively. The reduced mechanisms have given almost the same accuracy as the full mechanism. However, the results can also indicate that fuel lean combustion chemistry for NH_3/H_2 still needs more optimisation especially for low NH_3 fraction fuel blends.

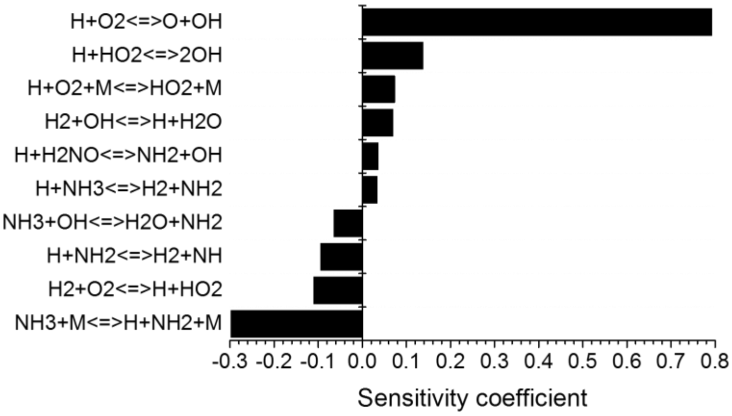


Figure 5-38 Sensitivity analysis of flame speed by the mechanism developed in the current study

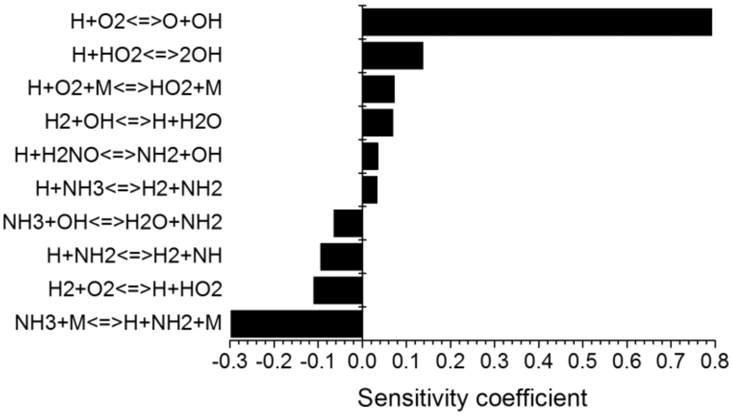


Figure 5-39 Sensitivity analysis of flame speed by the mechanism of the Mathieu mechanism

To illustrate the difference between different mechanisms, sensitivity analyses were performed. Taking stoichiometric conditions for instance, sensitivity analyses are illustrated in Figure 5-38~Figure 5-43 for the combustion of a blend with 61.5% NH_3 concentration. As shown in Figure 5-38 and Figure 5-39, the most-sensitive reactions for the flame speed calculation are almost the same for the improved mechanism and Mathieu's mechanism, which have produced the most accurate predictions as in Figure 5-35~Figure 5-37. It can be seen that that the most influential promoting reactions $H+O_2=O+OH$ and $H+HO_2=2OH$ and the most inhibiting reaction $NH_3+M=H+NH_2+M$ has the largest impacts on the predictions of flame speed in all the six mechanisms. The difference between them is that reaction $H+O_2=O+OH$ plays a more prominent role whereas the reaction $NH_3+M=H+NH_2+M$ is less prominent in the Duynslaegher mechanism than in the improved mechanism and Mathieu's mechanism. This illustrates the reason why Duynslaegher's mechanism predicts a faster flame speed than the mechanism of present study.

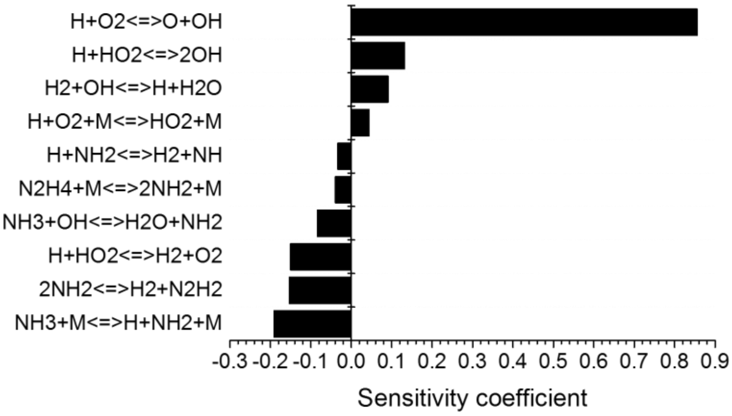


Figure 5-40 Sensitivity analysis of flame speed by the mechanism of the Duynslaegher mechanism

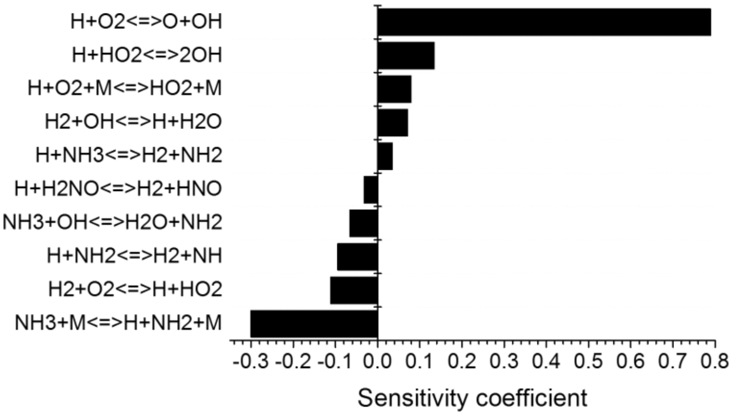


Figure 5-41 Sensitivity analysis of flame speed by the reduced mechanism Mech. 6

As for the reduced mechanisms, most of the main sensible elementary reactions are the same as the full mechanism. For instance, the sensitivity analysis of Mech. 6 and Mech. 7 are almost the same with the full mechanism as shown in the comparison of Figure 5-38, Figure 5-41 and Figure 5-42. In Mech. 8 the reaction HO_2+NH_2=H_2NO+OH plays a more prominent inhibiting reaction compared to the other two reduced mechanism, which accounts for relatively lower flame speed calculations than the full mechanism and the reduced mechanisms Mech. 6 and Mech. 7. In fact, differences between rate constants of some key reactions produce an important impact on flame speed calculation. For instance, concerning the most-sensitive reaction H+O_2=O+OH, the rate constant is $k=1.04*10^{14}$ exp(15286/RT) in the mechanism of the present study and the Mathieu mechanism while in Duynslaegher mechanism the value is $k= 9.750*10^{13}$exp(14850/RT). This case shows how these differences can alter the performance when predicting laminar flame speed.

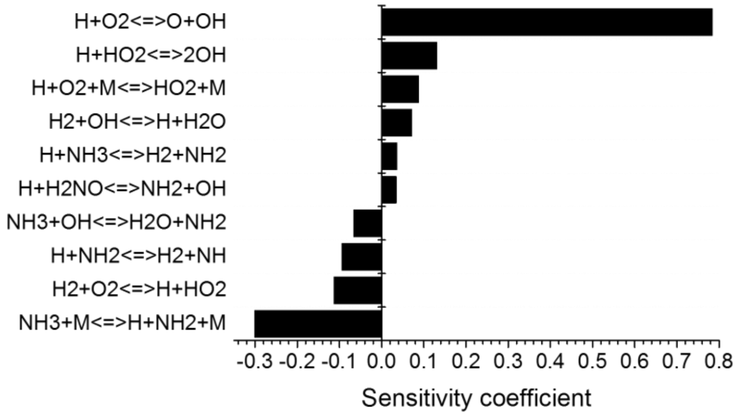


Figure 5-42 Sensitivity analysis of flame speed by the reduced mechanism Mech. 7

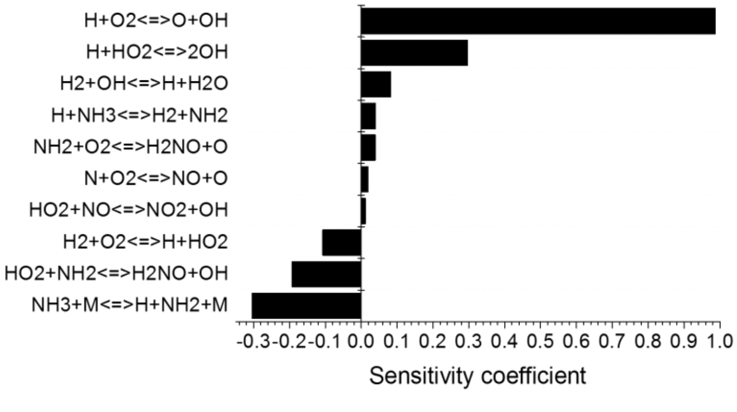


Figure 5-43 Sensitivity analysis of flame speed by the reduced mechanism Mech. 8

To validate the NH_3/H_2 combustion chemistry further for practical gas turbine application, elevated pressure conditions were also investigated. Recently, Hayakawa et al. [32] derived the unstretched laminar flame speed of premixed ammonia flames experimentally at various pressures up to 0.5 MPa. Therefore, the chemical-kinetics mechanisms developed in the present study was appraised against this experimental dataset, as shown in Figure 5-44 and Figure 5-45. The results show that the flame speed decreases with the increase of pressure, which is consistent with the conclusions in previous studies [31, 32]. The main reason for this effect is that under different pressure conditions, the sensitive elementary reaction will vary. As a result, the decrease in flame speed can be attributed to higher burning rates at high pressure conditions as observed in experiments [32, 227]. It can be observed in the figures that the improved mechanism, the reduced mechanisms and Mathieu’s mechanism show good agreement with the data under elevated conditions (all the average relative errors less than 15%), while the Duynslaegher mechanism shows a significant deviation from experimental data as shown in the figures.

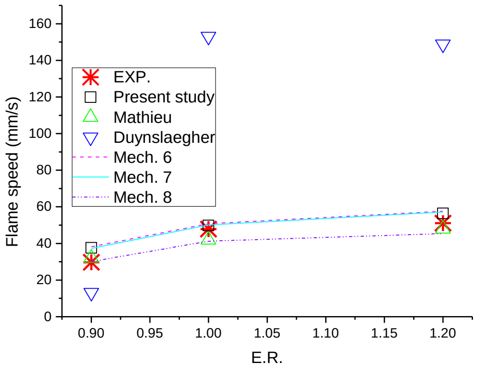


Figure 5-44 Flame speed calculation of ammonia (p=0.3 MPa). Experiments as in [32]

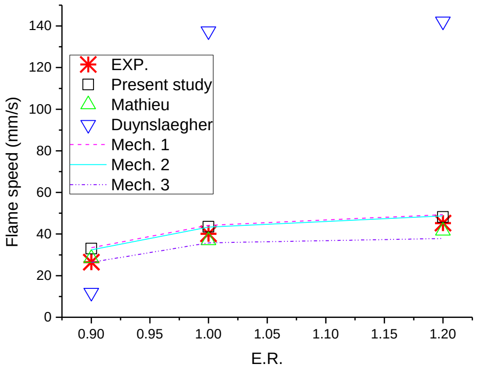


Figure 5-45 Flame speed calculation of ammonia (p=0.5 MPa). Experiments as in [32]

5.3.3 Ignition Delay Times Verification

The ignition delay time is another important parameter which describes autoignition properties of the combustion phenomenon. For operational aspects of gas turbine, it is crucial to avoid pre-ignition phenomena due to the variation of the fuel auto-ignition delay time. Therefore, the ignition delay time is one of the fundamental parameters that helps validate chemical kinetic models and aids the design of combustors utilising NH_3/H_2 in gas turbines. Thus, computational predictions of ignition delay times are usually compared with shock-tube experiments [228-230]. In this study, ignition delay times were modelled with a closed homogeneous reactor in CHEMKIN PRO. In this model, the ignition delay time can be defined based on different criteria such as the time at which a certain species reaches the maximum concentration or the time at which an inflection point appears in pressure or temperature profiles [44, 228, 230]. In the present work, ignition delay times were extracted as the time corresponding to the steepest rate of the OH* generation. The model was calculated at constant volume and adiabatic conditions. In the simulation, the ammonia and oxidiser mixtures are highly diluted (98.0-99.0%) to minimize effects of viscosity, heat transfer and non-equilibrium corresponding to the shock-tube experimental conditions [231]. The numerical work was carried out under high pressure conditions with different temperatures and equivalence ratios to simulate the experimental results provided by Mathieu et al, [44]. The mechanism developed in the present study was tested to validate its accuracy in predicting the ignition delay times.

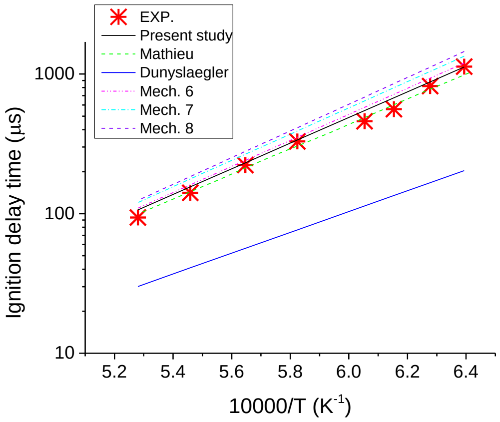


Figure 5-46 Ignition delay times of NH_3 mixtures diluted in 99% Ar at around 30 atm, E.R.=0.5. Experiments from [44]

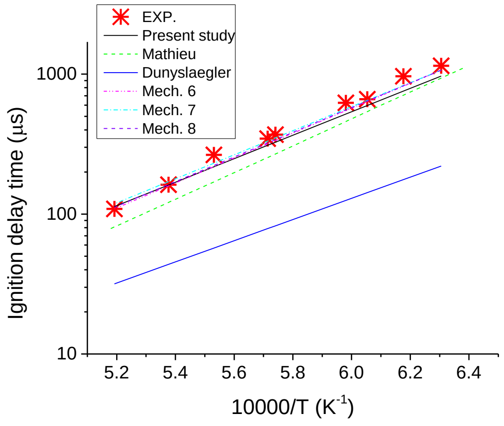


Figure 5-47 Ignition delay times of NH_3 mixtures diluted in 99% Ar at around 30 atm, E.R.=1. Experiments from [44]

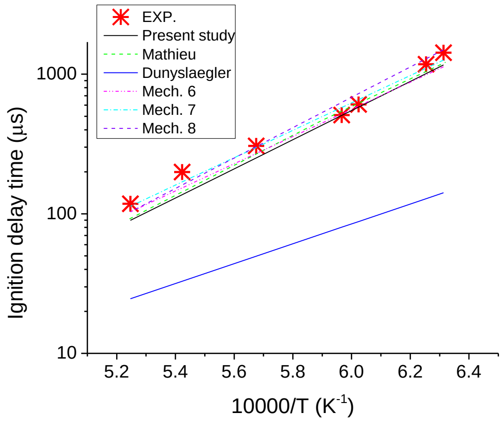


Figure 5-48 Ignition delay times of NH_3 mixtures diluted in 99% Ar at around 30 atm, E.R.=2. Experiments from [44]

Figure 5-46~Figure 5-48 show the ignition delay time calculations using the improved chemical-kinetics mechanism together with Mathieu's, the Duynslaegher's mechanisms under high pressure conditions and the reduced mechanisms relevant to gas turbine operation. Generally, under all equivalence ratios studied both the improved mechanism and Mathieu's mechanism show excellent agreement with the ignition delay time data. Specifically, the improved mechanism prediction in this study shows a good accuracy with an average relative error of 10% in fuel lean conditions. The reduced mechanisms predict a bit higher data than experiments. For stoichiometric conditions the improved mechanism slightly under-predicted the ignition delay times with an average relative error of 10% whilst Mathieu's mechanism predicts smaller ignition delay times than those obtained during the experiments. For fuel rich conditions both mechanisms show equal accuracy under high pressure conditions. On the other hand, the Duynslaegher mechanism shows poorer performance throughout.

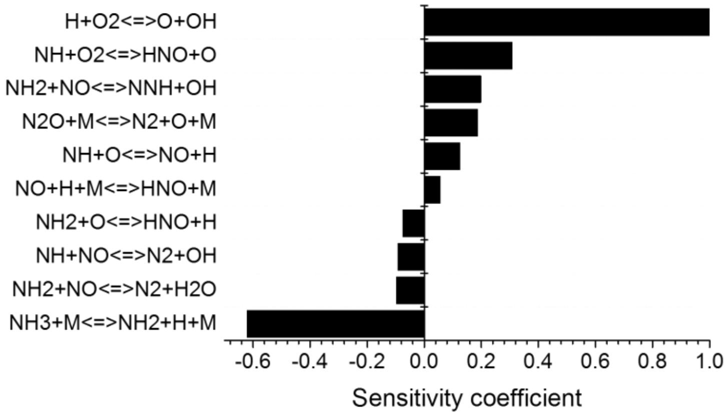


Figure 5-49 Sensitivity analysis of OH with the mechanism of present study (E.R.=1, 30 atm, 1700 K)

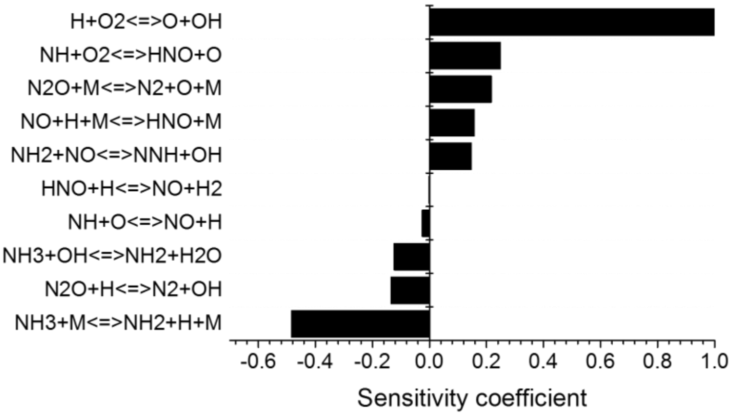


Figure 5-50 Sensitivity analysis of OH with the Mathieu mechanism (E.R.=1, 30 atm, 1700 K)

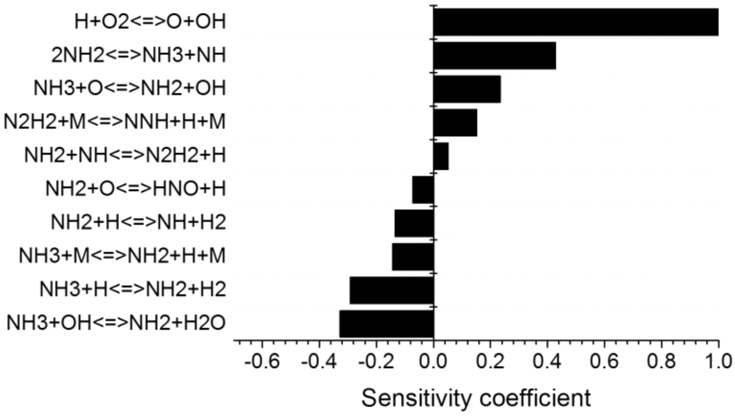


Figure 5-51 Sensitivity analysis of OH with the Duynslaegher mechanism (E.R.=1, 30 atm, 1700 K)

To illustrate the difference between the chemical mechanisms for ignition chemistry even further, sensitivity analysis was also undertaken. Taking the equivalence ratio of

1.00 for example, as shown in Figure 5-49~Figure 5-54, under 30atm it can be seen that the reaction $H+O_2=O+OH$ plays the most prominent role in all the three mechanisms. The second most sensitive reaction is the same in both the improved and Mathieu's mechanisms. A noticeable difference amongst the three mechanisms is that $NH_3+OH=NH_2+H_2O$ is the most inhibiting reaction, whilst $NH_3+M=NH_2+H+M$ is the most inhibiting reaction in the Duynslaegher mechanism. Another difference is that the N_2H_2 species plays a more important role in the Duynslaegher mechanism than in the other two. These differences account for the deviation from experimental data for the prediction results of Duynslaegher mechanism. As for the reduced mechanisms, most of the sensitive reactions are the same as for the full mechanism. For example, the three most promoting reactions and the three most inhibiting reactions are the same with the full mechanism, which leads to close ignition delay time results compared to the full mechanism as in Figure 5-46~Figure 5-48.

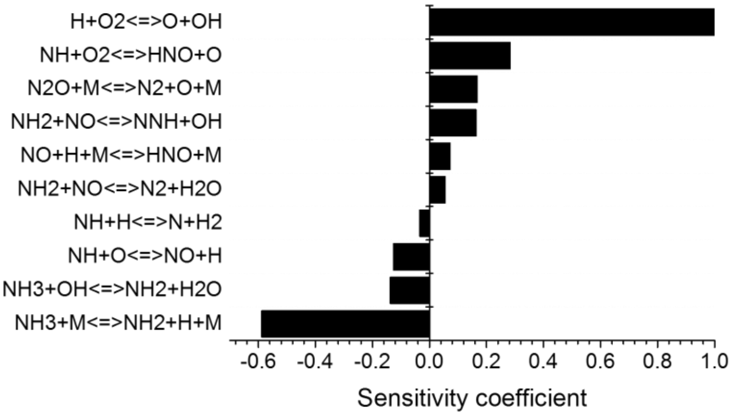


Figure 5-52 Sensitivity analysis of OH with the reduced mechanism Mech. 6 (E.R.=1, 30 atm, 1700 K)

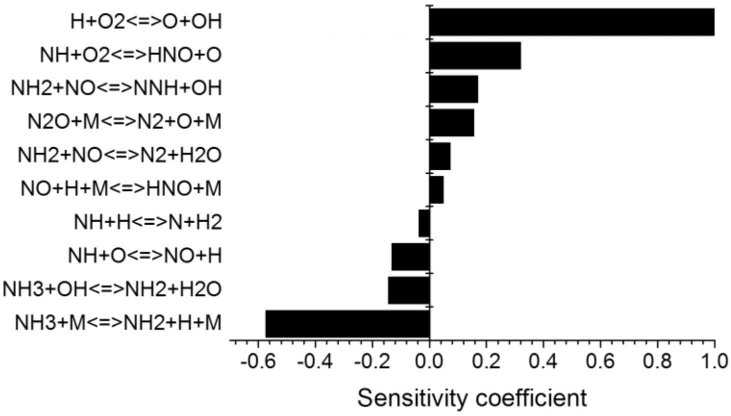


Figure 5-53 Sensitivity analysis of OH with the reduced mechanism Mech. 7 (E.R.=1, 30 atm, 1700 K)

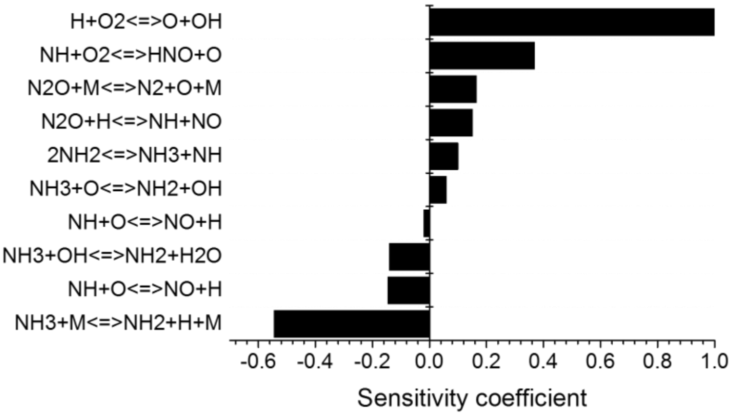


Figure 5-54 Sensitivity analysis of OH with the reduced mechanism Mech. 8 (E.R.=1, 30 atm, 1700 K)

5.4 Summary

In this chapter, a comprehensive comparison of different recent detailed ammonia combustion mechanisms was performed to study the premixed combustion of ammonia/hydrogen fuels. 12 detailed chemical mechanisms tested in previous literature were employed to determine their performance for the prediction of laminar flame speed, NO_x emission and ignition delay times using ammonia/hydrogen blends.

First, laminar flame speed calculation under atmospheric pressure conditions, different initial NH_3 concentrations in the ammonia/hydrogen fuel mixtures and different equivalence ratios were studied using these mechanisms. Elevated pressure conditions of ammonia combustion at different equivalence ratios were also simulated with different mechanisms against the results from literature. Results show that the Mathieu mechanism has the best agreement with the experimental data within the range of initial conditions tested. In addition, emission analyses of diluted ammonia/ hydrogen/ oxygen/argon flames have been modelled at different initial ammonia contents, equivalence ratios and working pressures. The best agreements of NO_x emission calculation with experimental results were achieved by using the Tian mechanism, Klippenstein mechanism and Mendiara mechanism. Sensitivity and pathway analyses were also carried out to identify reactions that require more attention in future development of combustion models. Simulation prediction using the Tian mechanism shows industrial high pressure conditions can lead to substantial decrease of NO_x emission. Finally, ignition delay time predictions for highly diluted ammonia showed that the Tian mechanism and Mathieu mechanism both yielded quite good performance.

Thus, for future practical industrial use of combustion chemistry of ammonia/hydrogen fuels, both the Mathieu and Tian mechanisms are promising. For flame propagation, the Mathieu mechanism showed the best performance while the Tian mechanism can give acceptable flame speed predictions especially for fuel-rich and high ammonia concentration flames. On the other hand, though the Tian mechanism showed the best performance in NO_x emission prediction, the Mathieu mechanism can also give acceptable NO_x prediction for NH_3/H_2 fuel mixtures. The choice can depend on the specific conditions to be analysed according to the results provided in this study. In the future, experimental studies and optimisation of these mechanisms are still needed for a deeper insight into the ammonia chemistry under practical gas turbine conditions. There will be also a need to reduce detailed ammonia/hydrogen combustion mechanisms to apply them to 3D-CFD simulation for gas turbine research.

Furthermore, an improved chemical-kinetics mechanism model was proposed for ammonia/hydrogen premixed combustion. The mechanism was developed mainly by improving the Mathieu mechanism in terms of NO_x emission calculations. The chemical-kinetic model was then tested to simulate ammonia/hydrogen flames against experimental data in Duynslaegher’s study for various equivalence ratios, pressures and initial ammonia contents. Results show that the general performance of the improved kinetic model is better than the the Mathieu mechanism and significantly better than the Duynslaegher mechanism. Then the proposed mechanism was validated for laminar flame speed calculations under different ammonia concentrations in NH_3/H_2 fuel blends and equivalence ratios ranging from fuel lean to fuel rich conditions. Laminar flame speed of ammonia combustion under high pressure conditions were also used to provide further validation of the proposed mechanism. Results demonstrate that the mechanism developed in the present study provides the best performance in terms of predicting flame speed under gas turbine conditions. For ignition delay time calculation, the improved kinetic model has also shown good results for highly diluted ammonia mixtures under high pressure conditions. Thus, the improved chemical-kinetics mechanism model has been shown to be capable of predicting different essential properties of ammonia/hydrogen combustion under gas turbine related conditions.

CHAPTER 6

Premixed Ammonia/Hydrogen Swirl Combustion for Gas Turbines

Chapter 6

In previous sections, initial chemical kinetics studies of NH_3/H_2 combustion have been carried out numerically. Combustion of this fuel blends with proper injection strategies is highly related to the emission and stability performance of practical gas turbine combustors. Therefore, in this chapter the main aim is to provide a first insight into practical combustor issues, using a premixed combustion generic burner and practically-relevant swirl-number, investigating ammonia/hydrogen blends. A series of experimental and numerical tests carried out to determine the combustion complexity of ammonia/hydrogen swirl combustion under rich conditions. A preliminary investigation into the effect of elevated ambient conditions is also explored for gas turbine applications. The results will permit a better understanding of such a process aiming at the development and implementation of an industrially based system to provide sustainable energy.

6.1 Setup

6.1.1 Experimental Study

Experiments were performed at the Gas Turbine Research Centre (GTRC). For the present project a High Pressure Optical Chamber (HPOC) was fitted with a generic lean pre-mixed swirl burner, Figure 6-1. The facility consists of a swirler/nozzle, combustor, and exhaust sections, in which premixed gas, consisting of H_2/NH_3 mixtures and air flows through a swirler housed swirler/nozzle section. The swirl-stabilized generic burner utilised in this study was operated at either atmospheric conditions with confinement of the exit nozzle. A cylindrical quartz confinement tube was utilised with an expansion ratio of 2.5:1 from the burner exit nozzle to the quartz confinement tube (ID =100 mm). The nozzle diameter is 40 mm and the 9 radial-tangential swirl inlets yields a swirl number of 0.8 [233, 234]. The campaign was initiated setting a blend of 60%NH_3-40%H_2 (%vol) which shows an unstable nature. Thus, the programme was continued with a 70%NH_3-30%H_2 (%vol) blend which demonstrated stable combustion behaviour. Test points were evaluated at a power output of 39.3 kW under atmospheric pressure, Table 6-1. Each point was analysed at 3 different inlet temperatures (288±5 K, 400±7 K and 484±10 K). In order to characterise the impact of dilution in the post-combustion zone and observe the impact on chemical reactivity, 63.7 g/s of bypass air were used for comparison purposes with the cases evaluated at 288 K inlet temperature.

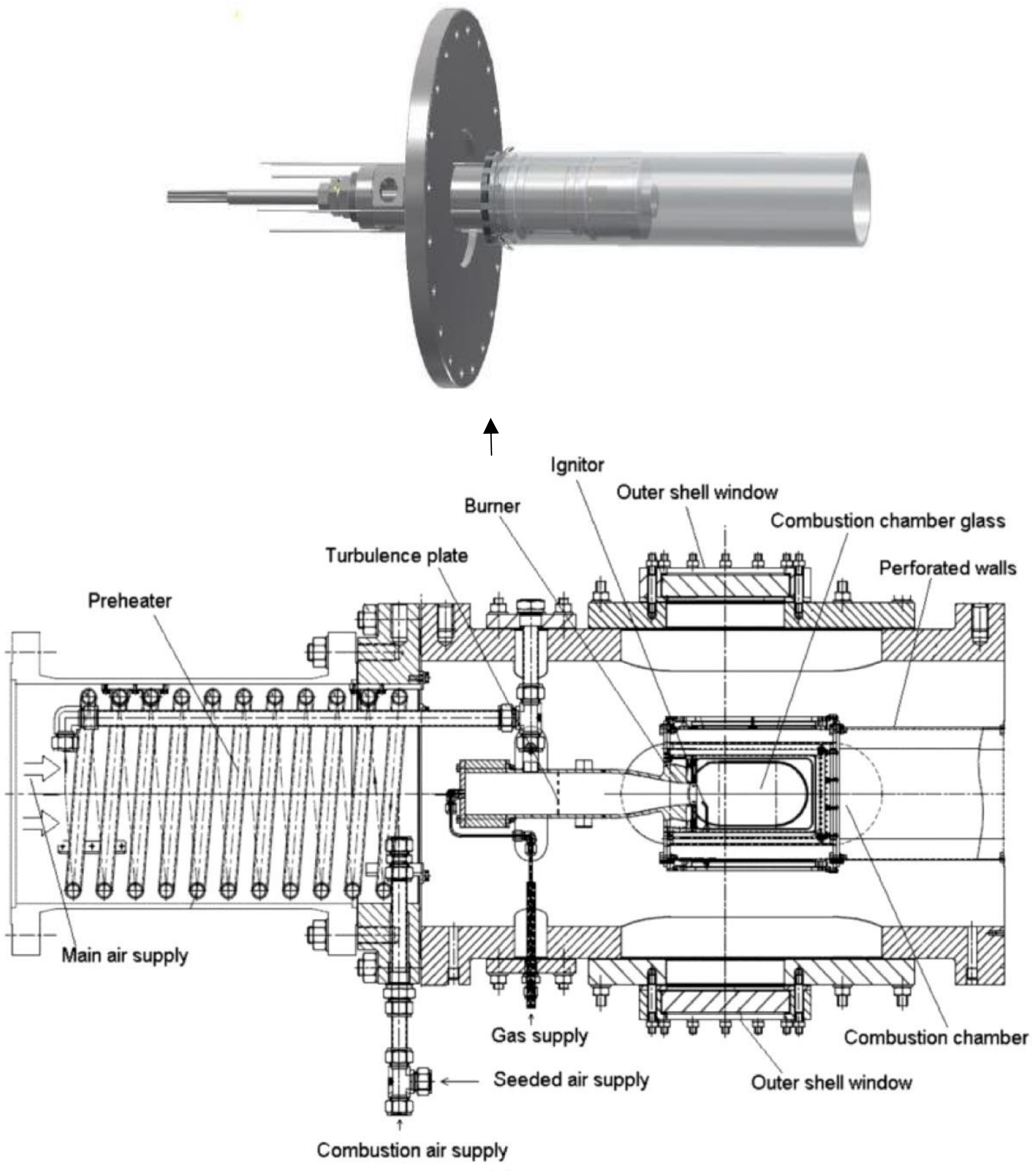


Figure 6-1 Drawing of Generic Swirl Burner and Experimental Rig [232]

OH chemiluminescense measurements were taken for all conditions. A Dantec Dynamics Hi Sense Mk II CCD camera with a 1.3 megapixel resolution was coupled to a Hamamatsu C9546-03L image intensifier. A specialty 78 mm focal length lens (F-stop = f/3.8) capable of capturing light in the UV wavelength range was installed on the image intensifier along with a narrow band pass filter centred at 307 nm (FWHM = 10 nm). Results were processes via Abel Deconvolution. An Avigilon 5 Mp H.264 HD camera was used to capture the flame during various stability stages and provide qualitative insights of the flame behaviour.

Table 6-1 Test points matrix. Each test point was evaluated at 3 different temperatures and 3 different pressures

Case	Mass NH_3 [g/s]	Mass H_2 [g/s]	Mass O_2 [g/s]	Mass Air [g/s]	Stoichiometry
1	1.321	0.067	2.403	10.314	1.00
2	1.321	0.067	2.187	9.387	1.10
3	1.321	0.067	2.005	8.604	1.20
4	1.321	0.067	1.920	8.240	1.25
5	1.321	0.067	1.849	7.938	1.30
6	1.321	0.067	1.718	7.375	1.40

An integrated Signal Instruments equipment comprising several analysers was used. The system is comprised of: a heated vacuum chemiluminescense analyser (Signal 4000VM) to quantify NO_x concentrations, calibrated to 37.1 ppm NO and 1.9 ppm NO_2; a system for quantifying trace concentrations of NH_3 in the flue gas, which forms a subsystem to the 4000VM NO_x analyser; a paramagnetic O_2 sensor (up to 22.5%). Measured errors have been account to ~5%.

6.1.2 Numerical Analysis

6.1.2.1 Chemical Reactor Network (CRN)

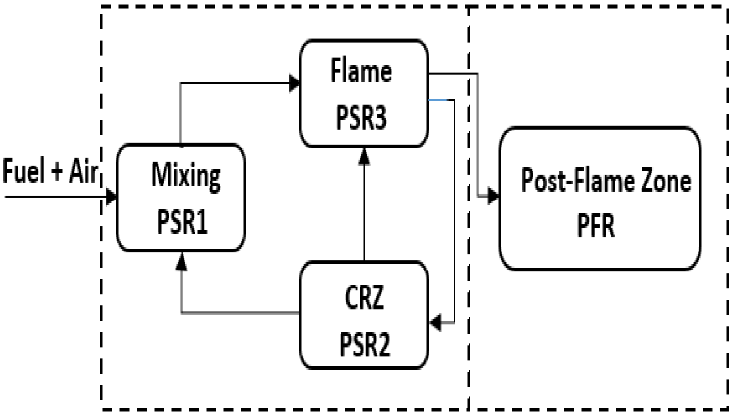


Figure 6-2 Gas Turbine Network

A 1D simulation was conducted using a Chemical Reactor Network (CRN) model, which has shown to be viable for gas turbine simulations previously [174]. The reactor network has two clusters, Figure 6-2. The first cluster represents the swirling flame with a central recirculation zone (CRZ) whose recirculation was set at 20% of the product gases. Recirculation strength was approximated from previous experimental campaigns using similar burners [233, 234]. The second cluster uses a single Plug Flow Reactor for post-flame processes along a 0.1 m duct. The detailed chemical kinetic mechanism established in chapter 5 was used in this numerical study. Simulations were conducted using PRO-CHEMKIN. As inlet conditions, the simulation was carried out using atmospheric and preheated temperatures as in the experimental trials. The model was calibrated to the experiments in order to determine heat losses that mainly accounted to the primary combustion zone. Mass flow rates and chemical composition were set as in the experimental campaign under atmospheric pressure conditions.

6.1.2.2 Gas Turbine Cycle Simulation

Combustion results from the CRN using the improved reaction model were used as inputs into a newly developed mathematical model for design and off design gas turbine analyses [235]. The enhanced version of the mathematical model considers the variation of the turbine polytropic efficiency due to operational regime changes. Moreover, to better understand the influence of fuel enthalpy, this parameter was introduced into the mathematical model for simulation of the flow behaviour, heat transfer and energy transformation. After implementing the adjustments in the mathematical model, coefficient b is calculated using the following equation:

$$b = \frac{\dot{m}_{fuel}}{\dot{m}_2} = \frac{c_{p_{cp}} \cdot (T_{3t} - T_0) - c_{p_{air}} \cdot (T_{2t} - T_0)}{\eta_{cc} \cdot (LHV + h_{fuel}) - c_{p_{cp}} \cdot (T_{3t} - T_0) \cdot (1 + \alpha) - \alpha \cdot (h_{cc2} - h_{cc1})} \qquad 6\text{-}1$$

Where T_{3t} is the inlet turbine temperature [K], T_0 the ambient temperature [K], T_{2t} the outlet compressor temperature [K], α the water vapour mass flow specified to fuel mass flow at the chamber inlet (if any), h_{cc2} and h_{cc1} the enthalpy of water vapor at the combustion chamber outlet and inlet, respectively [kJ/kg]. The coefficient is used to determine the heat supplied, overall specific work and temperature at the end of the expansion process are all set as functions of this parameter.

An industrial Rolls-Royce Allison 501-KB5 gas turbine was employed in the study. For model validation, the same input parameters utilised during the test campaign of the reference gas turbine plant [236] were applied, with error values within the range of experimental uncertainty for the operating conditions considered.

In addition to the reference gas turbine plant data [236], the values of pressure drop in the compressor and the combustion chamber were also quantified, as well as the polytropic efficiencies of the compressor and turbine, the combustion efficiency and mechanical efficiency. An inlet temperature of 567K and 9.67 bar pressure are adopted for all calculations performed.

For the present study, a 70%NH_3-30%H_2 (vol) blend was used at 1.20 equivalence ratio, as this condition showed good emissions performance. Comparison was carried out with the engine running on pure methane at 0.65 equivalence ratio, representative condition of Dry Low NO_x (DLN) current technologies. Recommendations on further development are presented to ensure competitiveness of ammonia based technologies.

6.2 Results and Discussion

6.2.1 Experimental Results

Initial experimental trials demonstrated that blends with 40% hydrogen (vol) produce unstable flame features prone to flashback. Therefore, the blend was reduced to 30% hydrogen (vol), which according to theoretical calculations provides a LHV of ~28.3 MJ/kg, lower than the value of 50 MJ/kg obtained from methane. Stable combustion was still attainable, Figure 6-3.

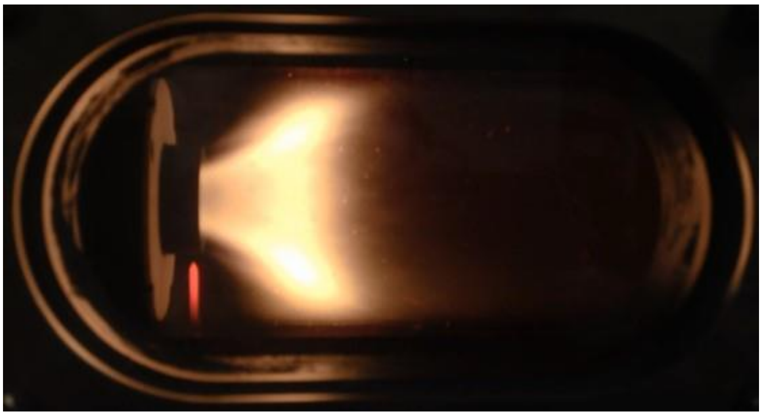


Figure 6-3 Representative stable combustion, case 3, table 6-1

OH* chemiluminescence identified the change in the position of the flame with considerably higher intensity in the production of radicals at $\varphi = 1.00$, Figure 6-4, beyond which OH intensity decays as a consequence of the reduced oxygen. Notwithstanding that oxygen has already been depleted relative to the stoichiometric condition for the higher equivalence ratio conditions, OH radical intensities still denote high values under fuel rich conditions, suggesting additional reactions with other oxygen-bound molecules.

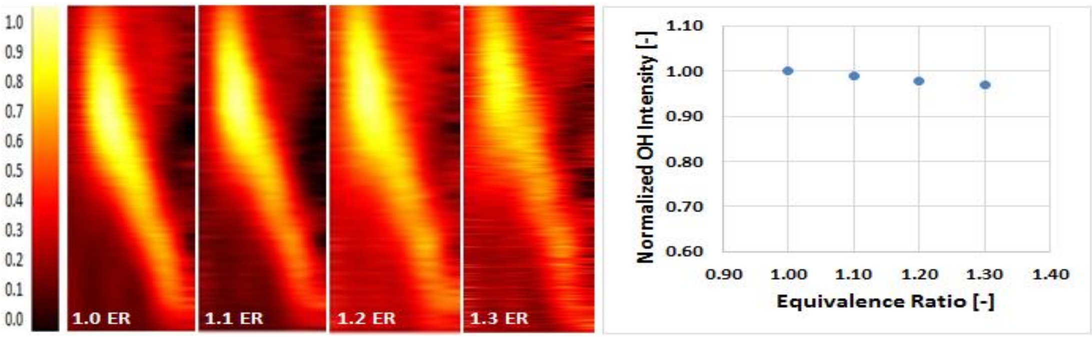


Figure 6-4 OH intensity comparison at different E.R. Normalized at highest value

When air was preheated at ~484 K, the high intensity boundary of the OH profile showed a considerable contraction of ~24% compared to atmospheric inlet temperature conditions, with most of the OH production located at the flame front, contrary to the atmospheric inlet temperature case where a considerable concentration of radicals remain free across the primary zone, Figure 6-5. Thus, as expected, the increase in inlet temperature compacts the flame front, rendering it more reactive and stable.

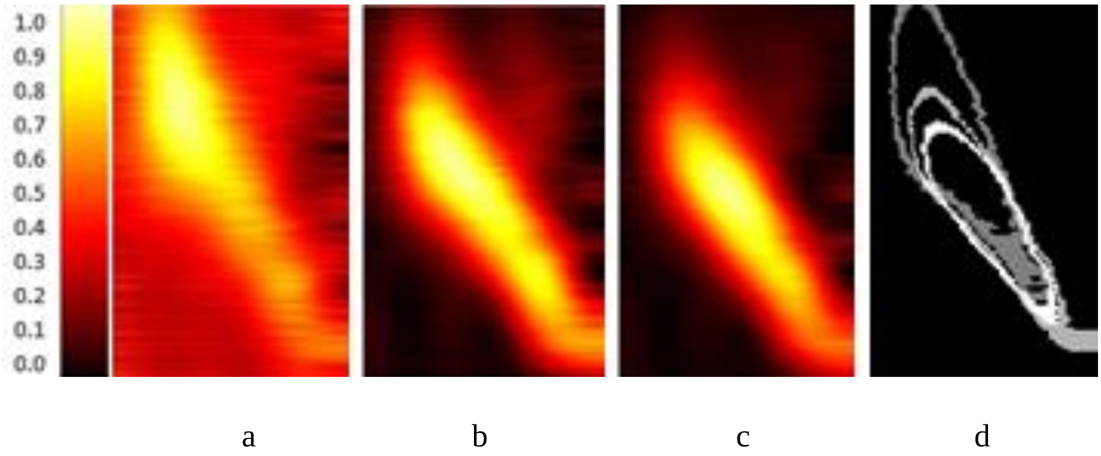


Figure 6-5 Impact of inlet temperature on OH chemiluminescence, case 3, table 6-1. a) 288 K; b) 400 K; c) 487 K; d) Comparison between high OH intensity (0.6-0.7 A.U.) profiles. Arbitrary Units [A.U.]

Finally, trials using by-pass air were carried out to observe the impact of additional cooling and extra post-combustion air in the combustion process at 288K inlet temperature conditions, Figure 6-6. By-pass air reduced the quartz casing temperature from 802±5 K to 444±7 K. The un-convoluted images show that there was a minor shift in the production of the OH species, from 1.0 to ~0.973 Normalized OH intensity, especially close to the flame envelope. Thus, the casing temperature does not have a critical impact on the flame performance, but as will be seen later, it does have it on the post-flame chemistry.

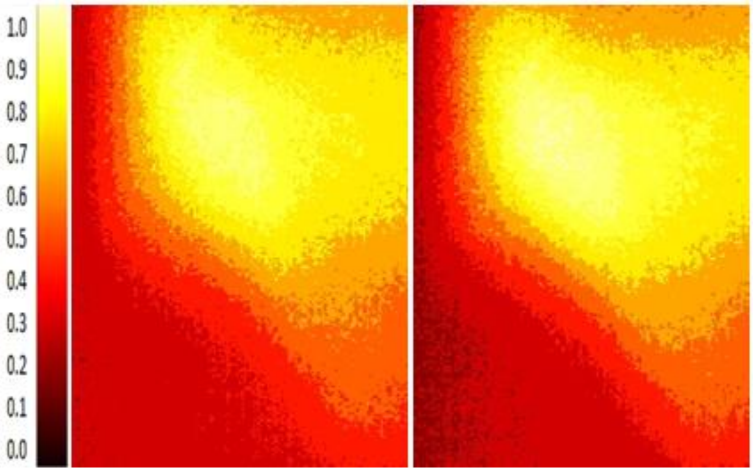


Figure 6-6 Impact of external cooling to the production of OH radicals in the main flame. Left) By-pass air condition; right) No bypass air

In terms of emissions, NO_x was primarily measured as this is the principal pollutant product of ammonia based fuel reactions, Figure 6-7. The results demonstrate that the increase in equivalence ratio decreases the production of NO_x in up to 4(O). It is evident that the reduction of oxygen is partially responsible for this shift, as less O_2 minimises the complete reaction of ammonia and hydrogen. However, the results provide evidence that ammonia based fuels can potentially be used at relatively high equivalence ratios in order to decrease the production of nitrogen oxides. Moreover, it is clear that the increase in inlet temperature augments emissions in ~2(O). Initial assumptions focused on the increase of flame temperature, thus boost of Zeldovich NO_x. Although adiabatic temperatures rise from 2033 to 2185K between cases (i.e. at E.R.=1.20), an increase in 2(O) was also linked to chemical reactions occurring during combustion. As from previous results, OH radicals have now been enhanced and compacted at the flame front, parameter likely linked to this effect will be discussed in the following sub-section. Finally, by-pass air seems to also keep a high NO_x concentration even at high equivalence ratios. The rationale of this phenomenon is based on the post-combustion recombination of hot, unburned ammonia with NO_x. One key finding, discussed next, is the enhancement of the reaction $NH_3+NO = H_2O+N_2$, which occurs when hot ammonia is present in the post-combustion zone. Due to the cooling effect of the by-pass air, unburned ammonia is cooled down, decreasing the previous reaction and letting high emission levels. This additional recombination of hot molecules provides guidelines on how to re-design current injection systems, thus ensuring that NO is minimised.

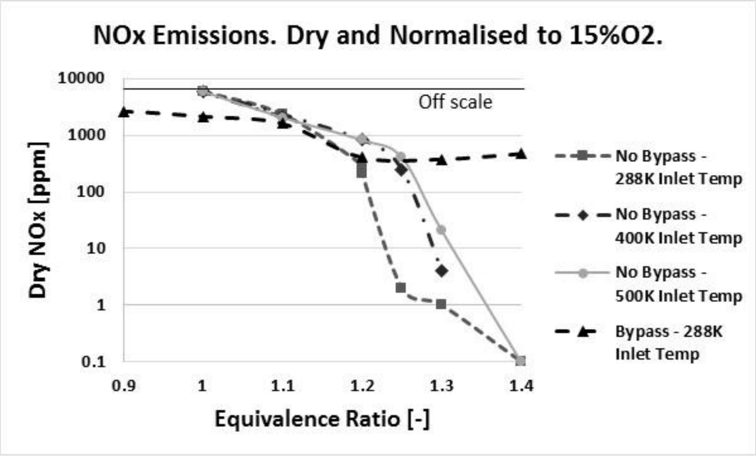


Figure 6-7 NO_x emission levels

6.2.2 Numerical Results

Using a calibrated model, predictions were conducted on the chemical reactions occurring at different conditions, specifically targeting an equivalence ratio of 1.20, case 3 Table 6-1. It is observed that the consumption of ammonia mainly occurs due to its reaction with OH radicals through the reaction NH_3+OH=NH_2+H_2O, followed by its reaction with other free radicals, i.e. H^+, O^-, etc. Although the change in temperature slightly alters the consumption of NH_3 through these reactions, *Figure 6-8*, it is clear that the consumption of ammonia has increased in ~4(O) at higher temperatures. This clearly correlates to previous findings, Figure 6-5, where OH radicals are more reactive at the flame front at higher inlet temperatures.

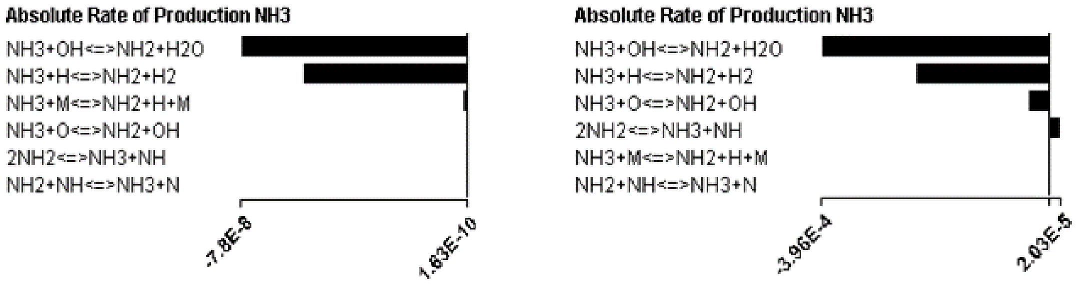


Figure 6-8 Absolute rate of production of NH_3 at the flame. Left) 288K; right) 488K.

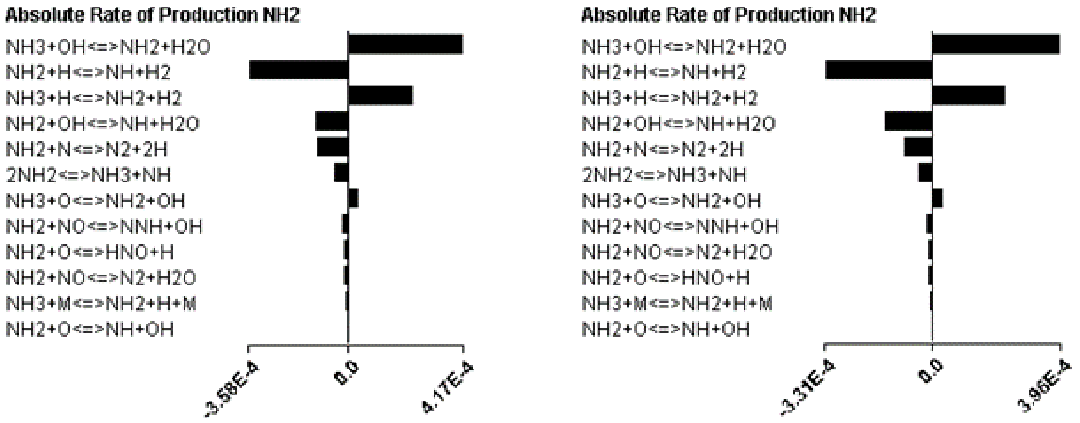


Figure 6-9 Absolute rate of production of NH_2 at the flame. Left) 288K; right) 488K.

On the contrary, NH_2, first main radical product of ammonia consumption, seems to remain as reactive as under atmospheric inlet temperature conditions, Figure 6-9. It is clear that the radical degrades into NH while producing extra water molecules. Interestingly, NO in the flame front starts reacting with the radical through the reaction NH_2+NO=N_2+H_2O, which in practise would need to be enhanced for minimization of pollutant emissions.

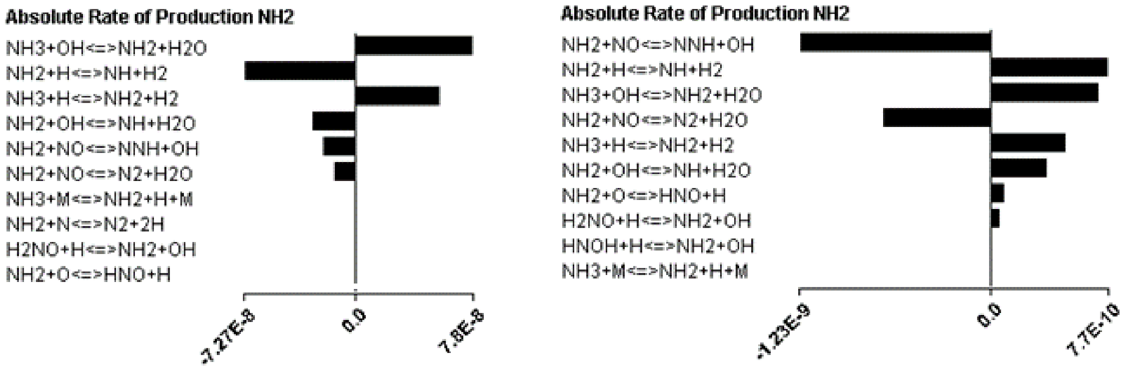


Figure 6-10 Absolute rate of production of NH_2 in the Post-flame region. Left) 288K; right) 488K.

However, the trend is completely different in the post-flame region, Figure 6-10, where at high temperatures the remaining unburned ammonia and hot hydrogen react with OH and NH molecules, respectively, to produce NH_2 molecules that interact with NO to form NNH and N_2+H_2O, thus enhancing the reduction of nitric oxides. Therefore, the higher temperature of the flame allows further recombination of species that will ensure that more NO is consumed, bringing down this emission in the post-flame zone.

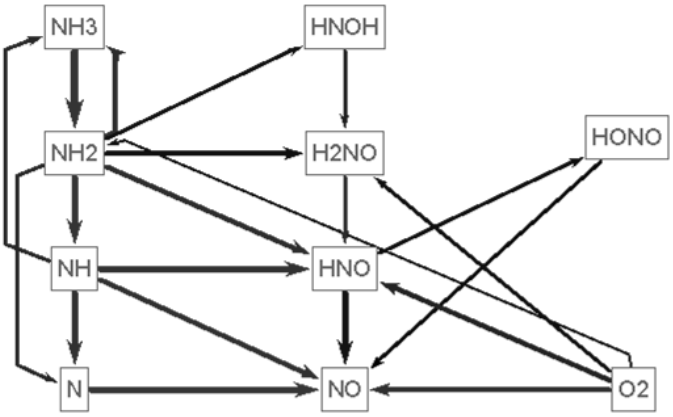


Figure 6-11 Reaction path for NO

Finally, the main reaction path of NO was also obtained for the primary zone, Figure 6-11, for the conditions at which the gas turbine cycle was calculated, i.e. 567K and 9.69bar. It is observed that once ammonia splits into NH_x radicals, these tend to produce HNO molecule that preludes the formation of NO, as expected. Since most of the NH_2 radicals have already reacted through the flame, i.e. as amidogen (NH_2) is highly reactive [237], the consumption of the pollutant is minimal in this region, whereas its reaction with hot NH_2 radicals formed in the post-flame zone allows further decrease of nitric oxides. Thus, these results evidence the need of having small hot ammonia and hydrogen quantities in the post-flame region to ensure that NO keeps reacting for its minimization.

6.2.3 Cycle Analyses

The cycle was initially calibrated using experimental tests from the manufacturer. Results showed good correlation between the numerical cycle and the manufacturer results, Figure 6-12. The results show that the relative error for the power calculated by the mathematical model and the value of the real turbine was 0.22% while the relative error for the efficiency was 0.07%.

When the model was used to compare the efficiency of the ammonia/hydrogen cycle, the first problem to solve was the power output at which the analysis needed to be performed. Due to the maximum permissible fuel flowrate of 0.367 kg/s, this value was set as inlet condition for the ammonia/hydrogen cycle. A rich fuel condition was predefined to ensure low NO_x emissions, as experimentally demonstrated, with a total air mass flowrate of 2.260 kg/s into the combustion chamber, setting the analysis at 1.20 equivalence ratio.

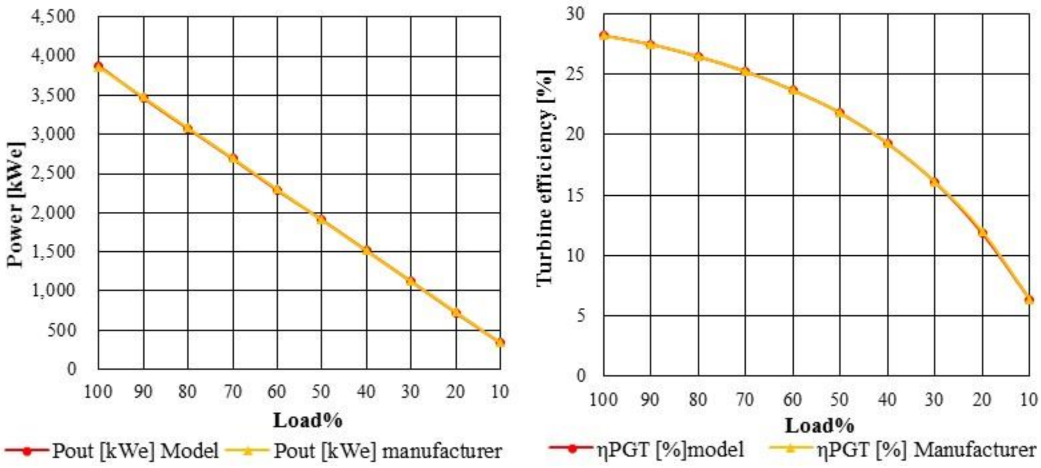


Figure 6-12 Correlation between the numerical model and an actual turbine using NG/air.

In order to compare such a system with current, high performance available technologies, a Dry Low NO_x (DLN) condition of 0.65 equivalence ratio using methane as fuel was used for comparison purposes. Thus, with a total fuel mass flowrate of 0.207 kg/s and an air flowrate of 5.480 kg/s into the combustion chamber, analyses were performed. A total air mass flowrate from the compressor was set at 14.990 kg/s, with a thermal power of 10.37 MW in both cases.

As expected, the reduced amount of air into the combustion process using the ammonia/hydrogen blend, i.e. only ~15%, led to a cycle efficiency of ~9.77% and turbine inlet temperatures of only 850 K, consequence of the excessive dilution that occurs after the primary combustion zone product of the remaining air coming from the main compressor. Results for DLN technologies show efficiencies in the range of 19.36%, i.e. since the system was designed to run at higher fuel flowrates, with air in the combustion primary zone accounting ~37% of the total available air flowrate, with turbine inlet temperatures of 1155 K.

Although it is clear that efficiencies can be increased by reducing dilution into the turbine, current calibration of the model cannot be employed for these further calculations, and a new set of tests needs to be performed under these conditions for such an aim. Moreover, it is evident from the previous analyses that although ammonia/hydrogen at this particular blend has potential for low emissions combustion, any equipment running on this blend needs to be re-designed accordingly to ensure higher efficiencies with greater flue gas temperatures or mass flowrates. On that point, further research is taking place via steam injection, which is out of the scope of this work.

6.3 Summary

Ammonia can be used as a fuel in gas turbines with stable combustion operation when hydrogen is added into the blend. A blend of 70%NH_3-30%H_2 (mol%) was found to produce stable flames, with low NO_x emissions at high equivalence ratios above 1.10. Results show a boost in the consumption of the radical at the flame front at high inlet temperatures representative of real gas turbine conditions. Contraction of the flame under these high inlet temperature conditions was evident, improving the combustion efficiency and leading to a faster consumption of species at the flame boundaries. This parameter ensured that hot, unburned ammonia was ready for further reaction with existing NO_x via its decomposition into NH_x radicals, reducing the pollutant and achieving low NO_x conditions. However, operation of gas turbines using both this blend and a simple Brayton cycle produces low efficiencies that cannot compete with current DLN technologies. Thus, further research and development are required to enable higher efficiencies.

CHAPTER 7

Summary of Results and Discussion

Chapter 7

In recent years, with the problem of decreasing fossil fuel reserves, climate change and pollution problems related to carbon emissions, studies on alternatives to fossil fuels become current among the various popular investigations on the subject of energy. Ammonia is a potential vector of energy that could be used for storage, transportation and cooling of integrated systems based on combustion processes, thus delivering good amounts of energy for industrial applications. Thus the combustion of ammonia as a fuel is an interesting topic as it yields less carbon dioxide emission and pollutants than conventional fossil fuels. Therefore, in this study to begin with, research has been dedicated to understanding the fundamental characteristics of ammonia-based fuels combustion and the reactions that occur through the process especially under practical conditions.

In the past, most developments focused on improving small- to medium-scale devices such as reciprocating engines, whilst as a key step in the realisation of ammonia as a viable energy vector is releasing the stored energy at the power levels required for commercial or grid-scale applications. Only quite few studies investigated the use of ammonia-based fuels in gas turbine engines to date. Thus, it is of great significance to develop new devices and techniques with gas turbines that can use green ammonia for power generation. Therefore, in this study, investigations were also performed to develop a gas-turbine combustor which burns a combination of NH_3 and other fuels, with the goal of achieving controlled emissions, identifying combustion characteristics to be used for new revolutionary designs.

As a summary, the most essential findings of this study are listed as follows.

- ➢ To determine the potential of using ammonia/methane blends for power generation, research was conducted to provide a reduced chemical reaction mechanism to assess ammonia/methane blends for further CFD studies. 5 reduced chemical kinetic mechanisms based on Konnov's mechanism were also obtained under the gas turbine operation relevant condition.
- ➢ The reduced mechanisms were examined with 0D (autoignition), 1D (laminar flame) and 2D (turbulent flame) modelling, under high temperature and pressure conditions which are met in gas turbine combustors. This provided a

comprehensive analyses of the reduced mechanism performance on ammonia/methane combustion kinetics description.

- Ignition delay time calculations with reduced mechanisms for highly diluted ammonia at high pressure showed relatively larger deviations from the shock tube experimental data while ignition delay time predictions for ammonia/methane blends showed with reduced mechanisms showed a better agreement with experimental data. These results indicated that the kinetics modelling still need to be refined for ammonia ignition chemistry.

- Furthermore, under high pressure (17atm) and different equivalence ratio conditions, ignition delay times predictions for ammonia/methane using Mech.1-4 demonstrated good performance against the full Konnov's mechanism while Mech.5 worked well only in the range of 0.5 to 1.25 equivalence ratios. From these calculations, it was deducted that attention needs to be carefully paid on the conditions of ammonia/methane combustion using the reduced mechanism.

- Ammonia/methane laminar burner-stabilised premixed flames were modelled using the reduced mechanisms. Combustion product calculations showed good accuracy of all reduced mechanisms and the full Konnov's mechanism. It was found that CO concentration tends to be high with the increase of methane in fuel mixture while NO concentration increases with the increase of ammonia.

- A 2D turbulent combustion simulation was also performed using the reduced chemical mechanisms. A variety of parameters were examined under gas turbine conditions using LES analyses. Temperature profiles, OH radicals, CO emissions and velocity magnitudes predicted with the four reduced mechanisms, showed satisfactory agreement with those obtained through the full Konnov's mechanism. Therefore, the Mech.4 was recommended as the kinetics model for future ammonia/methane simulations requiring extensive computational costs.

- To comprehensively investigate the properties of ammonia/methane combustion, the detailed chemical-kinetics of the Konnov mechanism were employed for ammonia/methane fuel blends with high ammonia content.

- From the ignition delay time calculations using the modified mechanism, it was found both the ammonia fraction in fuel blends and equivalence ratio have impact on the ignition delay time of ammonia/methane fuel blends. Significantly higher ignition delay time was identified using NH_3/CH_4 fuel blends than the equivalent for methane which can potentially help to prevent auto-ignition risk problems in gas turbine engines.

- Premixed ammonia/methane flames were also simulated by using a freely propagated laminar combustion model using this modified chemical mechanism. The characteristics of premixed ammonia/methane combustion were evaluated under different conditions.

- It was found a significant negative effect of ammonia fraction in the fuel blends on flame speed according to the laminar flame speed calculation results, especially under stoichiometric conditions. Due to the increase of ammonia fraction, ammonia/methane flame propagation is weakened, suggesting that the low flame speed of high NH_3 mixtures can limit the application and current designs of combustion devices, with the need of developing new techniques to promote stable operational conditions if using these blends.

- In the ammonia/methane laminar flames, emission characteristic results showed that when using ammonia as primary fuel in the blends, CO emission will be lower while NO_x emission will be rather high compared to pure methane. As NO_x emission is the main concern in utilising ammonia as fuel, further developing suitable techniques for practical device to reduce NO_x emissions is quite essential under operational conditions of gas turbine engines.

- Detailed analyses on the flame structures suggested that flame speed and peak value of OH, H, O and NH_2 are of the highest relevance. Specifically, a quasi-linear relation can be found between the NH_3/CH_4 flame speed and the maximum mole fraction of $OH+H+O+NH_2$ in the flames. This can help to explain that with more ammonia fraction in fuel blends, the reduction of flame speed results from decrease in chemical reactivity. NO and CO emissions were also found to have strong correlations with maximum radical concentrations like HNO and HCO in the reaction zone at different NH_3 fractions.

- Simulation results of ammonia/methane combustion under engine-relevant conditions showed that the increase of pressure has a negative effect on the flame propagation while temperature increase can promote the flame propagation. Specifically, under relative high temperature conditions, the effect of pressure tends to have more impact on the laminar flame speed. This suggests that under practical gas turbine operation conditions, pressure conditions will be an essential factor for the design and optimisation of performance of ammonia/methane combustion applications.
- The elevated pressure will decrease the NO and CO emissions, whilst increased initial temperature will lead to the augmentation of emissions. However, the decrease of total NO and CO emissions with the combined increased pressure and initial temperature suggests that pressure is a more important factor which affects the kinetics in practical engine operational conditions. In particular, for NO emissions the effect of inlet temperature on NO emission is rather slight compared to pressure, which indicates a good potential of using ammonia-based fuels under gas turbine operational relevant conditions.
- To explore the potential of using ammonia/hydrogen blends as an alternative fuel for future power generation, a comprehensive investigation were performed to provide assessment for chemical mechanisms of ammonia/hydrogen premixed combustion. 12 widely used detailed chemical mechanisms were employed to determine their performance for the prediction of laminar flame speed, NO_x emission and ignition delay times using ammonia/hydrogen blends.
- Laminar flame speed calculation for ammonia/hydrogen under different pressure, initial ammonia concentrations and equivalence ratios indicated that the Mathieu mechanism has the best agreement with the experimental data within the range of initial conditions tested. Thus the Mathieu mechanism is recommended for ammonia/hydrogen fuels' flame speed simulation studies.
- Simulation for emission analyses of diluted ammonia/hydrogen premixed flames have been performed against experimental data with different conditions. In terms of NO_x emission the best predictions were achieved by

using the Tian mechanism, Klippenstein mechanism and Mendiara mechanism. Sensitivity and pathway analyses were also carried out to identify reactions that require more attention in future development of combustion models. Simulation prediction using the Tian mechanism showed industrial high pressure conditions can lead to substantial decrease of NO_x emission.

- The ignition delay time prediction showed that the Tian mechanism and the Mathieu mechanism both yielded quite good performance. As the detailed results were provided, the choice of the kinetics model in practical use can be depended on the specific conditions accordingly.
- An improved chemical kinetics mechanism model was proposed for ammonia/hydrogen premixed combustion based on the Mathieu mechanism in terms of NO_x emission prediction.
- Simulation was carried out under low pressure conditions with various ammonia/hydrogen ratios and equivalence ratios to simulate the experimental results of premixed ammonia/hydrogen combustion from literature. From the predictions, the chemical mechanism developed in present study showed the best performance among the three mechanisms used for comparison. Moreover, the largest discrepancy occurred in the only condition using fuel lean mixtures, indicating that further development of reaction mechanism is needed for fuel lean combustion conditions.
- The proposed mechanism was validated against experimental data for laminar flame speed calculations under different ammonia concentrations in fuel blends and equivalence ratios ranging from fuel lean to fuel rich conditions. Specifically, validation under elevated pressure conditions indicated that the mechanism developed in present study is promising for practical gas turbine application.
- The improved mechanism has also been proved good accuracy for highly diluted ammonia mixtures ignition delay under high pressure conditions (30atm) under all different equivalence ratios studied. Thus, the improved chemical-kinetics mechanism model has been shown to be capable of predicting different essential properties of ammonia/hydrogen combustion

under gas turbine related conditions.

- In the present study, experimental campaigns were designed to understand the stability and potential of premixed ammonia/hydrogen blends in swirl combustion devices utilised in large gas turbines. A first assessment of the suitability of a chosen 70%NH_3-30%H_2 (%vol) blend for utilisation were performed by established optical generic swirl-burner enabled studies. Impact of equivalence ratio, ambient temperature (<484±10 K) and bypass air were also studied with a focus on NO_x reduction, one of the main challenges for ammonia combustion.

- OH chemiluminescence denoted that when inlet air was preheated from atmospheric condition of 288 K to 484 K, with most of the OH production located at the flame front, the increase in inlet temperature has compacted the flame front, making it more stable and reactive.

- The results demonstrated that the increase in equivalence ratio decreases the production of NO_x under fuel rich conditions whilst the increase in inlet temperature augments NO_x emissions. As for cooling effect of the by-pass air, it was found that unburned ammonia is cooled down, decreasing the previous reaction and letting high emission levels. This additional recombination of hot molecules provides guidelines on how to re-design current injection systems, thus ensuring that NO is minimized.

- A numerical GT cycle model was developed alongside the experimental investigation. The results demonstrate that the blend has considerable potential as a fuel substitute with reasonable combustion stability and significant reduction of emissions for the cases without bypass air. However, emissions are still above those recommended for gas turbine cycles, with a theoretical cycle that still produces low efficiencies compared to DLN methane, highlighting the requirement for new injection techniques to reduce NO_x/unburned NH_3 in the flue gases whilst ensuring increased power outputs.

CHAPTER 8

Conclusions and Future Work

Chapter 8

8.1 Conclusions

The overall objective of this work was to characterise combustion phenomena of ammonia-based fuels and its utilisation in a swirl stabilised combustion system for future power generation. The main conclusions of the present study can be summarised as follows,

- In order to improve ammonia combustion rate for power applications, methane, as a combustion promoter, has been proposed to be co-fired with ammonia. The Konnov's kinetics model was reduced and verified for ammonia/methane combustion under practical gas turbine conditions, providing a good predictive capability with much less computational run-time suitable for more practical CFD simulation use. Fundamental flame studies investigating the effect of burning ammonia/methane fuel mixtures provided deep insight into combustion characteristics of ammonia substitution on the ammonia/methane flames. On the one hand, emission characteristic results showed that when using ammonia as primary fuel in the blends, CO emission and NO emission are relatively low, suggesting the feasibility of ammonia substituting methane in a large proportion. On the other hand, it can be also concluded that practical engine operational-relevant conditions (elevated pressure and initial temperature) have a prominent impact on the reduction of CO and NO emissions, indicating a good potential of using ammonia-based fuels under gas turbine industrial conditions.

- Elaboration study of chemical mechanisms for ammonia/hydrogen fuel blends was performed to reproduce the fundamental combustion phenomena and distinguish their potential to be used in combustion systems. Comprehensive comparison of various combustion properties with different recent detailed ammonia combustion mechanisms has identified both Mathieu's and Tian's mechanisms are promising for future practical industrial use as their satisfying prediction performance. An improved chemical mechanism was proposed based on the Mathieu's mechanism mainly to get better agreement with experimental data in terms of NO_x emission calculations for ammonia/hydrogen flames. Comprehensive verification of the established mechanism in flame propagation, ignition and emissions has showed its capability of predicting different essential properties for ammonia/hydrogen combustion under gas turbine related conditions.

- A series of experimental and numerical tests were performed using a premixed combustion generic burner and practically-relevant swirl-number, investigating ammonia/hydrogen blends. Results demonstrated that ammonia can be used as a fuel in gas turbines with stable combustion operation when hydrogen is added into the blend. The blend of 70%NH_3-30%H_2 was found to produce stable flames within the generic swirl burner employed, generating relatively low NO_x emissions under fuel-rich conditions. Finally, at high equivalence ratios and higher inlet temperatures representative of real gas turbine conditions, improving the combustion efficiency and reducing the NO_x pollutant can be achieved.

8.2 Future Work

In the present research, we mainly proposed the framework of utilising ammonia-based fuels such as ammonia/methane and ammonia/hydrogen for combustion applications. Based on the present work some related future studies can be taken into consideration.

- More experimental and modelling work will be needed for chemical kinetics of ammonia/methane flames since data for ammonia as the primary fuel in the ammonia/methane blends are rather limited. Developing detailed chemical mechanisms and more comprehensive evaluation of the mechanisms for such fuels are quite necessary especially under various practical conditions.

- Fundamental studies of ammonia/hydrogen fuel blends combustion are needed especially at high pressures in order to provide guide designs of combustion chambers. For instance, autoignition of fuel blends in high-pressure conditions needs to be investigated with various equivalence ratios and compositions.

- More verification is needed on the mechanism reduction in order to fulfil future practical simulation studies. On the one hand, simulation of industrial devices with high resolution can lead to prohibiting computational cost with detailed mechanisms or even reduced mechanism, especially for complex geometries like gas turbine combustors. Turbulent combustion in real devices is a highly nonlinear complex system, so sometimes the deviations produced from reduced chemistry can translate in nonnegligible errors in 3D simulations. Therefore, careful investigations will be in need to settle more delicate reduced chemistry for future works.

- New combustion technologies can be explored to reduce NO_x of ammonia-based fuels combustion such as moderate or intense low oxygen dilution (MILD), catalytic combustion, plasma assisted combustion, etc.

- 3D simulation of full scale for swirl combustor can be performed as the implementation of 2D LES simulations has been proved feasible in this work. 3D simulations can provide better details of swirl flames for flame behaviour and aerodynamic flow motion especially in the shear layer region. Other benefits of such models also include the velocity profile of three dimensions at any plane even inside the nozzle.

- As for the swirl combustor, better injection strategies are needed to improve ammonia/hydrogen combustion to achieve high flame stability and lower emissions. Different swirl numbers would be possible choices for application in gas turbine power generation utilising ammonia fuel blends.

- More advanced diagnosis technologies need to be included in future experimental work, for example LDV, PLID or tomographic PIV techniques, with which important practical engineering issues such as NO_x emissions, instabilities and stabilities regimes can be deeply analysed.

- Experimental and numerical studies will be conducted on an annular combustor for an auxiliary power unit. This will be used to test the ammonia fuels in a real gas turbine system.

- Ammonia can also be utilised by mixing other fuels e.g. biofuels, as blended alternative fuel. This can be investigated to enhance the combustion performance and also reduced carbon emissions.

Appendix A

Mech.1

```
ELEM H C O N AR
END
SPECIES
!KD->  C2H4O C2 C CH3CO3 CH3CO3H
!KD->  C2H5O2H CH3CO2 CH3CO2H N2O3 C2N2
!KD->  NO3 HNO3 CNN HCNN N2O4
!KD->  HNNO HCNH NCN HNCN H2CNO
!KD->  CH3NO CH2CHOW C2H3O CH3HCOW C3H6OH
!KD->  O2C3H6OH C3H5O2 C3H5O2H NC3H7O2 NC3H7O2H
!KD->  IC3H7O2 IC3H7O2H IC3H7O NC3H7O C3H2
!KD->  C3H6O C2H5CHO C2H5CO C4H2 C4H
!KD->  H2C4O C6H6 C6H5O C6H5 AR
H H2 O O2 OH
HO2 H2O H2O2 CO CO2
HCO CH3 CH4 C2H6 CH2O
C2H5 CH2 CH3O CH2OH CH
C2H2 C2H4 C2H3 CH3OH CH3HCO
C2H CH2CO HCCO SCH2 C2O
CH3CO CH3O2 CH3O2H C2H5O2 C2H5OH
C2H5O SC2H5O PC2H5O CH2HCO CN
H2CN N NH HCN NO
HCNO HOCN HNCO NCO N2O
NH2 HNO NO2 NNH NH3
N2H2 HONO N2H3 N2H4 NH2OH
HNOH H2NO C3H5O C3H6 C3H8
IC3H7 NC3H7 C3H3 SC3H5 PC3H4
TC3H5 C3H5 C3H4 IC4H7 C4H6
C4H4 IC4H5 NC4H5 C4H8 T2C4H8
C2C4H8 IC4H3 NC4H3 N2
END
```

REACTIONS, A_i ((cm^3/mol)$^{(r-1)}$/s), β_i, E_i (cal/mol)

```
! CH + N2 = HCN + N      3.68E+05 1.42 20723
!KD-> CH+N2=NCN+H                 3.00E+12      0.0     22157.
!KD-> CN+N2O=NCN+NO               6.000E+13      0.0    15360.0
!KD->      DUPLICATE
!KD-> CN+N2O=NCN+NO               1.800E+10      0.0     1450.0
!KD->      DUPLICATE
!KD-> CN + NCO = NCN + CO         1.800E+13      0          0
!KD-> C2O + N2 = NCN + CO         7.00E+11      0      17000
!KD-> CH + N2 = HNCN              1.65E+21     -3.62    14196
!KD-> HNCN + M = H + NCN + M        1.79E+28     -3.44    64502
!KD-> HNCN + O = NO + HCN          1.22E+14      0.05      73.5
!KD-> HNCN + O = NH + NCO          5.60E+13      0.05      73.5
!KD-> HNCN + O = CN + HNO          9.36E+12      0.05      73.5
!KD-> HNCN + OH = NCN + H2O         8.28E+03      2.78     3135
!KD-> HNCN + O2 = HO2 + NCN         1.26E+08      1.28    24240
!KD-> NCN = N + CN               2.95E+30     -5.29   117090
```

```
!KD-> NCN = C + N2                2.66E+28     -5.32    83110
!KD-> NCN = CNN                   3.69E+29     -5.84    78410
!KD-> NCN + H = HCN +N              1.89E+14      0       8425
!KD-> NCN + O = CN + NO             2.54E+13      0.15      -34
!KD-> NCN + O = CO + N2             2.42E+02      2.32    -1135
!KD-> NCN + O = N + NCO             2.20E+09      0.42     -157
!KD-> NCN + N= N2 + CN              1.00E+13      0          0
!KD-> NCN + C = CN +CN              1.00E+13      0          0
!KD-> NCN + OH = HCN + NO             3.32E+10     -0.97     7290.
!KD->     DUPLICATE
!KD-> NCN + OH = HCN + NO             4.69E+10      0.44     4000.
!KD-> DUPLICATE
!KD-> NCN + O2 = NO + NCO             3.80E+09      0.51    24590
!KD-> NCN + CH = HCN +CN            3.21E+13      0       -860
!KD-> NCN + CN = C2N2 +N            1.25E+14      0       8020
!KD-> NCN + CH2 = H2CN + CN          7.99E+13      0       4630
H+H+M=H2+M                  7.000E+17    -1.0        0.0
H2/0.0/ N2/0.0/ H/0.0/ H2O/14.3/ CO/3.0/ CO2/3.0/
H+H+H2=H2+H2                1.000E+17    -0.6        0.0
H+H+N2=H2+N2                5.400E+18    -1.3        0.0
H+H+H=H2+H                3.200E+15     0.0        0.0
O+O+M=O2+M                  1.000E+17    -1.0        0.0
O/71.0/ O2/20.0/ NO/5.0/ N2/5.0/ N/5.0/ H2O/5.0/
O+H+M=OH+M                  6.200E+16    -0.6        0.0
H2O/5.0/
H2+O2=OH+OH                 2.500E+12     0.0    39000.0
O+H2=OH+H                 5.060E+04     2.67    6290.0
H+O2=OH+O                 9.750E+13     0.0    14850.0
H+O2(+M)=HO2(+M)             1.480E+12     0.6        0.0
LOW /3.50E+16 -0.41 -1116.0/
TROE /0.5 100000 10/
!KD->  AR/0.0/ H2O/10.6/ H2/1.5/ CO2/2.4/
H2O/10.6/ H2/1.5/ CO2/2.4/
!KD-> H+O2(+AR)=HO2(+AR)            1.480E+12     0.6        0.0
!KD->     LOW /7.00E+17 -0.8  0.0/
!KD->     TROE /0.45 10 100000/
H+OH+M=H2O+M                2.200E+22    -2.0        0.0
!KD->  H2O/6.4/ AR/0.38/ CO2/1.9/
H2O/6.4/        CO2/1.9/
H2+OH=H2O+H                 1.000E+08     1.6     3300.0
OH+OH=H2O+O                 1.500E+09     1.14     100.0
HO2+OH=H2O+O2                 2.890E+13     0.0     -500.0
HO2+O=OH+O2                 1.630E+13     0.0     -445.0
H+HO2=H2+O2                4.280E+13     0.0     1411.0
H+HO2=OH+OH                 1.700E+14     0.0      875.0
H+HO2=H2O+O                 3.000E+13     0.0     1720.0
HO2+HO2=H2O2+O2              4.200E+14     0.0    12000.0
DUPLICATE
HO2+HO2=H2O2+O2              1.300E+11     0.0    -1640.0
DUPLICATE
OH+OH(+M)=H2O2(+M)            7.200E+13    -0.37       0.0
```

```
LOW /2.2E+19 -0.76 0.0/
TROE /0.5 100000 10/
H2O/0.0/
OH+OH(+H2O)=H2O2(+H2O)        7.200E+13     -0.37       0.0
LOW /1.45E+18 0.0 0.0/
H2O2+OH=HO2+H2O              1.000E+12      0.0        0.0
DUPLICATE
H2O2+OH=HO2+H2O              5.800E+14      0.0     9560.0
DUPLICATE
H2O2+H=HO2+H2               1.700E+12      0.0     3755.0
H2O2+H=H2O+OH               1.000E+13      0.0     3575.0
H2O2+O=HO2+OH               2.800E+13      0.0     6400.0
N2+O=NO+N                  1.800E+14      0.0    76100.0
N+O2=NO+O                  9.000E+09      1.0     6500.0
NO+M=N+O+M                  9.640E+14      0.0   148300.0
N2 /1.5/ NO /3.0/ CO2/2.5/
NO+NO=N2+O2                 3.000E+11      0.0    65000.0
N2O(+M)=N2+O(+M)             1.260E+12      0.0    62620.0
LOW / 4.000E+14 0.0 56640.0/
O2/1.4/ N2/1.7/ H2O/12.0/ NO/3.0/ N2O/3.5/
N2O+O=N2+O2                 1.000E+14      0.0    28200.0
N2O+O=NO+NO                 6.920E+13      0.0    26630.0
N2O+N=N2+NO                 1.000E+13      0.0    20000.0
N2O+NO=N2+NO2                2.750E+14      0.0    50000.0
NO+O(+M)=NO2(+M)             1.300E+15     -0.75       0.0
LOW /4.72E+24 -2.87 1551.0/
TROE /0.962 10.0 7962.0 /
!KD->    AR /0.6/ NO2 /6.2/ NO /1.8/ O2 /0.8/ N2O /4.4/ CO2/0/
NO2 /6.2/ NO /1.8/ O2 /0.8/ N2O /4.4/ CO2/0/
H2O /10.0/
NO+O(+CO2)=NO2(+CO2)          1.300E+15     -0.75       0.0
LOW /4.0E+22 -2.16 1051.0/
TROE /0.962 10.0 7962.0 /
NO2+O=NO+O2                 3.910E+12      0.0      -238.0
NO2+N=N2O+O                 8.400E+11      0.0        0.0
NO2+N=NO+NO                 1.000E+12      0.0        0.0
NO2+NO=N2O+O2                1.000E+12      0.0    60000.0
NO2+NO2=NO+NO+O2             3.950E+12      0.0    27590.0
!KD-> NO2+NO2=NO3+NO              1.130E+04      2.58   22720.0
!KD-> NO2+O(+M)=NO3(+M)            1.330E+13      0.0        0.0
!KD->    LOW / 1.49E+28 -4.08 2467.0 /
!KD->    TROE /0.86 10.0 2800.0 /
!KD->    H2O/10.0/ O2/0.8/ H2/2.0/ CO2 /0/
!KD-> NO2+O(+CO2)=NO3(+CO2)        1.330E+13      0.0        0.0
!KD->    LOW / 1.34E+28 -3.94 2277.0 /
!KD->    TROE /0.86 10.0 2800.0 /
!KD-> NO3=NO+O2                  2.500E+06      0.0    12120.0
!KD-> NO3+NO2=NO+NO2+O2           1.200E+11      0.0     3200.0
!KD-> NO3+O=NO2+O2                1.020E+13      0.0        0.0
!KD-> NO3+NO3=NO2+NO2+O2          5.120E+11      0.0     4870.0
!KD-> N2O4(+M)=NO2+NO2(+M)         4.050E+18     -1.1    12840.0
```

```
!KD->     LOW /1.96E+28  -3.8  12840./
!KD->     AR/0.8/ N2O4/2.0/ NO2/2.0/
!KD-> N2O4+O=N2O3+O2              1.210E+12     0.0       0.0
!KD-> NO2+NO(+M)=N2O3(+M)          1.600E+09     1.4       0.0
!KD->     LOW /1.0E+33  -7.7  0.0/
!KD->     N2/1.36/
!KD-> N2O3+O=NO2+NO2              2.710E+11     0.0       0.0
N2+M=N+N+M                  1.000E+28    -3.33   225000.0
N/5/ O/2.2/
NH+M=N+H+M                  2.650E+14     0.0    75500.0
NH+H=N+H2                   3.200E+13     0.0      325.0
NH+N=N2+H                   9.000E+11     0.5       0.0
NH+NH=NNH+H                 5.100E+13     0.0       0.0
NH+NH=NH2+N                 5.950E+02     2.89   -2030.0
NH+NH=N2+H2                 1.000E+08     1.0       0.0
NH2+M=NH+H+M                3.160E+23    -2.0    91400.0
NH+H2=NH2+H                 1.000E+14     0.0    20070.0
NH2+N=N2+H+H                6.900E+13     0.0       0.0
NH2+NH=N2H2+H               1.500E+15    -0.5       0.0
NH2+NH=NH3+N                1.000E+13     0.0     2000.0
NH3+NH=NH2+NH2              3.160E+14     0.0    26770.0
NH2+NH2=N2H2+H2             1.000E+13     0.0     1500.0
N2H3+H=NH2+NH2              5.000E+13     0.0     2000.0
NH3+M=NH2+H+M               2.200E+16     0.0    93470.0
NH3+M=NH+H2+M               6.300E+14     0.0    93390.0
NH3+H=NH2+H2                5.420E+05     2.4     9920.0
NH3+NH2=N2H3+H2             1.000E+11     0.5    21600.0
NNH=N2+H                    3.000E+08     0.0       0.0
!   DUPLICATE
NNH+M=N2+H+M                1.000E+13     0.5     3060.0
!   DUPLICATE
NNH+H=N2+H2                 1.000E+14     0.0       0.0
NNH+N=NH+N2                 3.000E+13     0.0     2000.0
NNH+NH=N2+NH2               2.000E+11     0.5     2000.0
NNH+NH2=N2+NH3              1.000E+13     0.0       0.0
NNH+NNH=N2H2+N2             1.000E+13     0.0     4000.0
N2H2+M=NNH+H+M              5.000E+16     0.0    50000.0
H2O/15.0/ O2/2.0/ N2/2.0/ H2/2.0/
N2H2+M=NH+NH+M              3.160E+16     0.0    99400.0
H2O/15.0/ O2/2.0/ N2/2.0/ H2/2.0/
N2H2+H=NNH+H2               8.500E+04     2.63    -230.0
N2H2+N=NNH+NH               1.000E+06     2.0       0.0
N2H2+NH=NNH+NH2             1.000E+13     0.0     6000.0
N2H2+NH2=NH3+NNH            8.800E-02     4.05   -1610.0
N2H3+NH=N2H2+NH2            2.000E+13     0.0       0.0
N2H3+NNH=N2H2+N2H2          1.000E+13     0.0     4000.0
N2H3+M=NH2+NH+M             5.000E+16     0.0    60000.0
N2H3+M=N2H2+H+M             1.000E+16     0.0    37000.0
N2H3+H=N2H2+H2              1.000E+13     0.0       0.0
N2H3+H=NH+NH3               1.000E+11     0.0       0.0
N2H3+N=N2H2+NH              1.000E+06     2.0       0.0
```

```
N2H3+NH2=NH3+N2H2            1.000E+11     0.5        0.0
N2H3+N2H2=N2H4+NNH           1.000E+13     0.0     6000.0
N2H3+N2H3=NH3+NH3+N2         3.000E+12     0.0        0.0
N2H3+N2H3=N2H4+N2H2          1.200E+13     0.0        0.0
N2H4(+M)=NH2+NH2(+M)         5.000E+14     0.0    60000.0
LOW/1.50E+15 0.0 39000.0 /
N2/2.4/ NH3/3.0/ N2H4/4.0/
N2H4+M=N2H3+H+M              1.000E+15     0.0    63600.0
N2/2.4/ NH3/3.0/ N2H4/4.0/
N2H4+H=N2H3+H2               7.000E+12     0.0     2500.0
N2H4+H=NH2+NH3               2.400E+09     0.0     3100.0
N2H4+N=N2H3+NH               1.000E+10     1.0     2000.0
N2H4+NH=NH2+N2H3             1.000E+09     1.5     2000.0
N2H4+NH2=N2H3+NH3            1.800E+06     1.71   -1380.0
N+OH=NO+H                    2.800E+13     0.0        0.0
N2O+H=N2+OH                  2.200E+14     0.0    16750.0
N2O+H=NH+NO                  6.700E+22    -2.16   37155.0
N2O+H=NNH+O                  5.500E+18    -1.06   47290.0
!KD-> N2O+H=HNNO             8.000E+24    -4.39   10530.0
N2O+OH=N2+HO2                1.000E+14     0.0    30000.0
HNO+NO=N2O+OH                8.500E+12     0.0    29580.0
!KD-> HNO+NO+NO=HNNO+NO2           1.600E+11     0.0     2090.0
!KD-> NH+NO+M=HNNO+M               1.630E+23    -2.6     1820.0
!KD-> HNNO+H=N2O+H2                2.000E+13     0.0        0.0
!KD-> HNNO+H=NH2+NO                1.000E+12     0.0        0.0
!KD-> HNNO+O=N2O+OH                2.000E+13     0.0        0.0
!KD-> HNNO+OH=H2O+N2O              2.000E+13     0.0        0.0
!KD-> HNNO+OH=HNOH+NO              1.000E+12     0.0        0.0
!KD-> HNNO+NO=N2+HONO              2.600E+11     0.0     1610.0
!KD-> HNNO+NO=NNH+NO2              3.200E+12     0.0      540.0
!KD-> HNNO+NO=N2O+HNO              1.000E+12     0.0        0.0
!KD-> HNNO+NO2=N2O+HONO            1.000E+12     0.0        0.0
!KD-> HNNO+NO2=NNH+NO3             1.000E+13     0.0    17000.0
NO2+H=NO+OH                  1.320E+14     0.0      362.0
NO2+OH=HO2+NO                1.810E+13     0.0     6676.0
NO2+HO2=HONO+O2              4.640E+11     0.0     -479.0
NO2+H2=HONO+H                7.330E+11     0.0    28800.0
NO2+NH=N2O+OH                8.650E+10     0.0    -2270.0
NO2+NH=NO+HNO                1.245E+11     0.0    -2270.0
!KD-> NO3+H=NO2+OH                 6.620E+13     0.0        0.0
!KD-> NO3+OH=NO2+HO2               1.210E+13     0.0        0.0
!KD-> NO3+HO2=HNO3+O2              5.550E+11     0.0        0.0
!KD-> NO3+HO2=NO2+OH+O2            1.510E+12     0.0        0.0
!KD-> N2O4+H2O=HONO+HNO3           2.520E+14     0.0    11590.0
!KD-> N2O3+H2O=HONO+HONO           3.790E+13     0.0     8880.0
H+NO(+M)=HNO(+M)             1.520E+15    -0.41       0.0
LOW /4.00E+20 -1.75 0.0 /
!KD->    H2O/10.0/ O2/1.5/ AR/0.75/ H2/2.0/ CO2/3.0/
H2O/10.0/ O2/1.5/          H2/2.0/ CO2/3.0/
HNO+H=NO+H2                  4.460E+11     0.72     655.0
HNO+OH=NO+H2O                1.300E+07     1.88    -956.0
```

```
HNO+O=OH+NO                 5.000E+11     0.5     2000.0
HNO+O=NO2+H                 5.000E+10     0.0     2000.0
HNO+O2=NO+HO2                 2.200E+10     0.0     9140.0
HNO+N=NO+NH                 1.000E+11     0.5     2000.0
HNO+N=H+N2O                 5.000E+10     0.5     3000.0
HNO+NH=NH2+NO                 5.000E+11     0.5       0.0
HNO+NH2=NH3+NO                2.000E+13     0.0     1000.0
HNO+HNO=N2O+H2O               3.630E-03     3.98    1190.0
HNO+HNO=HNOH+NO               2.000E+08     0.0     4170.0
HNO+NO2=HONO+NO               6.020E+11     0.0     2000.0
NO+OH(+M)=HONO(+M)            2.000E+12    -0.05    -721.0
LOW / 5.08E+23 -2.51 -67.6 /
TROE /0.62 10.0 100000.0 /
!KD->    H2O/10.0/ O2/2.0/ AR/0.75/ H2/2.0/ CO2/0.0/
H2O/10.0/ O2/2.0/         H2/2.0/ CO2/0.0/
NO+OH(+CO2)=HONO(+CO2)        2.000E+12    -0.05    -721.0
LOW / 1.70E+23 -2.3 -246.0 /
TROE /0.62 10.0 100000.0 /
NO2+H+M=HONO+M                1.400E+18    -1.5      900.0
HONO+H=HNO+OH                 5.640E+10     0.86    4970.0
HONO+H=NO+H2O                 8.120E+06     1.89    3840.0
HONO+O=OH+NO2                 1.200E+13     0.0     5960.0
HONO+OH=H2O+NO2               1.690E+12     0.0     -517.0
HONO+NH=NH2+NO2               1.000E+13     0.0       0.0
HONO+HONO=H2O+NO2+NO          1.000E+13     0.0     8540.0
HONO+NH2=NO2+NH3              5.000E+12     0.0       0.0
!KD-> NO2+OH(+M)=HNO3(+M)          2.410E+13     0.0       0.0
!KD->    LOW / 6.42E+32 -5.49 2350.0 /
!KD->    TROE /1.0 10.0 1168.0 /
!KD->    H2O/10.0/ O2/2.0/ AR/0.75/ H2/2.0/ CO2/0.0/
!KD-> NO2+OH(+CO2)=HNO3(+CO2)      2.410E+13     0.0       0.0
!KD->    LOW / 5.80E+32 -5.4 2186.0 /
!KD->    TROE /1.0 10.0 1168.0 /
!KD-> NO+HO2+M=HNO3+M              1.500E+24    -3.5     2200.0
!KD-> HNO3+H=H2+NO3               5.560E+08     1.53   16400.0
!KD-> HNO3+H=H2O+NO2              6.080E+01     3.29    6290.0
!KD-> HNO3+H=OH+HONO              3.820E+05     2.3     6980.0
!KD-> HNO3+OH=NO3+H2O             1.030E+10     0.0    -1240.0
NH3+O=NH2+OH                 1.100E+06     2.1     5210.0
NH3+OH=NH2+H2O                5.000E+07     1.6      950.0
NH3+HO2=NH2+H2O2              3.000E+11     0.0    22000.0
NH2+HO2=NH3+O2                1.650E+04     1.55    2027.0
NH2+O=H2+NO                 5.000E+12     0.0       0.0
NH2+O=HNO+H                 4.500E+13     0.0       0.0
NH2+O=NH+OH                 7.000E+12     0.0       0.0
NH2+OH=NH+H2O                 9.000E+07     1.5     -460.0
NH2+OH=NH2OH                  1.790E+13     0.2       0.0
NH2+HO2=HNO+H2O               5.680E+15    -1.12     707.0
NH2+HO2=H2NO+OH               2.910E+17    -1.32    1248.0
NH2+O2=HNO+OH                 1.000E+13     0.0    26290.0
NH2+O2=H2NO+O                 6.000E+13     0.0    29880.0
```

```
NH2+NO=NNH+OH              2.290E+10     0.425    -814.0
NH2+NO=N2+H2O              2.770E+20    -2.65     1258.0
NH2+NO=H2+N2O              1.000E+13     0.0     33700.0
NH2+NO2=N2O+H2O            1.620E+16    -1.44      270.0
NH2+NO2=H2NO+NO            6.480E+16    -1.44      270.0
NH+O=NO+H                  7.000E+13     0.0        0.0
NH+O=N+OH                  7.000E+12     0.0        0.0
NH+OH=HNO+H                2.000E+13     0.0        0.0
NH+OH=N+H2O                2.000E+09     1.2        0.0
NH+OH=NO+H2                2.000E+13     0.0        0.0
NH+HO2=HNO+OH              1.000E+13     0.0     2000.0
NH+O2=HNO+O                4.000E+13     0.0    17880.0
NH+O2=NO+OH                4.500E+08     0.79    1190.0
NH+H2O=HNO+H2              2.000E+13     0.0    13850.0
NH+N2O=N2+HNO              2.000E+12     0.0     6000.0
NNH+O=NH+NO                2.000E+14     0.0     4000.0
NH+NO=N2+OH                6.100E+13    -0.50     120.0
N2H4+O=N2H2+H2O            8.500E+13     0.0     1200.0
N2H4+O=N2H3+OH             2.500E+12     0.0     1200.0
N2H4+OH=N2H3+H2O           3.000E+10     0.68    1290.0
N2H4+OH=NH3+H2NO           3.670E+13     0.0        0.0
N2H4+HO2=N2H3+H2O2         4.000E+13     0.0     2000.0
N2H3+O=N2H2+OH             2.000E+13     0.0     1000.0
N2H3+O=NNH+H2O             3.160E+11     0.5        0.0
N2H3+O=NH2+HNO             1.000E+13     0.0        0.0
N2H3+OH=N2H2+H2O           3.000E+10     0.68    1290.0
N2H3+OH=NH3+HNO            1.000E+12     0.0    15000.0
N2H3+O2=N2H2+HO2           3.000E+12     0.0        0.0
N2H3+HO2=N2H2+H2O2         1.000E+13     0.0     2000.0
N2H3+HO2=N2H4+O2           8.000E+12     0.0        0.0
N2H3+NO=HNO+N2H2           1.000E+12     0.0        0.0
N2H2+O=NH2+NO              1.000E+13     0.0        0.0
N2H2+O=NNH+OH              2.000E+13     0.0     1000.0
N2H2+OH=NNH+H2O            5.920E+01     3.4    -1360.0
N2H2+HO2=NNH+H2O2          1.000E+13     0.0     2000.0
N2H2+NO=N2O+NH2            3.000E+10     0.0        0.0
NNH+O=N2+OH                1.700E+16    -1.23     500.0
NNH+OH=N2+H2O              2.400E+22    -2.88    2444.0
NNH+O2=N2+HO2              1.200E+12    -0.34     150.0
NNH+O2=N2O+OH              2.900E+11    -0.34     150.0
NNH+HO2=N2+H2O2            1.000E+13     0.0     2000.0
NNH+NO=N2+HNO              5.000E+13     0.0        0.0
NH2OH+OH=HNOH+H2O          2.500E+13     0.0     4250.0
H2NO+M=H2+NO+M             7.830E+27    -4.29   60300.0
H2O/10.0/
H2NO+M=HNO+H+M             2.800E+24    -2.83   64915.0
H2O/10.0/
H2NO+M=HNOH+M              1.100E+29    -3.99   43980.0
H2O/10.0/
H2NO+H=HNO+H2              3.000E+07     2.0     2000.0
H2NO+H=NH2+OH              5.000E+13     0.0        0.0
```

```
H2NO+O=HNO+OH              3.000E+07    2.0    2000.0
H2NO+OH=HNO+H2O            2.000E+07    2.0    1000.0
H2NO+HO2=HNO+H2O2          2.900E+04    2.69   -1600.0
H2NO+NH2=HNO+NH3           3.000E+12    0.0    1000.0
H2NO+O2=HNO+HO2            3.000E+12    0.0    25000.0
H2NO+NO=HNO+HNO            2.000E+07    2.0    13000.0
H2NO+NO2=HONO+HNO          6.000E+11    0.0    2000.0
HNOH+M=HNO+H+M             2.000E+24    -2.84  58935.0
H2O/10.0/
HNOH+H=HNO+H2              4.800E+08    1.5    380.0
HNOH+H=NH2+OH              4.000E+13    0.0    0.0
HNOH+O=HNO+OH              7.000E+13    0.0    0.0
DUPLICATE
HNOH+O=HNO+OH              3.300E+08    1.5    -360.0
DUPLICATE
HNOH+OH=HNO+H2O            2.400E+06    2.0    -1190.0
HNOH+HO2=HNO+H2O2          2.900E+04    2.69   -1600.0
HNOH+NH2=HNO+NH3           1.800E+06    1.94   -1150.0
HNOH+NO2=HONO+HNO          6.000E+11    0.0    2000.0
HNOH+O2=HNO+HO2            3.000E+12    0.0    25000.0
HNOH+HNO=NH2OH+NO          1.000E+12    0.0    3000.0
!END
CO+HO2=CO2+OH              1.500E+14    0.0    23650.0
CO+OH=CO2+H                1.170E+07    1.354  -725.0
CO+O+M=CO2+M               6.160E+14    0.0    3000.0
!KD->  H2/2.5/ H2O/6.2/ CO/1.875/ CO2/3.75/ AR/0.88/
H2/2.5/ H2O/6.2/ CO/1.875/ CO2/3.75/
CH4/3.2/ CH3OH/7.5/
CO+O2=CO2+O                2.500E+12    0.0    47800.0
HCO+M=H+CO+M               1.560E+14    0.0    15760.0
!KD->  H2/2.5/ H2O/6.2/ CO/1.875/ CO2/3.75/ AR/1.0/
H2/2.5/ H2O/6.2/ CO/1.875/ CO2/3.75/
CH4/3.2/ CH3OH/7.5/
HCO+OH=CO+H2O              1.000E+14    0.0    0.0
HCO+O=CO+OH                3.000E+13    0.0    0.0
HCO+O=CO2+H                3.000E+13    0.0    0.0
HCO+H=CO+H2                9.000E+13    0.0    0.0
HCO+O2=CO+HO2              2.700E+13    0.0    1190.0
HCO+CH3=CO+CH4             1.200E+14    0.0    0.0
HCO+HO2=CO2+OH+H           3.000E+13    0.0    0.0
HCO+HCO=CH2O+CO            3.000E+13    0.0    0.0
HCO+HCO=H2+CO+CO           2.200E+13    0.0    0.0
CH4(+M)=CH3+H(+M)          2.400E+16    0.0    104913.0
LOW /4.5E+17 0.0 90800/
TROE /1.0 10.0 1350.0 7830.0/
CH4/0.0/ H2/2.0/ CO/2.0/ CO2/3.0/ H2O/5.0/
CH4(+CH4)=CH3+H(+CH4)      2.400E+16    0.0    104913.0
LOW /8.4E+18 0.0 90800/
TROE /0.31 2210.0 90/
CH4+HO2=CH3+H2O2           9.000E+12    0.0    24641.0
CH4+OH=CH3+H2O             1.548E+07    1.83   2774.0
```

```
CH4+O=CH3+OH                7.200E+08     1.56     8485.0
CH4+H=CH3+H2                1.300E+04     3.0     8050.0
CH4+CH2=CH3+CH3             4.300E+12     0.0     10038.0
CH4+O2=CH3+HO2              4.000E+13     0.0     56900.0
CH3+M=CH2+H+M               2.720E+36     -5.31   117100.0
!KD->  H2/2.5/ H2O/6.2/ CO/1.875/ CO2/3.75/ AR/1.0/
H2/2.5/ H2O/6.2/ CO/1.875/ CO2/3.75/
CH4/3.2/ CH3OH/7.5/
CH3+M=CH+H2+M               1.000E+16     0.0     85240.0
!KD->  H2/2.5/ H2O/6.2/ CO/1.875/ CO2/3.75/ AR/0.88/
H2/2.5/ H2O/6.2/ CO/1.875/ CO2/3.75/
CH4/3.2/ CH3OH/7.5/
CH3+HO2=CH3O+OH             1.800E+13     0.0        0.0
CH3+OH=CH2OH+H              2.640E+19     -1.8     8068.0
CH3+OH=CH3O+H               5.740E+12     -0.23    13931.0
CH3+OH=CH2+H2O              8.900E+18     -1.8     8067.0
CH3+OH=CH2O+H2              3.190E+12     -0.53    10810.0
CH3+O=H+CH2O                8.430E+13     0.0        0.0
CH3+O2=CH2O+OH              3.400E+11     0.0     8940.0
CH3+O2=CH3O+O               1.320E+14     0.0     31400.0
CH3+CH3=C2H5+H              5.000E+12     0.099   10600.0
CH3+CH3(+M)=C2H6(+M)        9.210E+16     -1.174    636.0
LOW /1.13E+36 -5.246 1705/
TROE /0.405 1120.0 69.6/
H2/2.0/ CO/2.0/ CO2/3.0/ H2O/5.0/
CH3+CH3O=CH4+CH2O           2.409E+13     0.0        0.0
CH3+CH2OH=CH4+CH2O          8.500E+13     0.0        0.0
CH3+H=SCH2+H2               6.000E+13     0.0     15100.0
CH3+O2(+M)=CH3O2(+M)        7.800E+08     1.2        0.0
LOW/5.8E+25 -3.30 0.0/
TROE /0.495 2325.5 10/
CH3+CH3=C2H4+H2             1.000E+14     0.0     32000.0
CH3+OH=SCH2+H2O             7.200E+13     0.0     2780.0
CH2+OH=CH2O+H               2.500E+13     0.0        0.0
CH2+O=CO+H2                 4.800E+13     0.0        0.0
CH2+O=CO+H+H                7.200E+13     0.0        0.0
CH2+O=CH+OH                 3.000E+14     0.0     11920.0
CH2+O=HCO+H                 3.000E+13     0.0        0.0
CH2+H=CH+H2                 3.120E+13     0.0     -1340.0
CH2+O2=HCO+OH               4.300E+10     0.0     -500.0
CH2+O2=CO2+H2               6.900E+11     0.0     500.0
CH2+O2=CO2+H+H              1.600E+12     0.0     1000.0
CH2+O2=CO+H2O               1.900E+10     0.0     -1000.0
CH2+O2=CO+OH+H              8.600E+10     0.0     -500.0
CH2+O2=CH2O+O               5.000E+13     0.0     9000.0
CH2+CO2=CH2O+CO             1.100E+11     0.0     1000.0
CH2+CH2=C2H2+H2             1.580E+15     0.0     11950.0
CH2+CH2=C2H2+H+H            2.000E+14     0.0     11000.0
CH2+CH2=CH3+CH              2.400E+14     0.0     9940.0
CH2+CH2=C2H3+H              2.000E+13     0.0        0.0
CH2+CH3=C2H4+H              4.200E+13     0.0        0.0
```

```
CH2+CH=C2H2+H              4.000E+13     0.0       0.0
!KD-> CH2+C=CH+CH              1.620E+12     0.67   46800.0
!KD-> CH2+M=C+H2+M               1.600E+14     0.0    64000.0
CH2+M=CH+H+M               5.600E+15     0.0    89600.0
SCH2+M=CH2+M               6.000E+12     0.0       0.0
!KD->  H2/2.5/ H2O/5.0/ CO/1.875/ CO2/3.75/ AR/0.6/ CH4/1.2/
H2/2.5/ H2O/5.0/ CO/1.875/ CO2/3.75/        CH4/1.2/
C2H2/8.0/ C2H4/4.0/ C2H6/3.6/ H/33.3/
SCH2+O2=CO+OH+H             3.000E+13     0.0       0.0
SCH2+H=CH+H2               3.000E+13     0.0       0.0
SCH2+O=CO+H+H               1.500E+13     0.0       0.0
SCH2+O=CO+H2               1.500E+13     0.0       0.0
SCH2+OH=CH2O+H              3.000E+13     0.0       0.0
SCH2+HO2=CH2O+OH             3.000E+13     0.0       0.0
SCH2+H2O2=CH3O+OH            3.000E+13     0.0       0.0
SCH2+H2O=>CH3OH             1.800E+13     0.0       0.0
SCH2+CH2O=CH3+HCO            1.200E+12     0.0       0.0
SCH2+HCO=CH3+CO             1.800E+13     0.0       0.0
SCH2+CH3=C2H4+H             1.800E+13     0.0       0.0
SCH2+CH4=CH3+CH3            4.000E+13     0.0       0.0
SCH2+C2H6=CH3+C2H5           1.200E+14     0.0       0.0
SCH2+CO2=CH2O+CO             3.000E+12     0.0       0.0
SCH2+CH2CO=C2H4+CO           1.600E+14     0.0       0.0
CH+OH=HCO+H                3.000E+13     0.0       0.0
CH+O=CO+H                4.000E+13     0.0       0.0
!KD-> CH+O=C+OH                1.520E+13     0.0     4730.0
!KD-> H2O+C=CH+OH                7.800E+11     0.67   39300.0
CH+O2=HCO+O                4.900E+13     0.0       0.0
CH+O2=CO+OH                4.900E+13     0.0       0.0
CH+CO2=HCO+CO               3.220E-02     4.44   -3530.0
CH+CH4=C2H4+H              3.900E+14    -0.4       0.0
CH+CH3=C2H3+H              3.000E+13     0.0       0.0
CH2+OH=CH+H2O              1.130E+07     2.0     3000.0
!KD-> CH+H=C+H2                 7.900E+13     0.0      160.0
CH+H2O=CH2O+H              1.170E+15    -0.75      0.0
CH+H2O=CH2OH               5.700E+12     0.0     -760.0
CH+CH2O=CH2CO+H             1.000E+14     0.0     -515.0
CH3O+M=CH2O+H+M             5.400E+13     0.0    13500.0
!KD->  H2/2.5/ H2O/6.2/ CO/1.875/ CO2/3.75/ AR/0.88/
H2/2.5/ H2O/6.2/ CO/1.875/ CO2/3.75/
CH4/3.2/ CH3OH/7.5/
CH3O+HO2=CH2O+H2O2           3.000E+11     0.0       0.0
CH3O+OH=CH2O+H2O            1.800E+13     0.0       0.0
CH3O+O=CH2O+OH             1.800E+12     0.0       0.0
CH3O+H=CH2O+H2             1.800E+13     0.0       0.0
CH3O+O2=CH2O+HO2            2.200E+10     0.0     1750.0
CH3O+CH2O=CH3OH+HCO          1.000E+11     0.0     2980.0
CH3O+CO=CH3+CO2             6.810E-18     9.2    -2850.0
CH3O+HCO=CH3OH+CO           9.000E+13     0.0       0.0
CH3O+C2H5=CH2O+C2H6          2.410E+13     0.0       0.0
CH3O+C2H3=CH2O+C2H4          2.410E+13     0.0       0.0
```

```
CH3O+C2H4=CH2O+C2H5           1.200E+11      0.0      6750.0
CH3O+H=CH2OH+H              3.400E+06      1.6        0.0
CH3O+H=SCH2+H2O             1.000E+12      0.0        0.0
CH2O+M=HCO+H+M              5.000E+35     -5.54    96680.0
!KD->  H2/2.5/ H2O/6.2/ CO/1.875/ CO2/3.75/ AR/1.0/
H2/2.5/ H2O/6.2/ CO/1.875/ CO2/3.75/
CH4/3.2/ CH3OH/7.5/
CH2O+M=CO+H2+M              1.100E+36     -5.54    96680.0
!KD->  H2/2.5/ H2O/6.2/ CO/1.875/ CO2/3.75/ AR/1.0/
H2/2.5/ H2O/6.2/ CO/1.875/ CO2/3.75/
CH4/3.2/ CH3OH/7.5/
CH2O+HO2=HCO+H2O2            4.110E+04      2.5     10210.0
CH2O+OH=HCO+H2O             3.433E+09      1.18     -447.0
CH2O+O=HCO+OH              4.100E+11      0.57     2760.0
CH2O+H=HCO+H2              1.260E+08      1.62     2166.0
CH2O+O2=HCO+HO2             6.000E+13      0.0     40650.0
CH2O+CH3=HCO+CH4            7.800E-08      6.1      1970.0
C2H6(+M)=C2H5+H(+M)          8.850E+20     -1.228  102210.0
LOW /6.90E+42 -6.431 107175.0/
SRI /47.61 16182.0 3371.0/
!KD->  H2/2.0/ H2O/6.0/ CH4/2.0/ CO/1.5/ CO2/2.0/ C2H6/3.0/ AR/0.7/
H2/2.0/ H2O/6.0/ CH4/2.0/ CO/1.5/ CO2/2.0/ C2H6/3.0/
C2H6+HO2=C2H5+H2O2           1.330E+13      0.0     20535.0
C2H6+OH=C2H5+H2O            7.200E+06      2.0       870.0
C2H6+O=C2H5+OH              1.000E+09      1.5      5800.0
C2H6+H=C2H5+H2              1.400E+09      1.5      7400.0
C2H6+H=CH3+CH4              5.400E+04      0.0     11630.0
C2H6+O2=C2H5+HO2            6.000E+13      0.0     52000.0
C2H6+CH3=C2H5+CH4           1.470E-07      6.0      6060.0
C2H6+CH2=CH3+C2H5           6.500E+12      0.0      7911.0
C2H6+C2H3=C2H4+C2H5          8.566E-02      4.14     2543.0
C2H6+HCO=CH2O+C2H5           4.700E+04      2.72    18235.0
C2H5(+M)=C2H4+H(+M)          1.110E+10      1.037   36767.0
LOW /4.0E+33 -4.99 40000.0/
TROE /0.832 10 1203.0/
!KD->  H2/2.0/ CO/2.0/ CO2/3.0/ H2O/5.0/ CH4/2.0/ C2H6/0.0/ AR/0.7/
H2/2.0/ CO/2.0/ CO2/3.0/ H2O/5.0/ CH4/2.0/ C2H6/0.0/
C2H5(+C2H6)=C2H4+H(+C2H6)      8.200E+13      0.0     39880.0
LOW /1.0E+18 0.0 33380.0/
TROE /0.75 97.0 1379.0/
C2H5+HO2=C2H4+H2O2           1.800E+12      0.0        0.0
C2H5+OH=C2H4+H2O            2.409E+13      0.0        0.0
C2H5+OH=>CH3+CH2O+H           2.409E+13      0.0        0.0
C2H5+O=CH2O+CH3             4.240E+13      0.0        0.0
C2H5+O=CH3HCO+H             5.300E+13      0.0        0.0
C2H5+O=C2H4+OH              3.460E+13      0.0        0.0
C2H5+H=C2H4+H2              1.700E+12      0.0        0.0
C2H5+O2=C2H4+HO2            2.560E+19     -2.77     1980.0
C2H5+CH3=C2H4+CH4           1.100E+12      0.0        0.0
C2H5+C2H5=C2H4+C2H6          1.400E+12      0.0        0.0
C2H5+HO2=C2H5O+OH            3.000E+13      0.0        0.0
```

```
C2H4+M=C2H2+H2+M             3.500E+16     0.0     71530.0
!KD->     H2/2.5/ H2O/6.2/ CO/1.875/ CO2/3.75/ AR/1.0/
H2/2.5/ H2O/6.2/ CO/1.875/ CO2/3.75/
CH4/3.2/ CH3OH/7.5/
C2H4+M=C2H3+H+M              2.600E+17     0.0     96570.0
!KD->     H2/2.5/ H2O/6.2/ CO/1.875/ CO2/3.75/ AR/1.0/
H2/2.5/ H2O/6.2/ CO/1.875/ CO2/3.75/
CH4/3.2/ CH3OH/7.5/
C2H4+OH=C2H3+H2O             5.530E+05     2.31     2900.0
C2H4+O=CH3+HCO               8.100E+06     1.88      180.0
C2H4+H=C2H3+H2               4.490E+07     2.12    13366.0
C2H4+O2=C2H3+HO2             4.000E+13     0.0     61500.0
C2H4+C2H4=C2H5+C2H3          1.860E+14     0.0     64200.0
C2H4+CH3=C2H3+CH4            4.200E+12     0.0     11100.0
C2H4+O=CH2HCO+H              4.700E+06     1.88      180.0
C2H4+O=CH2O+CH2              3.000E+04     1.88      180.0
C2H4+O=CH2CO+H2              6.700E+05     1.88      180.0
C2H4+O=C2H3+OH               1.510E+07     1.91     3790.0
C2H4+OH=CH2O+CH3             2.000E+12     0.0       960.0
C2H4+OH(+M)=PC2H5O(+M)       5.420E+12     0.0         0.0
LOW /1.19E+27 -3.1 0.0/
C2H4+HO2=C2H3+H2O2           1.120E+13     0.0     30400.0
C2H4+CH3O=C2H3+CH3OH         1.000E+11     0.0     10000.0
C2H3(+M)=C2H2+H(+M)          2.100E+14     0.0     39740.0
LOW /4.15E+41 -7.5 45500.0/
TROE /0.65 100000 10/
!KD->  H2/2.0/ CO/2.0/ CO2/3.0/ H2O/5.0/ CH4/2.0/ C2H6/3.0/ AR/0.7/
H2/2.0/ CO/2.0/ CO2/3.0/ H2O/5.0/ CH4/2.0/ C2H6/3.0/
C2H3+HO2=>CH3+CO+OH          3.000E+13     0.0         0.0
C2H3+OH=C2H2+H2O             3.000E+13     0.0         0.0
C2H3+H=C2H2+H2               1.200E+13     0.0         0.0
C2H3+O=CH3+CO                1.000E+13     0.0         0.0
C2H3+O2=CH2O+HCO             1.700E+29    -5.312    6500.0
C2H3+CH=CH2+C2H2             5.000E+13     0.0         0.0
C2H3+CH3=C2H2+CH4            2.050E+13     0.0         0.0
C2H3+C2H=C2H2+C2H2           3.000E+13     0.0         0.0
C2H3+HCO=C2H4+CO             9.034E+13     0.0         0.0
C2H3+CH2O=C2H4+HCO           5.420E+03     2.81     5862.0
C2H3+C2H3=C2H2+C2H4          1.450E+13     0.0         0.0
C2H3+O=C2H2+OH               1.000E+13     0.0         0.0
C2H3+O=CH2+HCO               1.000E+13     0.0         0.0
C2H3+O=CH2CO+H               1.000E+13     0.0         0.0
C2H3+OH=CH3HCO               3.000E+13     0.0         0.0
C2H3+O2=C2H2+HO2             5.190E+15    -1.26     3310.0
DUPLICATE
C2H3+O2=C2H2+HO2             2.120E-06     6.0      9484.0
DUPLICATE
C2H3+O2=CH2HCO+O             3.500E+14    -0.61     5260.0
C2H3+CH2=C2H2+CH3            3.000E+13     0.0         0.0
C2H2=C2H+H                   2.373E+32    -5.28   130688.0
C2H2+O2=HCCO+OH              2.000E+08     1.5     30100.0
```

```
C2H2+O2=C2H+HO2              1.200E+13     0.0     74520.0
C2H2+OH=C2H+H2O              3.385E+07     2.0     14000.0
C2H2+OH=CH2CO+H              1.100E+13     0.0      7170.0
C2H2+O=CH2+CO                1.200E+06     2.1      1570.0
C2H2+O=HCCO+H                5.000E+06     2.1      1570.0
C2H2+CH3=C2H+CH4             1.800E+11     0.0     17290.0
C2H2+O=C2H+OH                3.000E+14     0.0     25000.0
C2H2+OH=CH3+CO               4.830E-04     4.0     -2000.0
C2H2+HO2=CH2CO+OH            6.100E+09     0.0      7950.0
C2H2+O2=HCO+HCO              4.000E+12     0.0     28000.0
C2H+OH=HCCO+H                2.000E+13     0.0         0.0
!KD-> C2H+OH=C2+H2O              4.000E+07     2.0      8000.0
C2H+O=CO+CH                  1.450E+13     0.0       460.0
C2H+O2=HCO+CO                9.000E+12     0.0         0.0
C2H+H2=C2H2+H                7.880E+05     2.39      346.0
C2H+O2=CO+CO+H               9.000E+12     0.0         0.0
C2H+O2=HCCO+O                6.000E+11     0.0         0.0
CH2CO(+M)=CH2+CO(+M)         3.000E+14     0.0     71000.0
LOW /2.300E+15   0.0  57600.0/
!KD->     H2/2.5/ H2O/6.2/ CO/1.875/ CO2/3.75/ AR/1.0/
H2/2.5/ H2O/6.2/ CO/1.875/ CO2/3.75/
CH4/3.2/ CH3OH/7.5/
CH2CO+O2=CH2O+CO2            2.000E+13     0.0     61500.0
CH2CO+HO2=>CH2O+CO+OH        6.000E+11     0.0     12738.0
CH2CO+O=HCCO+OH              1.000E+13     0.0      8000.0
CH2CO+OH=CH2OH+CO            1.000E+13     0.0         0.0
CH2CO+H=CH3+CO               3.280E+10     0.851    2840.0
CH2CO+CH3=C2H5+CO            2.400E+12     0.0      8000.0
CH2CO+CH2=C2H4+CO            2.900E+12     0.0      3800.0
CH2CO+CH2=HCCO+CH3           3.600E+13     0.0     11000.0
CH2CO+CH3=HCCO+CH4           7.500E+12     0.0     13000.0
CH2CO+OH=CH2O+HCO            2.800E+13     0.0         0.0
CH2CO+H=HCCO+H2              1.800E+14     0.0      8600.0
CH2CO+O=HCO+HCO              7.500E+11     0.0      1350.0
CH2CO+O=HCO+CO+H             7.500E+11     0.0      1350.0
CH2CO+O=CH2O+CO              7.500E+11     0.0      1350.0
CH2CO+OH=HCCO+H2O            7.500E+12     0.0      2000.0
HCCO+M=CH+CO+M               6.000E+15     0.0     58821.0
!KD->     H2/2.5/ H2O/6.2/ CO/1.875/ CO2/3.75/ AR/0.88/
H2/2.5/ H2O/6.2/ CO/1.875/ CO2/3.75/
CH4/3.2/ CH3OH/7.5/
HCCO+OH=HCO+CO+H             1.000E+13     0.0         0.0
HCCO+OH=C2O+H2O              3.000E+13     0.0         0.0
HCCO+O=CO+CO+H               1.000E+14     0.0         0.0
HCCO+O=CH+CO2                2.950E+13     0.0      1110.0
HCCO+H=CH2+CO                1.500E+14     0.0         0.0
HCCO+O2=CO2+CO+H             5.400E+11     0.0       850.0
HCCO+CH2=C2H+CH2O            1.000E+13     0.0      2000.0
HCCO+CH2=C2H3+CO             3.000E+13     0.0         0.0
HCCO+CH3=C2H4+CO             2.000E+12     0.0         0.0
HCCO+CH=CO+C2H2              5.000E+13     0.0         0.0
```

```
HCCO+HCCO=CO+C2H2+CO          1.000E+13     0.0        0.0
HCCO+OH=HCO+HCO               1.000E+13     0.0        0.0
HCCO+O2=CO+CO+OH              5.400E+11     0.0      850.0
HCCO+O2=CO2+HCO               5.400E+11     0.0      850.0
CH3OH(+M)=CH3+OH(+M)          1.700E+16     0.0    90885.0
LOW /6.60E+16 0.0 65730.0/
TROE /0.82 200.0 1438.0/
CH3OH+HO2=CH2OH+H2O2          9.640E+10     0.0    12580.0
CH3OH+OH=CH2OH+H2O            1.440E+06     2.0     -840.0
CH3OH+OH=CH3O+H2O             1.000E+13     0.0     1700.0
CH3OH+O=CH2OH+OH              1.630E+13     0.0     5030.0
CH3OH+H=CH2OH+H2              1.640E+07     2.0     4520.0
CH3OH+CH3=CH2OH+CH4           3.190E+01     3.17    7172.0
CH3OH+CH3=CH3O+CH4            1.450E+01     3.1     6935.0
CH3OH+C2H5=C2H6+CH3O          1.440E+01     3.1     8942.0
CH3OH+H=CH3+H2O               2.000E+14     0.0     5300.0
CH3OH+O=CH3O+OH               1.000E+13     0.0     4680.0
CH3OH+CH3=C2H6+OH             2.000E+12     0.0    15000.0
CH3OH+CH3O=CH2OH+CH3OH        3.000E+11     0.0     4070.0
CH3OH(+M)=CH2OH+H(+M)         1.380E+16     0.0    95950.0
LOW /5.35E+16 0.0 70800.0/
TROE /0.82 200.0 1438.0/
CH3OH+H=H2+CH3O               4.000E+13     0.0     6095.0
CH3OH+O2=CH2OH+HO2            2.050E+13     0.0    44900.0
CH3OH+C2H5=C2H6+CH2OH         3.190E+01     3.2     9161.0
CH2OH+M=CH2O+H+M              1.140E+43    -8.0    43000.0
H2O/16.0/ CH4/3.0/ CO2/3.75/  CO/1.875/  H2/2.5/   CH3OH/6.0/
CH2OH+H=CH2O+H2               1.000E+13     0.0        0.0
CH2OH+O2=CH2O+HO2             1.500E+15    -1.0        0.0
DUPLICATE
CH2OH+O2=CH2O+HO2             7.200E+13     0.0     3570.0
DUPLICATE
H+CH2OH=SCH2+H2O              1.000E+12     0.0        0.0
CH2OH+O=CH2O+OH               9.000E+13     0.0        0.0
CH2OH+OH=CH2O+H2O             1.000E+13     0.0        0.0
CH2OH+HO2=CH2O+H2O2           1.210E+13     0.0        0.0
CH2OH+CH2OH=CH3OH+CH2O        4.820E+12     0.0        0.0
CH2OH+CH2OH=CH2O+CH2O+H2      1.000E+15    -0.7        0.0
CH2OH+HCO=CH3OH+CO            1.210E+14     0.0        0.0
CH2OH+CH2O=CH3OH+HCO          5.490E+03     2.8     5900.0
CH2OH+CH3O=CH3OH+CH2O         2.400E+13     0.0        0.0
CH3O+CH3O=CH3OH+CH2O          2.320E+13     0.0        0.0
CH3HCO=CH3+HCO                7.100E+15     0.0    81790.0
CH3HCO+HO2=CH3CO+H2O2         3.000E+12     0.0    12000.0
CH3HCO+OH=CH3CO+H2O           2.300E+10     0.73   -1100.0
CH3HCO+O=CH3CO+OH             5.800E+12     0.0     1800.0
CH3HCO+H=CH3CO+H2             4.100E+09     1.16    2400.0
CH3HCO+O2=CH3CO+HO2           3.000E+13     0.0    39200.0
CH3HCO+CH3=CH3CO+CH4          7.600E+00     3.4     3740.0
CH3HCO+H=CH2HCO+H2            7.000E+08     1.5     7400.0
CH3HCO+O=CH2HCO+OH            5.000E+08     1.5     5800.0
```

```
CH3HCO+OH=CH2HCO+H2O          2.000E+14     0.0     6000.0
CH3HCO+HO2=CH2HCO+H2O2        3.000E+13     0.0    15000.0
CH3HCO+CH2=CH3CO+CH3          1.660E+12     0.0     3510.0
CH3HCO+CH3=CH2HCO+CH4         1.580E+00     4.0     7720.0
CH3HCO+CH3O=CH3CO+CH3OH       5.000E+12     0.0        0.0
CH3HCO+C2H5=CH3CO+C2H6        1.260E+12     0.0     8500.0
CH3HCO+C2H3=CH3CO+C2H4        8.130E+10     0.0     3680.0
CH2HCO=CH3CO                  1.600E+11     0.0    21600.0
CH3HCO+CH2HCO=CH3CO+CH3HCO    3.000E+12     0.0    11200.0
CH3CO(+M)=CH3+CO(+M)          2.800E+13     0.0    17150.0
LOW /6.0E+15 0.0 14070.0/
TROE /0.5 100000 10/
!KD->    H2/2.5/ H2O/6.2/ CO/1.875/ CO2/3.75/ AR/0.88/
H2/2.5/ H2O/6.2/ CO/1.875/ CO2/3.75/
CH4/3.2/ CH3OH/7.5/
CH3CO+H=CH2CO+H2              1.150E+13     0.0        0.0
CH3CO+H=CH3+HCO               2.150E+13     0.0        0.0
CH3CO+O=CH2CO+OH              4.000E+13     0.0        0.0
CH3CO+O=CH3+CO2               1.500E+14     0.0        0.0
CH3CO+CH3=C2H6+CO             3.300E+13     0.0        0.0
CH3CO+CH3=CH4+CH2CO           6.100E+12     0.0        0.0
CH2HCO+H=CH2CO+H2             2.000E+13     0.0        0.0
CH2HCO+O2=CH2O+OH+CO          1.800E+10     0.0        0.0
CH2HCO+O2=CH2CO+HO2           1.500E+11     0.0        0.0
CH2HCO=CH2CO+H                1.580E+13     0.0    35200.0
C2H5O=CH3+CH2O                1.000E+15     0.0    21600.0
C2H5O+O2=CH3HCO+HO2           3.600E+10     0.0     1090.0
C2H5O=CH3HCO+H                2.000E+14     0.0    23300.0
C2H5O+OH=CH3HCO+H2O           1.000E+14     0.0        0.0
C2H5O+H=CH3HCO+H2             1.000E+14     0.0        0.0
C2H5O+O=CH3HCO+OH             1.210E+14     0.0        0.0
C2H5O+HO2=CH3HCO+H2O2         1.000E+14     0.0        0.0
C2H5O+C2H5O=C2H5OH+CH3HCO     5.000E+13     0.0        0.0
C2H5O+PC2H5O=C2H5OH+CH3HCO    5.000E+13     0.0        0.0
C2H5O+SC2H5O=C2H5OH+CH3HCO    5.000E+13     0.0        0.0
SC2H5O+M=CH3HCO+H+M           5.000E+13     0.0    21860.0
SC2H5O+H=CH3HCO+H2            2.000E+13     0.0        0.0
SC2H5O+OH=CH3HCO+H2O          1.500E+13     0.0        0.0
SC2H5O+O=CH3HCO+OH            9.040E+13     0.0        0.0
SC2H5O+O2=CH3HCO+HO2          8.400E+15    -1.20       0.0
DUPLICATE
SC2H5O+O2=CH3HCO+HO2          4.800E+14     0.0     5000.0
DUPLICATE
SC2H5O+HO2=CH3HCO+H2O2        1.000E+13     0.0        0.0
SC2H5O+SC2H5O=C2H5OH+CH3HCO   3.500E+13     0.0        0.0
SC2H5O+PC2H5O=C2H5OH+CH3HCO   5.000E+13     0.0        0.0
PC2H5O=SC2H5O                 1.000E+11     0.0    27000.0
PC2H5O+PC2H5O=C2H5OH+CH3HCO   3.400E+13     0.0        0.0
C2H5OH=CH2OH+CH3              3.100E+15     0.0    80600.0
C2H5OH+OH=SC2H5O+H2O          3.000E+13     0.0     5960.0
C2H5OH+OH=C2H5O+H2O           1.138E+06     2.0      914.0
```

```
C2H5OH+OH=PC2H5O+H2O          2.563E+06     2.06     860.0
C2H5OH+O=SC2H5O+OH            6.000E+05     2.46    1850.0
C2H5OH+O=C2H5O+OH             4.820E+13     0.0     6856.0
C2H5OH+O=PC2H5O+OH            5.000E+12     0.0     4411.0
C2H5OH+H=C2H5+H2O             5.900E+11     0.0     3450.0
C2H5OH+H=SC2H5O+H2            4.400E+12     0.0     4570.0
C2H5OH+HO2=SC2H5O+H2O2        2.000E+13     0.0    17000.0
C2H5OH+CH3=SC2H5O+CH4         4.000E+11     0.0     9700.0
C2H5OH+CH3=PC2H5O+CH4         3.000E+00     4.0    10480.0
C2H5OH+CH3=C2H5O+CH4          8.000E+10     0.0     9400.0
C2H5OH+CH3O=SC2H5O+CH3OH      2.000E+11     0.0     7000.0
C2H5OH+CH2O=C2H5O+CH3O        1.500E+12     0.0    79500.0
C2H5OH+C2H5O=C2H5OH+SC2H5O    2.000E+11     0.0     7000.0
C2H5OH=C2H5+OH                5.000E+16     0.0    91212.0
C2H5OH=C2H4+H2O               1.000E+14     0.0    76706.0
C2H5OH+O2=PC2H5O+HO2          4.000E+13     0.0    50900.0
C2H5OH+O2=SC2H5O+HO2          4.000E+13     0.0    51200.0
C2H5OH+O2=C2H5O+HO2           2.000E+13     0.0    56000.0
C2H5OH+H=PC2H5O+H2            2.000E+12     0.0     9500.0
C2H5OH+H=C2H5O+H2             1.760E+12     0.0     4570.0
C2H5OH+HO2=H2O2+C2H5O         1.000E+11     0.0    15500.0
C2H5OH+HO2=H2O2+PC2H5O        1.000E+11     0.0    12500.0
C2H5OH+C2H5=PC2H5O+C2H6       1.500E+12     0.0    11700.0
C2H5OH+C2H5=SC2H5O+C2H6       4.000E+13     0.0    10000.0
C2H5OH+CH2OH=SC2H5O+CH3OH     4.000E+11     0.0     9700.0
!KD-> C+OH=CO+H               5.000E+13     0.0        0.0
!KD-> C+O2=CO+O               1.200E+14     0.0     4000.0
!KD-> C+CH3=C2H2+H            5.000E+13     0.0        0.0
!KD-> C+CH2=C2H+H             5.000E+13     0.0        0.0
CH2O+CH3O2=HCO+CH3O2H         2.000E+12     0.0    11660.0
CH3O2+H=CH3O+OH               9.600E+13     0.0        0.0
CH3O2+OH=CH3OH+O2             6.000E+13     0.0        0.0
CH3O2+CH3=CH3O+CH3O           2.400E+13     0.0        0.0
CH3O2+CH3O2=>CH2O+CH3OH+O2    2.700E+10     0.0     -780.0
CH3O2+CH3O2=>CH3O+CH3O+O2     2.800E+10     0.0     -780.0
CH3O2+H2O2=CH3O2H+HO2         2.400E+12     0.0    10000.0
CH3O2H=CH3O+OH                6.000E+14     0.0    42300.0
CH3O2+HO2=CH3O2H+O2           2.290E+11     0.0    -1550.0
CH3O2H+OH=CH3O2+H2O           1.150E+12     0.0     -380.0
CH4+CH3O2=CH3+CH3O2H          1.810E+11     0.0    18600.0
C2H6+CH3O2=C2H5+CH3O2H        2.950E+11     0.0    14940.0
CH3OH+CH3O2=CH2OH+CH3O2H      1.810E+12     0.0    13800.0
CH3O2H+O=OH+CH3O2             2.000E+13     0.0     4750.0
!KD-> CH3CO+O2=CH3CO3         1.000E+10     0.0    -2700.0
!KD-> CH3HCO+CH3CO3=CH3CO+CH3CO3H    1.200E+11     0.0     4900.0
!KD-> CH3HCO+C2H5O2=CH3CO+C2H5O2H    1.150E+11     0.0    10000.0
C2H5+O2(+M)=C2H5O2(+M)        2.200E+10     0.772   -570.0
LOW /7.10E+42 -8.24 4270.0 /
C2H5O2=C2H4+HO2               5.620E+11     0.0    28900.0
!KD-> C2H5O2+HO2=C2H5O2H+O2         3.400E+11     0.0    -1300.0
!KD-> C2H5O2H=C2H5O+OH              4.000E+15     0.0    43000.0
```

```
!KD-> C2H5O2H+O=OH+C2H5O2          2.000E+13     0.0     4750.0
!KD-> C2H5O2H+OH=C2H5O2+H2O        2.000E+12     0.0     -370.0
!KD-> CH4+C2H5O2=CH3+C2H5O2H       1.140E+13     0.0    20460.0
!KD-> CH4+CH3CO3=CH3+CH3CO3H       1.140E+13     0.0    20460.0
!KD-> C2H4+C2H5O2=C2H3+C2H5O2H     1.000E+12     0.0    25000.0
!KD-> C2H4+CH3CO3=C2H3+CH3CO3H     3.000E+12     0.0    29000.0
!KD-> CH3CO3+HO2=CH3CO3H+O2        1.000E+12     0.0        0.0
!KD-> CH3CO3H=>CH3CO2+OH           1.150E+13     0.0    32550.0
!KD-> CH3CO3H=>CH3+CO2+OH          2.000E+14     0.0    40150.0
!KD-> CH3CO3+CH3O2=>CH3CO2+CH3O+O2  1.080E+15     0.0     3600.0
!KD-> CH3CO3+CH3O2=>CH3CO2H+CH2O+O2  2.470E+09     0.0    -4200.0
!KD-> CH3CO3+HO2=>CH3CO2+OH+O2     2.590E+11     0.0    -2080.0
!KD-> CH3CO3+CH3CO3=>CH3CO2+CH3CO2+O2  1.690E+12    0.0    -1060.0
!KD-> CH3CO2+M=>CH3+CO2+M          8.700E+15     0.0    14400.0
!KD-> CH3CO2H=CH4+CO2              7.080E+13     0.0    74600.0
!KD-> CH3CO2H=CH2CO+H2O            4.470E+14     0.0    79800.0
!KD-> CH3CO2H+OH=CH3CO2+H2O        2.400E+11     0.0     -400.0
!KD-> CH3OH+C2H5O2=CH2OH+C2H5O2H   6.300E+12     0.0    19360.0
!KD-> CH3OH+CH3CO3=CH2OH+CH3CO3H   6.300E+12     0.0    19360.0
!KD-> CH2O+C2H5O2=HCO+C2H5O2H      1.300E+11     0.0     9000.0
!KD-> CH2O+CH3CO3=HCO+CH3CO3H      1.000E+12     0.0    10560.0
C2H4+CH3O2=C2H3+CH3O2H       1.000E+13     0.0    25000.0
CH3HCO+CH3O2=CH3CO+CH3O2H    1.150E+11     0.0    10000.0
C2H5OH+CH3O2=SC2H5O+CH3O2H   1.000E+13     0.0    10000.0
C2H5+CH3O2=C2H5O+CH3O        2.410E+13     0.0        0.0
!KD-> C2H4+HO2=C2H4O+OH            2.200E+12     0.0    17200.0
!KD-> C2H4+CH3O=C2H4O+CH3          1.000E+11     0.0    14500.0
!KD-> C2H4+CH3O2=C2H4O+CH3O        7.000E+11     0.0    14500.0
!KD-> C2H4O=>CH3HCOW               1.600E+13     0.0    54300.0
!KD-> CH3HCOW+M=>CH3HCO+M          1.000E+14     0.0        0.0
!KD-> CH3HCOW=>CH3+HCO             5.000E+08     0.0        0.0
!KD-> C2H4O+H=H2+C2H3O             8.000E+13     0.0     9740.0
!KD-> C2H4O+H=H2O+C2H3             5.000E+09     0.0     5030.0
!KD-> C2H4O+H=C2H4+OH              9.510E+10     0.0     5030.0
!KD-> C2H4O+CH2HCO=CH3HCO+C2H3O    1.000E+11     0.0    14000.0
!KD-> C2H4O+CH3=CH4+C2H3O          1.070E+12     0.0    11900.0
!KD-> C2H4O+O=OH+C2H3O             1.910E+12     0.0     5300.0
!KD-> C2H4O+OH=H2O+C2H3O           1.780E+13     0.0     3600.0
!KD-> C2H3O=>CH2CHOW               1.000E+11     0.0    10000.0
!KD-> C2H3O=>CH3+CO                8.000E+11     0.0    10000.0
!KD-> C2H3O+H+M=>C2H4O+M           4.000E+15     0.0        0.0
!KD-> CH2CHOW+M=>CH2HCO+M          1.000E+14     0.0        0.0
!KD-> CH2CHOW=>CH3+CO              1.000E+08     0.0        0.0
!KD-> CH2CHOW=>OH+C2H2             1.000E+11     0.0    17000.0
!KD-> CH2CHOW=>CH2CO+H             1.000E+08     0.0        0.0
!KD-> C2H4O+O2=HO2+C2H3O           1.000E+14     0.0    52000.0
!KD-> C2H4O+HO2=H2O2+C2H3O         5.000E+13     0.0    18000.0
!KD-> CH3HCOW+O2=>HO2+CH3CO        1.000E+14     0.0        0.0
!KD-> CH2CHOW+O2=>HO2+CH2CO        1.000E+14     0.0        0.0
CH2+C2H2=H+C3H3              1.200E+13     0.0     6620.0
CH2+C2H4=C3H6                3.160E+12     0.0     5280.0
```

```
SCH2+C2H4=>C3H6              1.000E+14     0.0        0.0
CH2+C3H8=CH3+IC3H7           1.500E+00     3.46    7470.0
CH2+C3H8=CH3+NC3H7           9.000E-01     3.65    7150.0
SCH2+C2H2=C3H3+H             1.800E+14     0.0        0.0
C2H3+CH2=C3H4+H              3.000E+13     0.0        0.0
C2H3+C2H2=C4H4+H             1.930E+12     0.0     6000.0
C2H3+C2H3=C4H6               7.230E+13     0.0        0.0
C2H2+CH3=SC3H5               1.610E+40    -8.58   20331.0
C2H2+CH3=C3H5                2.610E+46    -9.82   36951.0
C2H2+CH3=C3H4+H              6.740E+19    -2.08   31591.0
CH2CO+C2H3=C3H5+CO           1.000E+12     0.0     3000.0
HCCO+C2H2=C3H3+CO            1.000E+11     0.0     3000.0
C3H8(+M)=C2H5+CH3(+M)        1.100E+17     0.0    84400.0
LOW /7.83E+18 0.0 65000.0/
C3H8+O2=NC3H7+HO2            4.000E+13     0.0    50870.0
C3H8+O2=IC3H7+HO2            4.000E+13     0.0    47690.0
C3H8+HO2=NC3H7+H2O2          4.760E+04     2.55   16490.0
C3H8+HO2=IC3H7+H2O2          9.640E+03     2.6    13910.0
C3H8+OH=NC3H7+H2O            3.160E+07     1.80     934.0
C3H8+OH=IC3H7+H2O            7.060E+06     1.90    -159.0
C3H8+O=NC3H7+OH              3.715E+06     2.4     5505.0
C3H8+O=IC3H7+OH              5.495E+05     2.5     3140.0
C3H8+H=NC3H7+H2              1.336E+06     2.54    6756.0
C3H8+H=IC3H7+H2              1.300E+06     2.4     4470.0
C3H8+CH3=NC3H7+CH4           9.000E-01     3.65    7150.0
C3H8+CH3=IC3H7+CH4           1.500E+00     3.46    5480.0
C3H8+C2H5=NC3H7+C2H6         9.000E-01     3.65    9140.0
C3H8+C2H5=IC3H7+C2H6         1.200E+00     3.46    7470.0
C3H8+C2H3=NC3H7+C2H4         6.000E+02     3.3    10502.0
C3H8+C2H3=IC3H7+C2H4         1.000E+03     3.1     8829.0
C3H8+IC3H7=NC3H7+C3H8        8.440E-03     4.2     8720.0
C3H8+C3H5=NC3H7+C3H6         2.350E+02     3.3    19800.0
C3H8+C3H5=IC3H7+C3H6         7.840E+01     3.3    18200.0
C3H8+CH3O=NC3H7+CH3OH        4.340E+11     0.0     6460.0
C3H8+CH3O=IC3H7+CH3OH        1.450E+11     0.0     4570.0
NC3H7=C2H4+CH3               1.260E+13     0.0    30404.0
NC3H7+O2=C3H6+HO2            1.000E+12     0.0     5000.0
IC3H7=C2H4+CH3               1.000E+12     0.0    34500.0
IC3H7+O2=C3H6+HO2            2.754E+10     0.0    -2151.0
C3H6=C3H5+H                  4.570E+14     0.0    88900.0
C3H6=SC3H5+H                 7.590E+14     0.0   101300.0
C3H6=TC3H5+H                 1.450E+15     0.0    98060.0
C3H6=C2H3+CH3                1.100E+21    -1.2    97720.0
!KD-> C3H6+HO2=C3H6O+OH            1.050E+12     0.0    14210.0
C3H6+HO2=C3H5+H2O2           9.640E+03     2.6    13910.0
C3H6+HO2=SC3H5+H2O2          7.500E+09     0.0    12570.0
C3H6+HO2=TC3H5+H2O2          3.000E+09     0.0     9930.0
C3H6+OH=C3H5+H2O             3.120E+06     2.0     -300.0
C3H6+OH=SC3H5+H2O            2.140E+06     2.0     2780.0
C3H6+OH=TC3H5+H2O            1.110E+06     2.0     1450.0
C3H6+O=C2H5+HCO              6.833E+06     1.57    -628.0
```

```
C3H6+O=CH3+CH3CO            9.111E+06     1.57     -628.0
C3H6+O=C2H4+CH2O            4.555E+06     1.57     -628.0
NC3H7=C3H6+H               1.000E+14     0.0     37286.0
C3H6+H=IC3H7               5.704E+09     1.16     874.0
C3H6+H=C3H5+H2              6.457E+12     0.0     4445.0
C3H6+H=SC3H5+H2             7.810E+05     2.5     12280.0
C3H6+O2=SC3H5+HO2           1.950E+12     0.0     39000.0
C3H6+O2=TC3H5+HO2           1.950E+12     0.0     39000.0
C3H6+O2=C3H5+HO2            1.950E+12     0.0     39000.0
C3H6+CH3=C3H5+CH4           2.210E+00     3.5      5680.0
C3H6+CH3=SC3H5+CH4          1.350E+00     3.5     12850.0
C3H6+CH3=TC3H5+CH4          8.400E-01     3.5     11660.0
C3H6+C2H5=C3H5+C2H6         2.230E+00     3.5      6640.0
!KD-> C3H6O=C2H5+HCO             2.450E+13     0.0     58500.0
!KD-> C3H6O=C2H5CHO              1.820E+14     0.0     58500.0
!KD-> C3H6O=CH3+CH3CO            4.540E+13     0.0     59900.0
!KD-> C3H6O=CH3+CH2HCO           2.450E+13     0.0     58820.0
!KD-> C3H6O=CH3+C2H3O            8.000E+15     0.0     92010.0
!KD-> C2H5CHO=C2H5+HCO           2.450E+16     0.0     73000.0
!KD-> C2H5CHO+O=C2H5CO+OH          5.680E+12     0.0      1540.0
!KD-> C2H5CHO+OH=C2H5CO+H2O        1.210E+13     0.0        0.0
!KD-> C2H5CHO+HO2=C2H5CO+H2O2      1.520E+09     0.0        0.0
!KD-> C2H5CHO+C2H5=C2H5CO+C2H6     5.000E+10     0.0      6290.0
!KD-> C2H5CO=C2H5+CO             5.890E+12     0.0     14400.0
C3H5+O2=>CH2O+CH2HCO         5.000E+12     0.0     19190.0
C3H5+H=C3H4+H2              1.800E+13     0.0        0.0
C3H5+O=>C2H4+CO+H           1.807E+14     0.0        0.0
C3H5+CH3=C3H4+CH4           3.000E+12    -0.32    -130.0
C3H5+C2H5=C3H4+C2H6         9.640E+11     0.0     -130.0
C3H5+C2H3=C3H4+C2H4         2.400E+12     0.0        0.0
C3H5+C2H3=C3H6+C2H2         4.800E+12     0.0        0.0
SC3H5+O2=CH3HCO+HCO         4.340E+12     0.0        0.0
SC3H5+HO2=>CH2CO+CH3+OH      4.500E+12     0.0        0.0
SC3H5+H=C3H4+H2             3.333E+12     0.0        0.0
SC3H5+O=>CH2CO+CH3          1.807E+14     0.0        0.0
SC3H5+CH3=C3H4+CH4          1.000E+11     0.0        0.0
SC3H5+C2H5=C3H4+C2H6        1.000E+11     0.0        0.0
SC3H5+C2H3=C3H4+C2H4        1.000E+11     0.0        0.0
TC3H5+O2=CH3CO+CH2O         4.335E+11     0.0        0.0
TC3H5+HO2=>CH2CO+CH3+OH      4.500E+12     0.0        0.0
TC3H5+H=C3H4+H2             3.333E+12     0.0        0.0
TC3H5+O=>HCCO+CH3+H         1.807E+14     0.0        0.0
TC3H5+CH3=C3H4+CH4          1.000E+11     0.0        0.0
TC3H5+C2H5=C3H4+C2H6        1.000E+11     0.0        0.0
TC3H5+C2H3=C3H4+C2H4        1.000E+11     0.0        0.0
C3H4+M=C3H3+H+M             2.000E+18     0.0     80000.0
H2O/16.0/ CO2/3.75/ CO/1.875/ H2/2.5/ CH4/3.0/ C3H6/16.0/ C2H4/16.0/ C3H8/16.0/
C3H4(+M)=PC3H4(+M)          1.070E+14     0.0     64300.0
LOW /3.48E+17 0.0 48390.0/
C3H4+O2=C3H3+HO2            4.000E+13     0.0     61500.0
C3H4+HO2=>CH2CO+CH2+OH       8.000E+12     0.0     19000.0
```

```
C3H4+OH=CH2CO+CH3            3.120E+12     0.0     -397.0
C3H4+OH=C3H3+H2O             2.000E+07     2.0     1000.0
C3H4+O=C2H3+HCO              1.100E-02     4.613   -4243.0
C3H4+H=C3H5                  1.200E+11     0.69    3000.0
C3H4+H=TC3H5                 8.500E+12     0.0     2000.0
C3H4+H=C3H3+H2               2.000E+07     2.0     5000.0
C3H4+CH3=C3H3+CH4            2.000E+11     0.0     7700.0
PC3H4+M=C3H3+H+M             4.700E+18     0.0    80000.0
H2O/16.0/ CO2/3.75/ CO/1.875/ H2/2.5/ CH4/3.0/ C3H6/16.0/ C2H4/16.0/ C3H8/16.0/
PC3H4+O2=>HCCO+OH+CH2        2.000E+08     1.5    30100.0
PC3H4+O2=C3H3+HO2            5.000E+12     0.0    51000.0
PC3H4+HO2=>C2H4+CO+OH        3.000E+12     0.0    19000.0
PC3H4+OH=C3H3+H2O            2.000E+07     2.0     1000.0
PC3H4+OH=CH2CO+CH3           5.000E-04     4.5    -1000.0
PC3H4+O=CH2CO+CH2            6.400E+12     0.0     2010.0
PC3H4+O=C2H3+HCO             3.200E+12     0.0     2010.0
PC3H4+O=HCCO+CH3             6.300E+12     0.0     2010.0
PC3H4+O=>HCCO+CH2+H          3.200E+11     0.0     2010.0
PC3H4+H=TC3H5                6.500E+12     0.0     2000.0
PC3H4+H=C3H3+H2              2.000E+07     2.0     5000.0
PC3H4+H=C2H2+CH3             1.300E+05     2.5     1000.0
PC3H4+CH3=C3H3+CH4           1.500E+00     3.5     5600.0
PC3H4+C2H3=C3H3+C2H4         1.000E+12     0.0     7700.0
PC3H4+C3H5=C3H3+C3H6         1.000E+12     0.0     7700.0
!KD-> C3H3+H=C3H2+H2         5.000E+13     0.0     3000.0
C3H3+O=>C2H+HCO+H            7.000E+13     0.0        0.0
C3H3+O=>C2H2+CO+H            7.000E+13     0.0        0.0
!KD-> C3H3+OH=C3H2+H2O       1.000E+13     0.0        0.0
C3H3+O2=CH2CO+HCO            3.010E+10     0.0     2870.0
C3H3+CH=IC4H3+H              7.000E+13     0.0        0.0
C3H3+CH=NC4H3+H              7.000E+13     0.0        0.0
C3H3+CH2=C4H4+H              4.000E+13     0.0        0.0
!KD-> C3H3+C3H3=C6H5+H       2.000E+12     0.0        0.0
!KD-> CH+C2H2=C3H2+H         1.000E+14     0.0        0.0
!KD-> C3H2+O2=HCCO+CO+H      1.000E+14     0.0     3000.0
!KD-> C3H2+OH=C2H2+HCO       5.000E+13     0.0        0.0
!KD-> C3H2+CH2=IC4H3+H       3.000E+13     0.0        0.0
C4H8=IC4H7+H                 4.078E+18    -1.0    97350.0
C4H8=C2C4H8                  4.000E+11     0.0    60000.0
C4H8=T2C4H8                  4.000E+11     0.0    60000.0
C4H8=C3H5+CH3                1.000E+16     0.0    73000.0
C4H8=C2H3+C2H5               1.000E+19    -1.0    96770.0
C4H8+O2=IC4H7+HO2            4.000E+12     0.0    33200.0
C4H8+HO2=IC4H7+H2O2          1.000E+11     0.0    17060.0
C4H8+OH=NC3H7+CH2O           6.500E+12     0.0        0.0
C4H8+OH=CH3HCO+C2H5          1.000E+11     0.0        0.0
C4H8+OH=C2H6+CH3CO           1.000E+10     0.0        0.0
C4H8+OH=IC4H7+H2O            2.250E+13     0.0     2217.0
C4H8+O=C3H6+CH2O             2.505E+12     0.0        0.0
C4H8+O=CH3HCO+C2H4           1.250E+12     0.0      850.0
C4H8+O=C2H5+CH3CO            1.625E+13     0.0      850.0
```

```
C4H8+O=IC4H7+OH             9.600E+12     0.0     1970.0
C4H8+O=NC3H7+HCO            1.800E+05     2.5    -1029.0
C4H8+H=IC4H7+H2             5.000E+13     0.0     3900.0
C4H8+CH3=IC4H7+CH4          1.000E+11     0.0     7300.0
C4H8+C2H5=IC4H7+C2H6        1.000E+11     0.0     8000.0
C4H8+C3H5=IC4H7+C3H6        7.900E+10     0.0    12400.0
C4H8+SC3H5=IC4H7+C3H6       8.000E+10     0.0    12400.0
C4H8+TC3H5=IC4H7+C3H6       8.000E+10     0.0    12400.0
C2C4H8=T2C4H8               4.000E+13     0.0    62000.0
C2C4H8=C4H6+H2              1.000E+13     0.0    65500.0
C2C4H8=IC4H7+H              4.074E+18    -1.0    97350.0
C2C4H8=SC3H5+CH3            2.000E+16     0.0    95000.0
C2C4H8+OH=IC4H7+H2O         1.250E+14     0.0     3060.0
C2C4H8+OH=CH3HCO+C2H5       1.400E+13     0.0        0.0
C2C4H8+O=IC3H7+HCO          6.030E+12     0.0        0.0
C2C4H8+O=CH3HCO+C2H4        1.000E+12     0.0        0.0
C2C4H8+H=IC4H7+H2           1.000E+13     0.0     3500.0
C2C4H8+CH3=IC4H7+CH4        1.000E+11     0.0     8200.0
T2C4H8=IC4H7+H              4.074E+18    -1.0    97350.0
T2C4H8=SC3H5+CH3            2.000E+16     0.0    96000.0
T2C4H8+OH=IC4H7+H2O         1.000E+14     0.0     3060.0
T2C4H8+OH=CH3HCO+C2H5       1.500E+13     0.0        0.0
T2C4H8+O=IC3H7+HCO          6.030E+12     0.0        0.0
T2C4H8+O=CH3HCO+C2H4        1.000E+12     0.0        0.0
T2C4H8+H=IC4H7+H2           5.000E+12     0.0     3500.0
T2C4H8+CH3=IC4H7+CH4        1.000E+11     0.0     8200.0
IC4H7=C4H6+H                1.200E+14     0.0    49300.0
IC4H7=C2H4+C2H3             1.000E+14     0.0    49000.0
IC4H7+H=C4H6+H2             3.160E+12     0.0        0.0
IC4H7+O2=C4H6+HO2           1.000E+11     0.0        0.0
IC4H7+CH3=C4H6+CH4          1.000E+13     0.0        0.0
IC4H7+C2H3=C4H6+C2H4        4.000E+12     0.0        0.0
IC4H7+C2H5=C4H6+C2H6        4.000E+12     0.0        0.0
IC4H7+C2H5=C4H8+C2H4        5.000E+11     0.0        0.0
IC4H7+C2H5=T2C4H8+C2H4      5.000E+11     0.0        0.0
IC4H7+C2H5=C2C4H8+C2H4      5.000E+11     0.0        0.0
IC4H7+C3H5=C4H6+C3H6        4.000E+13     0.0        0.0
IC4H7+IC4H7=C4H6+C4H8       3.160E+12     0.0        0.0
C2H3+C2H4=C4H6+H            3.000E+12     0.0     1000.0
C4H6+H=NC4H5+H2             3.000E+07     2.0    13000.0
C4H6+H=IC4H5+H2             3.000E+07     2.0     6000.0
C4H6+OH=NC4H5+H2O           2.000E+07     2.0     5000.0
C4H6+OH=IC4H5+H2O           2.000E+07     2.0     2000.0
C4H6+O=C2H4+CH2CO           1.000E+12     0.0        0.0
C4H6+O=PC3H4+CH2O           1.000E+12     0.0        0.0
!KD-> C2H2+NC4H5=C6H6+H           2.800E+03     2.9     1400.0
NC4H5+OH=C4H4+H2O           2.000E+07     2.0     1000.0
NC4H5+H=C4H4+H2             3.000E+07     2.0     1000.0
NC4H5+H=IC4H5+H             1.000E+14     0.0        0.0
IC4H5=C4H4+H                2.000E+15     0.0    45000.0
NC4H5=C4H4+H                1.600E+14     0.0    41400.0
```

```
C4H4+OH=IC4H3+H2O            1.000E+07     2.0     2000.0
C4H4+OH=NC4H3+H2O            7.500E+06     2.0     5000.0
C4H4+H=NC4H3+H2              2.000E+07     2.0    15000.0
NC4H3+H=IC4H3+H              1.000E+14     0.0        0.0
IC4H3+CH2=C3H4+C2H           2.000E+13     0.0        0.0
IC4H3+O2=CH2CO+HCCO          1.000E+12     0.0        0.0
!KD-> IC4H3+OH=C4H2+H2O            3.000E+13     0.0        0.0
IC4H3+O=CH2CO+C2H            2.000E+13     0.0        0.0
!KD-> IC4H3+H=C4H2+H2              5.000E+13     0.0        0.0
!KD-> NC4H3+C2H2=C6H5              2.800E+03     2.9     1400.0
!KD-> NC4H3+M=C4H2+H+M             1.000E+16     0.0    59700.0
!KD->   H2O/16.0/   CO2/3.75/   CO/1.875/   H2/2.5/   CH4/3.0/   C3H6/16.0/   C2H4/16.0/
C3H8/16.0/
!KD-> IC4H3+M=C4H2+H+M             4.460E+15     0.0    46516.0
!KD->   H2O/16.0/   CO2/3.75/   CO/1.875/   H2/2.5/   CH4/3.0/   C3H6/16.0/   C2H4/16.0/
C3H8/16.0/
!KD-> IC4H3+O=H2C4O+H              2.000E+13     0.0        0.0
!KD-> H2C4O+H=C2H2+HCCO            5.000E+13     0.0     3000.0
!KD-> H2C4O+OH=CH2CO+HCCO          1.000E+07     2.0     2000.0
!KD-> C4H2+OH=H2C4O+H              6.660E+12     0.0     -410.0
C2H2+C2H2=IC4H3+H            2.200E+12     0.0    64060.0
C2H2+C2H2=NC4H3+H            1.000E+12     0.0    66000.0
C2H2+C2H2=C4H4               5.500E+12     0.0    37000.0
!KD-> C4H2(+M)=C4H+H(+M)           2.200E+14     0.0   116740.0
!KD->       LOW /3.50E+17  0.0  80065.0/
!KD->      H2O /16.0/ H2 /2.5/ CO /1.875/ CO2 /3.75/ CH4 /3.0/
!KD->      C3H6 /16.0/ C2H4 /16.0/ C3H8 /16.0/
!KD-> C4H2+O=C3H2+CO               2.700E+13     0.0     1720.0
!KD-> C2H2+C2H=C4H2+H              1.820E+14     0.0      467.0
C2H2+C2H=NC4H3               1.000E+13     0.0        0.0
!KD-> C4H+O2=C2H+CO+CO             1.000E+14     0.0        0.0
C2O+H=CH+CO                  1.320E+13     0.0        0.0
C2O+O=CO+CO                  5.200E+13     0.0        0.0
C2O+OH=CO+CO+H               2.000E+13     0.0        0.0
C2O+O2=CO+CO+O               2.000E+13     0.0        0.0
C2O+O2=CO+CO2                2.000E+13     0.0        0.0
!KD-> C2+H2=C2H+H                  6.600E+13     0.0     7950.0
!KD-> C2+O=C+CO                    3.600E+14     0.0        0.0
!KD-> C2+O2=CO+CO                  9.000E+12     0.0      980.0
!KD-> C2+OH=C2O+H                  5.000E+13     0.0        0.0
!KD-> C6H5+OH=C6H5O+H              5.000E+13     0.0        0.0
!KD-> C6H5+O2=C6H5O+O              2.600E+13     0.0     6120.0
!KD-> C6H5+HO2=C6H5O+OH            5.000E+13     0.0     1000.0
!KD-> C6H6+H=C6H5+H2               3.000E+12     0.0     8100.0
!KD-> C6H6+OH=C6H5+H2O             1.680E+08     1.42    1450.0
!KD-> C6H6+O=C6H5O+H               2.780E+13     0.0     4910.0
!KD-> C6H6+O2=C6H5O+OH             4.000E+13     0.0    34000.0
!KD-> H+C6H5=C6H6                  7.800E+13     0.0        0.0
C3H3+O=>C2H3+CO              3.800E+13     0.0        0.0
C3H3+O=CH2O+C2H              2.000E+13     0.0        0.0
C3H3+O2=>HCCO+CH2O           6.000E+12     0.0        0.0
```

```
C3H3+CH3=C2H5+C2H            1.000E+13     0.0    37500.0
C3H3+CH3=C4H6               5.000E+12     0.0        0.0
C3H6+C2H3=C3H5+C2H4          2.210E+00     3.5     4680.0
C3H6+C2H3=SC3H5+C2H4         1.350E+00     3.5    10860.0
C3H6+C2H3=TC3H5+C2H4         8.400E-01     3.5     9670.0
C3H6+CH3O=C3H5+CH3OH         9.000E+01     2.95   12000.0
CH2+C2H2=C3H4               1.200E+13     0.0     6620.0
C3H4+C3H4=C3H5+C3H3          5.000E+14     0.0    64700.0
C3H4+OH=CH2O+C2H3            1.700E+12     0.0     -300.0
C3H4+OH=HCO+C2H4             1.700E+12     0.0     -300.0
C3H4+O=CH2O+C2H2             1.000E+12     0.0        0.0
C3H4+O=>CO+C2H4              7.800E+12     0.0     1600.0
C3H4+C3H5=C3H3+C3H6          2.000E+12     0.0     7700.0
C3H4+C2H=C3H3+C2H2           1.000E+13     0.0        0.0
PC3H4=C2H+CH3               4.200E+16     0.0   100000.0
PC3H4+C2H=C3H3+C2H2          1.000E+13     0.0        0.0
!KD-> C3H2+O2=HCO+HCCO            1.000E+13     0.0        0.0
C2H2+C2H3=NC4H5             2.510E+05     1.9     2100.0
C2H3+C2H3=IC4H5+H            4.000E+13     0.0        0.0
IC4H5+H=C4H4+H2             3.000E+07     2.0     1000.0
!KD-> C4H2+H=C4H+H2              1.000E+14     0.0    35000.0
C4H6+OH=C3H5+CH2O            7.230E+12     0.0     -994.0
C4H8+IC4H7=IC4H7+C2C4H8       3.980E+10     0.0    12400.0
C4H8+IC4H7=IC4H7+T2C4H8       3.980E+10     0.0    12400.0
!KD-> C3H3+C3H3=C6H6             3.000E+11     0.0        0.0
!KD-> C3H3+C3H4=C6H6+H            1.400E+12     0.0    10000.0
C3H5+C2H5=C3H6+C2H4          2.600E+12     0.0     -130.0
C3H6+OH=C2H5+CH2O            8.000E+12     0.0        0.0
C3H6+OH=CH3+CH3HCO           3.400E+11     0.0        0.0
C3H5+O2=C3H4+HO2             1.200E+12     0.0    13550.0
CH2O+C3H5=HCO+C3H6           8.000E+10     0.0    12400.0
CH3HCO+C3H5=CH3CO+C3H6        3.800E+11     0.0     7200.0
C3H8+CH3O2=NC3H7+CH3O2H       6.030E+12     0.0    19380.0
C3H8+CH3O2=IC3H7+CH3O2H       1.990E+12     0.0    17050.0
!KD-> C3H8+C2H5O2=NC3H7+C2H5O2H     6.030E+12     0.0    19380.0
!KD-> C3H8+C2H5O2=IC3H7+C2H5O2H     1.990E+12     0.0    17050.0
!KD-> C3H8+IC3H7O2=NC3H7+IC3H7O2H   6.030E+12     0.0    19380.0
!KD-> C3H8+IC3H7O2=IC3H7+IC3H7O2H   1.990E+12     0.0    17050.0
!KD-> C3H8+NC3H7O2=NC3H7+NC3H7O2H   6.030E+12     0.0    19380.0
!KD-> C3H8+NC3H7O2=IC3H7+NC3H7O2H   1.990E+12     0.0    17050.0
!KD-> NC3H7+O2=NC3H7O2            4.820E+12     0.0        0.0
!KD-> IC3H7+O2=IC3H7O2            6.620E+12     0.0        0.0
!KD-> NC3H7+HO2=NC3H7O+OH          3.200E+13     0.0        0.0
!KD-> IC3H7+HO2=IC3H7O+OH          3.200E+13     0.0        0.0
!KD-> NC3H7+CH3O2=NC3H7O+CH3O      3.800E+12     0.0    -1200.0
!KD-> IC3H7+CH3O2=IC3H7O+CH3O      3.800E+12     0.0    -1200.0
!KD-> NC3H7+NC3H7O2=NC3H7O+NC3H7O   3.800E+12     0.0    -1200.0
!KD-> IC3H7+NC3H7O2=IC3H7O+NC3H7O   3.800E+12     0.0    -1200.0
!KD-> NC3H7+IC3H7O2=NC3H7O+IC3H7O   3.800E+12     0.0    -1200.0
!KD-> IC3H7+IC3H7O2=IC3H7O+IC3H7O   3.800E+12     0.0    -1200.0
!KD-> NC3H7O2+HO2=NC3H7O2H+O2      4.600E+10     0.0    -2600.0
```

```
!KD-> IC3H7O2+HO2=IC3H7O2H+O2       4.600E+10     0.0     -2600.0
!KD-> CH3+NC3H7O2=CH3O+NC3H7O       3.800E+12     0.0     -1200.0
!KD-> CH3+IC3H7O2=CH3O+IC3H7O       3.800E+12     0.0     -1200.0
!KD-> NC3H7O2H=NC3H7O+OH            4.000E+15     0.0     43000.0
!KD-> IC3H7O2H=IC3H7O+OH            4.000E+15     0.0     43000.0
!KD-> NC3H7O=C2H5+CH2O              5.000E+13     0.0     15700.0
!KD-> IC3H7O=CH3+CH3HCO             4.000E+14     0.0     17200.0
!KD-> C3H6+OH(+M)=C3H6OH(+M)        1.810E+13     0.0         0.0
!KD->     LOW /1.33E+30  -3.5  0.0/
!KD-> C3H6OH=>C2H5+CH2O             1.400E+09     0.0     17200.0
!KD-> C3H6OH=>CH3+CH3HCO            1.000E+09     0.0     17200.0
!KD-> C3H6OH+O2=O2C3H6OH            1.000E+12     0.0     -1100.0
!KD-> O2C3H6OH=>CH3HCO+CH2O+OH      1.000E+16     0.0     25000.0
C3H6+CH3O2=C3H5+CH3O2H        2.000E+12     0.0     17000.0
!KD-> C3H6+CH3O2=C3H6O+CH3O         4.000E+11     0.0     11720.0
!KD-> C3H6+C2H5O2=C3H5+C2H5O2H      3.200E+11     0.0     14900.0
!KD-> C3H6+C3H5O2=C3H5+C3H5O2H      3.200E+11     0.0     14900.0
!KD-> C3H6+C3H5O2=C3H6O+C3H5O       1.050E+11     0.0     14200.0
!KD-> C3H6+CH3CO3=C3H5+CH3CO3H      3.200E+11     0.0     14900.0
!KD-> C3H6+NC3H7O2=C3H5+NC3H7O2H    3.200E+11     0.0     14900.0
!KD-> C3H6+IC3H7O2=C3H5+IC3H7O2H    3.200E+11     0.0     14900.0
!KD-> C3H6+NC3H7O2=C3H6O+NC3H7O     1.700E+07     0.0         0.0
!KD-> C3H5+O2=C3H5O2                1.200E+10     0.0     -2300.0
C3H5+HO2=C3H5O+OH             9.000E+12     0.0         0.0
C3H5+CH3O2=C3H5O+CH3O         3.800E+11     0.0     -1200.0
!KD-> C3H5O2+CH3=C3H5O+CH3O         3.800E+11     0.0     -1200.0
!KD-> C3H5O2+C3H5=C3H5O+C3H5O       3.800E+11     0.0     -1200.0
!KD-> C3H5O2+HO2=C3H5O2H+O2         4.600E+10     0.0     -2600.0
!KD-> C3H5O2+HO2=>C3H5O+OH+O2       1.000E+12     0.0         0.0
!KD-> C3H5O2+CH3O2=>C3H5O+CH3O+O2   1.700E+11     0.0     -1000.0
!KD-> C3H5O2+C3H5O2=>C3H5O+C3H5O+O2 3.700E+12     0.0      2200.0
C3H5O=CH2O+C2H3               1.000E+14     0.0     21600.0
!KD-> C3H5O2H=C3H5O+OH              4.000E+15     0.0     43000.0
!KD-> CH2O+C3H5O2=HCO+C3H5O2H       1.300E+11     0.0     10500.0
!KD-> CH2O+NC3H7O2=HCO+NC3H7O2H     1.300E+11     0.0      9000.0
!KD-> CH2O+IC3H7O2=HCO+IC3H7O2H     1.300E+11     0.0      9000.0
!KD-> C2H4+NC3H7O2=C2H3+NC3H7O2H    7.100E+11     0.0     25000.0
!KD-> C2H4+IC3H7O2=C2H3+IC3H7O2H    7.100E+11     0.0     25000.0
!KD-> CH4+C3H5O2=CH3+C3H5O2H        1.140E+13     0.0     20460.0
!KD-> CH4+NC3H7O2=CH3+NC3H7O2H      1.140E+13     0.0     20460.0
!KD-> CH4+IC3H7O2=CH3+IC3H7O2H      1.140E+13     0.0     20460.0
!KD-> CH3OH+NC3H7O2=CH2OH+NC3H7O2H   6.300E+12     0.0     19360.0
!KD-> CH3OH+IC3H7O2=CH2OH+IC3H7O2H   6.300E+12     0.0     19360.0
!KD-> CH3HCO+C3H5O2=CH3CO+C3H5O2H    1.150E+11     0.0     10000.0
!KD-> CH3HCO+NC3H7O2=CH3CO+NC3H7O2H  1.150E+11     0.0     10000.0
!KD-> CH3HCO+IC3H7O2=CH3CO+IC3H7O2H  1.150E+11     0.0     10000.0
!KD-> C+N2+M=CNN+M                  1.120E+15     0.0         0.0
C2H+NO=HCN+CO                 6.000E+13     0.0       570.0
C2H+HCN=CN+C2H2               3.200E+12     0.0      1530.0
CH2+NO=HCN+OH                 5.000E+11     0.0      2870.0
HCN+M=H+CN+M                  3.570E+26    -2.6    124900.0
```

```
!KD-> C2N2+M=CN+CN+M              3.200E+16     0.0    94400.0
!KD-> CH+N2(+M)=HCNN(+M)          3.100E+12     0.15      0.0
!KD->     LOW / 1.30E+25 -3.16 740.0 /
!KD->     TROE /0.667 235.0 2117.0 4536.0 /
!KD->     H2O/10.0/ O2/2.0/ AR/0.75/ H2/2.0/
!KD-> HCNN+H=H2+CNN               5.000E+13     0.0       0.0
!KD-> HCNN+H=>CH2+N2              2.000E+13     0.0    3000.0
!KD-> HCNN+O=OH+CNN               2.000E+13     0.0    20000.0
!KD-> HCNN+O=CO+H+N2              5.000E+13     0.0    15000.0
!KD-> HCNN+O=HCN+NO               5.000E+13     0.0    15000.0
!KD-> HCNN+OH=H2O+CNN             1.000E+13     0.0     8000.0
!KD-> HCNN+OH=H+HCO+N2            1.000E+13     0.0    16000.0
!KD-> HCNN+O2=HO2+CNN             1.000E+12     0.0     4000.0
!KD-> HCNN+O2=>H+CO2+N2           4.000E+12     0.0       0.0
!KD-> HCNN+O2=HCO+N2O             4.000E+12     0.0       0.0
!KD-> CNN+O=CO+N2                 1.000E+13     0.0       0.0
!KD-> CNN+O=CN+NO                 1.000E+14     0.0    20000.0
!KD-> CNN+OH=H+CO+N2              1.000E+13     0.0     1000.0
!KD-> CNN+H=NH+CN                 5.000E+14     0.0    40000.0
!KD-> CNN+OH=HCN+NO               1.000E+12     0.0     1000.0
!KD-> CNN+H=HCN+N                 5.000E+13     0.0    25000.0
!KD-> CNN+O2=NO+NCO               1.000E+13     0.0     5000.0
HNO+CH3=NO+CH4                8.200E+05     1.87     954.0
HONO+CH3=NO2+CH4              8.100E+05     1.87    5504.0
H2NO+CH3=CH3O+NH2             2.000E+13     0.0       0.0
H2NO+CH3=HNO+CH4              1.600E+06     1.87    2960.0
HNOH+CH3=HNO+CH4              1.600E+06     1.87    2096.0
NH2OH+CH3=HNOH+CH4            1.600E+06     1.87    6350.0
NH2OH+CH3=H2NO+CH4            8.200E+05     1.87    5500.0
N2H2+CH3=NNH+CH4              1.600E+06     1.87    2970.0
N2H3+CH3=N2H2+CH4             8.200E+05     1.87    1818.0
N2H4+CH3=N2H3+CH4             3.300E+06     1.87    5325.0
CH4+NH=CH3+NH2                9.000E+13     0.0    20080.0
CH4+NH2=CH3+NH3               1.200E+13     0.0    15150.0
CH3+NH2=CH2+NH3               1.600E+06     1.87    7570.0
C2H6+NH=C2H5+NH2              7.000E+13     0.0    16700.0
C2H6+NH2=C2H5+NH3             9.700E+12     0.0    11470.0
C3H8+NH2=NC3H7+NH3            1.700E+13     0.0    10660.0
C3H8+NH2=IC3H7+NH3            4.500E+11     0.0     6150.0
!KD-> CH3+NO(+M)=CH3NO(+M)        1.000E+13     0.0       0.0
!KD->    LOW /1.90E+18 0.0 0.0/
!KD->    SRI /0.03 -790.0 1.0/
!KD-> CH3NO+H=H2CNO+H2            4.400E+08     1.5      377.0
!KD-> CH3NO+H=CH3+HNO             1.800E+13     0.0     2800.0
!KD-> CH3NO+O=H2CNO+OH            3.300E+08     1.5     3615.0
!KD-> CH3NO+O=CH3+NO2             1.700E+06     2.08      0.0
!KD-> CH3NO+OH=H2CNO+H2O          3.600E+06     2.0    -1192.0
!KD-> CH3NO+OH=CH3+HONO           2.500E+12     0.0     1000.0
!KD-> CH3NO+CH3=H2CNO+CH4         7.900E+05     1.87    5415.0
!KD-> CH3NO+NH2=H2CNO+NH3         2.800E+06     1.94    1073.0
!KD-> H2CNO=HNCO+H                2.300E+42    -9.11   53840.0
```

```
!KD-> H2CNO+O2=CH2O+NO2           2.900E+12    -0.31    17700.0
!KD-> H2CNO+H=CH3+NO            4.000E+13     0.0        0.0
!KD-> H2CNO+H=HCNO+H2             4.800E+08     1.5      -894.0
!KD-> H2CNO+O=HCNO+OH             3.300E+08     1.5      -894.0
!KD-> H2CNO+O=CH2O+NO             7.000E+13     0.0        0.0
!KD-> H2CNO+OH=CH2OH+NO           4.000E+13     0.0        0.0
!KD-> H2CNO+OH=HCNO+H2O           2.400E+06     2.0     -1192.0
!KD-> H2CNO+CH3=C2H5+NO           3.000E+13     0.0        0.0
!KD-> H2CNO+CH3=HCNO+CH4          1.600E+06     1.87    -1113.0
!KD-> H2CNO+NH2=HCNO+NH3          1.800E+06     1.94    -1152.0
CH3+NO2=CH3O+NO             1.400E+13     0.0        0.0
CH+NO2=HCO+NO               1.200E+14     0.0        0.0
CH2+NO2=CH2O+NO             4.200E+13     0.0        0.0
CN+NO=N2+CO                 1.000E+11     0.0        0.0
HNCO+M=H+NCO+M              5.000E+15     0.0    120000.0
HNCO+N=NH+NCO               4.000E+13     0.0    36000.0
CH3O+HNO=CH3OH+NO           3.160E+13     0.0        0.0
NCO+HO2=HNCO+O2             2.000E+13     0.0        0.0
N2O+CO=CO2+N2               2.510E+14     0.0    46000.0
N2O+CH2=CH2O+N2             1.000E+12     0.0        0.0
N2O+CH3=CH3O+N2             9.000E+09     0.0        0.0
N2O+HCO=CO2+H+N2            1.700E+14     0.0    20000.0
N2O+HCCO=CO+HCO+N2          1.700E+14     0.0    25500.0
N2O+C2H2=HCCO+H+N2          6.590E+16     0.0    61200.0
N2O+C2H3=CH2HCO+N2          1.000E+11     0.0        0.0
HOCN+O=NCO+OH               1.500E+04     2.64     4000.0
HOCN+H=NCO+H2               2.000E+07     2.0      2000.0
HOCN+H=NH2+CO               1.200E+08     0.61     2080.0
HOCN+OH=NCO+H2O             6.380E+05     2.0      2560.0
HOCN+CH3=NCO+CH4            8.200E+05     1.87     6620.0
HOCN+NH2=NCO+NH3            9.200E+05     1.94     3645.0
CN+NO2=CO+N2O               4.930E+14    -0.752    344.0
CN+NO2=CO2+N2               3.700E+14    -0.752    344.0
CN+CO2=NCO+CO               3.670E+06     2.16    26900.0
CN+NH3=HCN+NH2              9.200E+12     0.0     -357.0
HNCO+CN=HCN+NCO             1.500E+13     0.0        0.0
HONO+NCO=HNCO+NO2           3.600E+12     0.0        0.0
NCO+CH2O=HNCO+HCO           6.000E+12     0.0        0.0
!CH+N2=HCN+N                3.680E+07     1.42    20723.0
!KD-> NH2+C=CH+NH           5.800E+11     0.67    20900.0
!KD-> C+N2=CN+N             5.200E+13     0.0    44700.0
CH2+N2=HCN+NH               4.800E+12     0.0    35850.0
!KD-> C2+N2=CN+CN           1.500E+13     0.0    41700.0
H2CN+N=N2+CH2               6.000E+13     0.0      400.0
H2CN+H=HCN+H2               2.400E+08     1.5      -894.0
H2CN+O=HCN+OH               1.700E+08     1.5      -894.0
H2CN+O=HNCO+H               6.000E+13     0.0        0.0
H2CN+O=HCNO+H               2.000E+13     0.0        0.0
H2CN+M=HCN+H+M              3.000E+14     0.0    22000.0
H2CN+HO2=HCN+H2O2           1.400E+04     2.69    -1610.0
H2CN+O2=CH2O+NO             3.000E+12     0.0     6000.0
```

```
H2CN+CH3=HCN+CH4            8.100E+05     1.87    -1113.0
H2CN+OH=HCN+H2O             1.200E+06     2.0     -1192.0
H2CN+NH2=HCN+NH3             9.200E+05     1.94    -1152.0
!KD-> C+NO=CN+O               2.000E+13     0.0       0.0
CH+NO=HCN+O              8.690E+13     0.0       0.0
CH+NO=CN+OH              1.680E+12     0.0       0.0
CH+NO=CO+NH              9.840E+12     0.0       0.0
CH+NO=NCO+H              1.670E+13     0.0       0.0
CH2+NO=HNCO+H              2.500E+12     0.0     5970.0
CH2+NO=HCNO+H              3.800E+13    -0.36     576.0
CH2+NO=NH2+CO              2.300E+16    -1.43    1331.0
CH2+NO=H2CN+O              8.100E+07     1.42    4110.0
CH3+NO=HCN+H2O              2.400E+12     0.0    15700.0
CH3+NO=H2CN+OH              5.200E+12     0.0    24240.0
HCCO+NO=HCNO+CO              4.640E+13     0.0      700.0
HCCO+NO=HCN+CO2              1.390E+13     0.0      700.0
SCH2+NO=HCN+OH              1.000E+14     0.0       0.0
HCNO=HCN+O              4.200E+31    -6.12   61210.0
HCNO+H=HCN+OH              1.000E+14     0.0    12000.0
HCNO+H=HNCO+H              2.100E+15    -0.69    2850.0
HCNO+H=HOCN+H              1.400E+11    -0.19    2484.0
HCNO+H=NH2+CO              1.700E+14    -0.75    2890.0
HCNO+O=HCO+NO              7.000E+13     0.0       0.0
CH2+N=HCN+H              5.000E+13     0.0       0.0
CH2+N=NH+CH              6.000E+11     0.67   40500.0
CH+N=CN+H              1.670E+14    -0.09      0.0
!KD-> CH+N=C+NH              4.500E+11     0.65    2400.0
N+CO2=NO+CO              1.900E+11     0.0     3400.0
N+HCCO=HCN+CO              5.000E+13     0.0       0.0
CH3+N=H2CN+H              7.100E+13     0.0       0.0
!KD-> CH3+N=HCNH+H              1.200E+11     0.52     367.6
!KD-> HCNH=HCN+H              6.100E+28    -5.69   24270.0
!KD-> HCNH+H=H2CN+H              2.000E+13     0.0       0.0
!KD-> HCNH+H=HCN+H2              2.400E+08     1.5     -894.0
!KD-> HCNH+O=HNCO+H              7.000E+13     0.0       0.0
!KD-> HCNH+O=HCN+OH              1.700E+08     1.5     -894.0
!KD-> HCNH+OH=HCN+H2O             1.200E+06     2.0    -1192.0
!KD-> HCNH+CH3=HCN+CH4             8.200E+05     1.87   -1113.0
C2H3+N=HCN+CH2              2.000E+13     0.0       0.0
CN+H2O=HCN+OH              4.000E+12     0.0     7400.0
CN+H2O=HOCN+H              4.000E+12     0.0     7400.0
OH+HCN=HOCN+H              3.200E+04     2.45    12120.0
OH+HCN=HNCO+H              5.600E-06     4.71    -490.0
OH+HCN=NH2+CO              6.440E+10     0.0    11700.0
HOCN+H=HNCO+H              1.000E+13     0.0       0.0
HCN+O=NCO+H              1.380E+04     2.64    4980.0
HCN+O=NH+CO              3.450E+03     2.64    4980.0
HCN+O=CN+OH              2.700E+09     1.58   26600.0
CN+H2=HCN+H              2.000E+04     2.87    1600.0
CN+O=CO+N              1.900E+12     0.46     720.0
CN+O2=NCO+O              7.200E+12     0.0     -400.0
```

```
CN+OH=NCO+H                 4.000E+13     0.0        0.0
!KD-> CN+HCN=C2N2+H             1.510E+07     1.71     1530.0
CN+NO2=NCO+NO               5.320E+15    -0.752    344.0
CN+N2O=NCO+N2              6.000E+12     0.0     15360.0
!KD-> C2N2+O=NCO+CN             4.570E+12     0.0     8880.0
!KD-> C2N2+OH=HNCO+CN             1.860E+11     0.0     2900.0
!KD-> C2N2+OH=HOCN+CN             2.000E+12     0.0    19000.0
HNCO+H=H2+NCO              1.760E+05     2.41    12300.0
HNCO+H=NH2+CO              3.600E+04     2.49     2340.0
HNCO+M=NH+CO+M               1.100E+16     0.0     86000.0
N2/1.5/ O2/1.5/ H2O/18.6/
HNCO+O=NCO+OH               2.200E+06     2.11    11430.0
HNCO+O=NH+CO2              9.800E+07     1.41     8530.0
HNCO+O=HNO+CO               1.500E+08     1.57    44012.0
HNCO+OH=NCO+H2O              3.450E+07     1.5      3600.0
HNCO+OH=NH2+CO2             6.300E+10    -0.06    11645.0
HNCO+HO2=NCO+H2O2             3.000E+11     0.0     29000.0
HNCO+O2=HNO+CO2             1.000E+12     0.0     35000.0
HNCO+NH2=NCO+NH3             5.000E+12     0.0      6200.0
HNCO+NH=NCO+NH2             1.040E+15     0.0     39390.0
NCO+H=NH+CO                 5.360E+13     0.0        0.0
NCO+O=NO+CO                 4.200E+13     0.0        0.0
NCO+O=N+CO2                8.000E+12     0.0      2500.0
NCO+N=N2+CO                2.000E+13     0.0        0.0
NCO+OH=NO+HCO               5.000E+12     0.0     15000.0
NCO+M=N+CO+M               2.200E+14     0.0     54050.0
NCO+NO=N2O+CO              4.600E+18    -2.01      934.0
NCO+NO=N2+CO2             5.800E+18    -2.01      934.0
NCO+O2=NO+CO2              2.000E+12     0.0     20000.0
NCO+HCO=HNCO+CO              3.600E+13     0.0        0.0
NCO+NO2=CO+NO+NO              2.830E+13    -0.646    -326.0
NCO+NO2=CO2+N2O             3.570E+14    -0.646    -326.0
NCO+HNO=HNCO+NO              1.800E+13     0.0        0.0
NCO+NCO=CO+CO+N2             3.000E+12     0.0        0.0
NO+HCO=CO+HNO               7.240E+13    -0.4        0.0
NO2+CO=CO2+NO              9.000E+13     0.0     33800.0
NO2+HCO=H+CO2+NO             8.400E+15    -0.75     1930.0
CH3O+NO2=HONO+CH2O            3.000E+12     0.0        0.0
CH3O+NO=CH2O+HNO             1.300E+14    -0.7        0.0
NO2+CH2O=HONO+HCO             1.000E+10     0.0     15100.0
NO+CH2O=HNO+HCO              1.000E+13     0.0     40820.0
NO2+HCO=HONO+CO              1.000E+13     0.0        0.0
NO2+HCO=OH+NO+CO              1.000E+14     0.0        0.0
NCO+N=NO+CN                2.700E+18    -0.995   17200.0
CN+CH4=HCN+CH3              9.000E+04     2.64     -300.0
!KD-> C+NO=CO+N              2.800E+13     0.0        0.0
NH+CO2=HNO+CO              1.000E+13     0.0     14350.0
NCO+CH4=HNCO+CH3             1.000E+13     0.0      8130.0
!KD-> C+N2O=CN+NO              4.800E+12     0.0        0.0
CH+NH2=HCN+H+H              3.000E+13     0.0        0.0
CH+NH=HCN+H                5.000E+13     0.0        0.0
```

```
CH2+NH=HCN+H+H          3.000E+13    0.0       0.0
CH3+N=HCN+H+H           2.000E+11    0.0       0.0
CH3+N=HCN+H2            7.100E+12    0.0       0.0
CH4+N=NH+CH3            1.000E+13    0.0   24000.0
C3H3+N=HCN+C2H2         1.000E+13    0.0       0.0
CH+N2O=HCN+NO           1.340E+13    0.0    -510.0
CH+N2O=CO+H+N2          5.200E+12    0.0    -510.0
C2O+N2=>NCO+CN          7.000E+11    0.0   17000.0
END
```

Mech.2

```
ELEM H C O N AR
END
SPECIES
!KD->  C2H4O C2 C2O C CH3CO3
!KD->  CH3CO3H CH3O2H C2H5O2H C2H5O2 CH3CO2
!KD->  CH3CO2H N2O3 C2N2 NO3 HNO3
!KD->  CNN HCNN N2O4 NH2OH HNNO
!KD->  HCNH NCN HNCN H2CNO CH3NO
!KD->  CH2CHOW C2H3O CH3HCOW C3H6OH O2C3H6OH
!KD->  C3H5O2 C3H5O2H NC3H7O2 NC3H7O2H IC3H7O2
!KD->  IC3H7O2H IC3H7O NC3H7O C3H2 C3H6O
!KD->  C2H5CHO C2H5CO C4H2 C4H H2C4O
!KD->  NC4H5 T2C4H8 C2C4H8 NC4H3 C6H6
!KD->  C6H5O C6H5 AR
H H2 O O2 OH
HO2 H2O H2O2 CO CO2
HCO CH3 CH4 C2H6 CH2O
C2H5 CH2 CH3O CH2OH CH
C2H2 C2H4 C2H3 CH3OH CH3HCO
C2H CH2CO HCCO SCH2 CH3CO
CH3O2 C2H5OH C2H5O SC2H5O PC2H5O
CH2HCO CN H2CN N NH
HCN NO HCNO HOCN HNCO
NCO N2O NH2 HNO NO2
NNH NH3 N2H2 HONO N2H3
N2H4 HNOH H2NO C3H5O C3H6
C3H8 IC3H7 NC3H7 C3H3 SC3H5
PC3H4 TC3H5 C3H5 C3H4 IC4H7
C4H6 C4H4 IC4H5 C4H8 IC4H3
N2
END
```

REACTIONS, A_i ((cm^3/mol)$^{(r-1)}$/s), β_i, E_i (cal/mol)

```
! CH + N2 = HCN + N     3.68E+05 1.42 20723
!KD-> CH+N2=NCN+H              3.00E+12     0.0    22157.
!KD-> CN+N2O=NCN+NO            6.000E+13    0.0    15360.0
!KD->     DUPLICATE
!KD-> CN+N2O=NCN+NO            1.800E+10    0.0     1450.0
!KD->     DUPLICATE
```

```
!KD-> CN + NCO = NCN + CO          1.800E+13      0          0
!KD-> C2O + N2 = NCN + CO          7.00E+11       0      17000
!KD-> CH + N2 = HNCN               1.65E+21     -3.62    14196
!KD-> HNCN + M = H + NCN + M        1.79E+28     -3.44    64502
!KD-> HNCN + O = NO + HCN          1.22E+14      0.05      73.5
!KD-> HNCN + O = NH + NCO          5.60E+13      0.05      73.5
!KD-> HNCN + O = CN + HNO          9.36E+12      0.05      73.5
!KD-> HNCN + OH = NCN + H2O        8.28E+03      2.78     3135
!KD-> HNCN + O2 = HO2 + NCN        1.26E+08      1.28    24240
!KD-> NCN = N + CN                2.95E+30     -5.29   117090
!KD-> NCN = C + N2                2.66E+28     -5.32    83110
!KD-> NCN = CNN                   3.69E+29     -5.84    78410
!KD-> NCN + H = HCN +N            1.89E+14      0       8425
!KD-> NCN + O = CN + NO           2.54E+13      0.15      -34
!KD-> NCN + O = CO + N2           2.42E+02      2.32    -1135
!KD-> NCN + O = N + NCO           2.20E+09      0.42     -157
!KD-> NCN + N= N2 + CN            1.00E+13      0          0
!KD-> NCN + C = CN +CN            1.00E+13      0          0
!KD-> NCN + OH = HCN + NO          3.32E+10     -0.97     7290.
!KD->    DUPLICATE
!KD-> NCN + OH = HCN + NO          4.69E+10      0.44     4000.
!KD-> DUPLICATE
!KD-> NCN + O2 = NO + NCO          3.80E+09      0.51    24590
!KD-> NCN + CH = HCN +CN           3.21E+13      0        -860
!KD-> NCN + CN = C2N2 +N           1.25E+14      0        8020
!KD-> NCN + CH2 = H2CN + CN         7.99E+13      0        4630
H+H+M=H2+M                  7.000E+17    -1.0        0.0
H2/0.0/ N2/0.0/ H/0.0/ H2O/14.3/ CO/3.0/ CO2/3.0/
H+H+H2=H2+H2                1.000E+17    -0.6        0.0
H+H+N2=H2+N2                5.400E+18    -1.3        0.0
H+H+H=H2+H                 3.200E+15     0.0        0.0
O+O+M=O2+M                  1.000E+17    -1.0        0.0
O/71.0/ O2/20.0/ NO/5.0/ N2/5.0/ N/5.0/ H2O/5.0/
O+H+M=OH+M                  6.200E+16    -0.6        0.0
H2O/5.0/
H2+O2=OH+OH                 2.500E+12     0.0    39000.0
O+H2=OH+H                  5.060E+04     2.67     6290.0
H+O2=OH+O                  9.750E+13     0.0    14850.0
H+O2(+M)=HO2(+M)              1.480E+12     0.6        0.0
LOW /3.50E+16 -0.41 -1116.0/
TROE /0.5 100000 10/
!KD->  AR/0.0/ H2O/10.6/ H2/1.5/ CO2/2.4/
H2O/10.6/ H2/1.5/ CO2/2.4/
!KD-> H+O2(+AR)=HO2(+AR)           1.480E+12     0.6        0.0
!KD->    LOW /7.00E+17 -0.8  0.0/
!KD->    TROE /0.45 10 100000/
H+OH+M=H2O+M                2.200E+22    -2.0        0.0
!KD->  H2O/6.4/ AR/0.38/ CO2/1.9/
H2O/6.4/        CO2/1.9/
H2+OH=H2O+H                 1.000E+08     1.6     3300.0
OH+OH=H2O+O                 1.500E+09     1.14     100.0
```

```
HO2+OH=H2O+O2              2.890E+13    0.0     -500.0
HO2+O=OH+O2                1.630E+13    0.0     -445.0
H+HO2=H2+O2                4.280E+13    0.0     1411.0
H+HO2=OH+OH                1.700E+14    0.0      875.0
H+HO2=H2O+O                3.000E+13    0.0     1720.0
HO2+HO2=H2O2+O2            4.200E+14    0.0    12000.0
DUPLICATE
HO2+HO2=H2O2+O2            1.300E+11    0.0    -1640.0
DUPLICATE
OH+OH(+M)=H2O2(+M)         7.200E+13   -0.37       0.0
LOW /2.2E+19 -0.76 0.0/
TROE /0.5 100000 10/
H2O/0.0/
OH+OH(+H2O)=H2O2(+H2O)     7.200E+13   -0.37       0.0
LOW /1.45E+18 0.0 0.0/
H2O2+OH=HO2+H2O            1.000E+12    0.0        0.0
DUPLICATE
H2O2+OH=HO2+H2O            5.800E+14    0.0     9560.0
DUPLICATE
H2O2+H=HO2+H2              1.700E+12    0.0     3755.0
H2O2+H=H2O+OH              1.000E+13    0.0     3575.0
H2O2+O=HO2+OH              2.800E+13    0.0     6400.0
N2+O=NO+N                  1.800E+14    0.0    76100.0
N+O2=NO+O                  9.000E+09    1.0     6500.0
NO+M=N+O+M                 9.640E+14    0.0   148300.0
N2 /1.5/ NO /3.0/ CO2/2.5/
NO+NO=N2+O2                3.000E+11    0.0    65000.0
N2O(+M)=N2+O(+M)           1.260E+12    0.0    62620.0
LOW / 4.000E+14 0.0 56640.0/
O2/1.4/ N2/1.7/ H2O/12.0/ NO/3.0/ N2O/3.5/
N2O+O=N2+O2                1.000E+14    0.0    28200.0
N2O+O=NO+NO                6.920E+13    0.0    26630.0
N2O+N=N2+NO                1.000E+13    0.0    20000.0
N2O+NO=N2+NO2              2.750E+14    0.0    50000.0
NO+O(+M)=NO2(+M)           1.300E+15   -0.75       0.0
LOW /4.72E+24 -2.87 1551.0/
TROE /0.962 10.0 7962.0 /
!KD->    AR /0.6/ NO2 /6.2/ NO /1.8/ O2 /0.8/ N2O /4.4/ CO2/0/
NO2 /6.2/ NO /1.8/ O2 /0.8/ N2O /4.4/ CO2/0/
H2O /10.0/
NO+O(+CO2)=NO2(+CO2)       1.300E+15   -0.75       0.0
LOW /4.0E+22 -2.16 1051.0/
TROE /0.962 10.0 7962.0 /
NO2+O=NO+O2                3.910E+12    0.0     -238.0
NO2+N=N2O+O                8.400E+11    0.0        0.0
NO2+N=NO+NO                1.000E+12    0.0        0.0
NO2+NO=N2O+O2              1.000E+12    0.0    60000.0
NO2+NO2=NO+NO+O2           3.950E+12    0.0    27590.0
!KD-> NO2+NO2=NO3+NO            1.130E+04    2.58   22720.0
!KD-> NO2+O(+M)=NO3(+M)         1.330E+13    0.0       0.0
!KD->    LOW / 1.49E+28 -4.08 2467.0 /
```

```
!KD->    TROE /0.86 10.0 2800.0 /
!KD->    H2O/10.0/ O2/0.8/ H2/2.0/ CO2 /0/
!KD-> NO2+O(+CO2)=NO3(+CO2)        1.330E+13     0.0        0.0
!KD->    LOW / 1.34E+28 -3.94 2277.0 /
!KD->    TROE /0.86 10.0 2800.0 /
!KD-> NO3=NO+O2                  2.500E+06     0.0    12120.0
!KD-> NO3+NO2=NO+NO2+O2           1.200E+11     0.0     3200.0
!KD-> NO3+O=NO2+O2               1.020E+13     0.0        0.0
!KD-> NO3+NO3=NO2+NO2+O2          5.120E+11     0.0     4870.0
!KD-> N2O4(+M)=NO2+NO2(+M)        4.050E+18    -1.1    12840.0
!KD->     LOW /1.96E+28  -3.8  12840./
!KD->     AR/0.8/ N2O4/2.0/ NO2/2.0/
!KD-> N2O4+O=N2O3+O2              1.210E+12     0.0        0.0
!KD-> NO2+NO(+M)=N2O3(+M)         1.600E+09     1.4        0.0
!KD->     LOW /1.0E+33  -7.7  0.0/
!KD->     N2/1.36/
!KD-> N2O3+O=NO2+NO2              2.710E+11     0.0        0.0
N2+M=N+N+M                 1.000E+28    -3.33   225000.0
N/5/ O/2.2/
NH+M=N+H+M                 2.650E+14     0.0    75500.0
NH+H=N+H2                 3.200E+13     0.0      325.0
NH+N=N2+H                 9.000E+11     0.5        0.0
NH+NH=NNH+H                5.100E+13     0.0        0.0
NH+NH=NH2+N                5.950E+02     2.89    -2030.0
NH+NH=N2+H2                1.000E+08     1.0        0.0
NH2+M=NH+H+M                3.160E+23    -2.0    91400.0
NH+H2=NH2+H                1.000E+14     0.0    20070.0
NH2+N=N2+H+H               6.900E+13     0.0        0.0
NH2+NH=N2H2+H               1.500E+15    -0.5        0.0
NH2+NH=NH3+N               1.000E+13     0.0     2000.0
NH3+NH=NH2+NH2              3.160E+14     0.0    26770.0
NH2+NH2=N2H2+H2             1.000E+13     0.0     1500.0
N2H3+H=NH2+NH2              5.000E+13     0.0     2000.0
NH3+M=NH2+H+M               2.200E+16     0.0    93470.0
NH3+M=NH+H2+M               6.300E+14     0.0    93390.0
NH3+H=NH2+H2               5.420E+05     2.4      9920.0
NH3+NH2=N2H3+H2             1.000E+11     0.5    21600.0
NNH=N2+H                 3.000E+08     0.0        0.0
!    DUPLICATE
NNH+M=N2+H+M                1.000E+13     0.5     3060.0
!    DUPLICATE
NNH+H=N2+H2                1.000E+14     0.0        0.0
NNH+N=NH+N2                3.000E+13     0.0     2000.0
NNH+NH=N2+NH2               2.000E+11     0.5     2000.0
NNH+NH2=N2+NH3              1.000E+13     0.0        0.0
NNH+NNH=N2H2+N2             1.000E+13     0.0     4000.0
N2H2+M=NNH+H+M              5.000E+16     0.0    50000.0
H2O/15.0/ O2/2.0/ N2/2.0/ H2/2.0/
N2H2+M=NH+NH+M              3.160E+16     0.0    99400.0
H2O/15.0/ O2/2.0/ N2/2.0/ H2/2.0/
N2H2+H=NNH+H2               8.500E+04     2.63    -230.0
```

```
N2H2+N=NNH+NH               1.000E+06     2.0       0.0
N2H2+NH=NNH+NH2              1.000E+13     0.0     6000.0
N2H2+NH2=NH3+NNH             8.800E-02     4.05    -1610.0
N2H3+NH=N2H2+NH2             2.000E+13     0.0       0.0
N2H3+NNH=N2H2+N2H2            1.000E+13     0.0     4000.0
N2H3+M=NH2+NH+M              5.000E+16     0.0    60000.0
N2H3+M=N2H2+H+M              1.000E+16     0.0    37000.0
N2H3+H=N2H2+H2              1.000E+13     0.0       0.0
N2H3+H=NH+NH3               1.000E+11     0.0       0.0
N2H3+N=N2H2+NH              1.000E+06     2.0       0.0
N2H3+NH2=NH3+N2H2            1.000E+11     0.5       0.0
N2H3+N2H2=N2H4+NNH            1.000E+13     0.0     6000.0
N2H3+N2H3=NH3+NH3+N2          3.000E+12     0.0       0.0
N2H3+N2H3=N2H4+N2H2           1.200E+13     0.0       0.0
N2H4(+M)=NH2+NH2(+M)          5.000E+14     0.0    60000.0
LOW/1.50E+15 0.0 39000.0 /
N2/2.4/ NH3/3.0/ N2H4/4.0/
N2H4+M=N2H3+H+M              1.000E+15     0.0    63600.0
N2/2.4/ NH3/3.0/ N2H4/4.0/
N2H4+H=N2H3+H2              7.000E+12     0.0     2500.0
N2H4+H=NH2+NH3              2.400E+09     0.0     3100.0
N2H4+N=N2H3+NH              1.000E+10     1.0     2000.0
N2H4+NH=NH2+N2H3             1.000E+09     1.5     2000.0
N2H4+NH2=N2H3+NH3            1.800E+06     1.71    -1380.0
N+OH=NO+H                  2.800E+13     0.0       0.0
N2O+H=N2+OH                2.200E+14     0.0    16750.0
N2O+H=NH+NO                6.700E+22    -2.16   37155.0
N2O+H=NNH+O                5.500E+18    -1.06   47290.0
!KD-> N2O+H=HNNO                 8.000E+24    -4.39   10530.0
N2O+OH=N2+HO2               1.000E+14     0.0    30000.0
HNO+NO=N2O+OH               8.500E+12     0.0    29580.0
!KD-> HNO+NO+NO=HNNO+NO2          1.600E+11     0.0     2090.0
!KD-> NH+NO+M=HNNO+M             1.630E+23    -2.6     1820.0
!KD-> HNNO+H=N2O+H2              2.000E+13     0.0       0.0
!KD-> HNNO+H=NH2+NO              1.000E+12     0.0       0.0
!KD-> HNNO+O=N2O+OH              2.000E+13     0.0       0.0
!KD-> HNNO+OH=H2O+N2O             2.000E+13     0.0       0.0
!KD-> HNNO+OH=HNOH+NO             1.000E+12     0.0       0.0
!KD-> HNNO+NO=N2+HONO             2.600E+11     0.0     1610.0
!KD-> HNNO+NO=NNH+NO2             3.200E+12     0.0      540.0
!KD-> HNNO+NO=N2O+HNO             1.000E+12     0.0       0.0
!KD-> HNNO+NO2=N2O+HONO            1.000E+12     0.0       0.0
!KD-> HNNO+NO2=NNH+NO3            1.000E+13     0.0    17000.0
NO2+H=NO+OH                1.320E+14     0.0      362.0
NO2+OH=HO2+NO               1.810E+13     0.0     6676.0
NO2+HO2=HONO+O2              4.640E+11     0.0     -479.0
NO2+H2=HONO+H               7.330E+11     0.0    28800.0
NO2+NH=N2O+OH               8.650E+10     0.0    -2270.0
NO2+NH=NO+HNO               1.245E+11     0.0    -2270.0
!KD-> NO3+H=NO2+OH               6.620E+13     0.0       0.0
!KD-> NO3+OH=NO2+HO2              1.210E+13     0.0       0.0
```

```
!KD-> NO3+HO2=HNO3+O2              5.550E+11     0.0        0.0
!KD-> NO3+HO2=NO2+OH+O2            1.510E+12     0.0        0.0
!KD-> N2O4+H2O=HONO+HNO3           2.520E+14     0.0     11590.0
!KD-> N2O3+H2O=HONO+HONO           3.790E+13     0.0     8880.0
H+NO(+M)=HNO(+M)             1.520E+15     -0.41       0.0
LOW /4.00E+20 -1.75 0.0 /
!KD->     H2O/10.0/ O2/1.5/ AR/0.75/ H2/2.0/ CO2/3.0/
H2O/10.0/ O2/1.5/         H2/2.0/ CO2/3.0/
HNO+H=NO+H2                  4.460E+11     0.72     655.0
HNO+OH=NO+H2O                1.300E+07     1.88     -956.0
HNO+O=OH+NO                  5.000E+11     0.5      2000.0
HNO+O=NO2+H                  5.000E+10     0.0      2000.0
HNO+O2=NO+HO2                2.200E+10     0.0      9140.0
HNO+N=NO+NH                  1.000E+11     0.5      2000.0
HNO+N=H+N2O                  5.000E+10     0.5      3000.0
HNO+NH=NH2+NO                5.000E+11     0.5        0.0
HNO+NH2=NH3+NO               2.000E+13     0.0      1000.0
HNO+HNO=N2O+H2O              3.630E-03     3.98     1190.0
HNO+HNO=HNOH+NO              2.000E+08     0.0      4170.0
HNO+NO2=HONO+NO              6.020E+11     0.0      2000.0
NO+OH(+M)=HONO(+M)           2.000E+12     -0.05    -721.0
LOW / 5.08E+23 -2.51 -67.6 /
TROE /0.62 10.0 100000.0 /
!KD->     H2O/10.0/ O2/2.0/ AR/0.75/ H2/2.0/ CO2/0.0/
H2O/10.0/ O2/2.0/         H2/2.0/ CO2/0.0/
NO+OH(+CO2)=HONO(+CO2)       2.000E+12     -0.05    -721.0
LOW / 1.70E+23 -2.3 -246.0 /
TROE /0.62 10.0 100000.0 /
NO2+H+M=HONO+M               1.400E+18     -1.5      900.0
HONO+H=HNO+OH                5.640E+10     0.86     4970.0
HONO+H=NO+H2O                8.120E+06     1.89     3840.0
HONO+O=OH+NO2                1.200E+13     0.0      5960.0
HONO+OH=H2O+NO2              1.690E+12     0.0      -517.0
HONO+NH=NH2+NO2              1.000E+13     0.0        0.0
HONO+HONO=H2O+NO2+NO         1.000E+13     0.0      8540.0
HONO+NH2=NO2+NH3             5.000E+12     0.0        0.0
!KD-> NO2+OH(+M)=HNO3(+M)          2.410E+13     0.0        0.0
!KD->     LOW / 6.42E+32 -5.49 2350.0 /
!KD->     TROE /1.0 10.0 1168.0 /
!KD->     H2O/10.0/ O2/2.0/ AR/0.75/ H2/2.0/ CO2/0.0/
!KD-> NO2+OH(+CO2)=HNO3(+CO2)      2.410E+13     0.0        0.0
!KD->     LOW / 5.80E+32 -5.4 2186.0 /
!KD->     TROE /1.0 10.0 1168.0 /
!KD-> NO+HO2+M=HNO3+M              1.500E+24     -3.5      2200.0
!KD-> HNO3+H=H2+NO3                5.560E+08     1.53    16400.0
!KD-> HNO3+H=H2O+NO2               6.080E+01     3.29     6290.0
!KD-> HNO3+H=OH+HONO               3.820E+05     2.3      6980.0
!KD-> HNO3+OH=NO3+H2O              1.030E+10     0.0     -1240.0
NH3+O=NH2+OH                 1.100E+06     2.1      5210.0
NH3+OH=NH2+H2O               5.000E+07     1.6      950.0
NH3+HO2=NH2+H2O2             3.000E+11     0.0     22000.0
```

```
NH2+HO2=NH3+O2            1.650E+04     1.55     2027.0
NH2+O=H2+NO             5.000E+12     0.0        0.0
NH2+O=HNO+H             4.500E+13     0.0        0.0
NH2+O=NH+OH             7.000E+12     0.0        0.0
NH2+OH=NH+H2O            9.000E+07     1.5      -460.0
!KD-> NH2+OH=NH2OH              1.790E+13     0.2        0.0
NH2+HO2=HNO+H2O           5.680E+15    -1.12     707.0
NH2+HO2=H2NO+OH           2.910E+17    -1.32    1248.0
NH2+O2=HNO+OH            1.000E+13     0.0    26290.0
NH2+O2=H2NO+O            6.000E+13     0.0    29880.0
NH2+NO=NNH+OH            2.290E+10     0.425   -814.0
NH2+NO=N2+H2O            2.770E+20    -2.65    1258.0
NH2+NO=H2+N2O            1.000E+13     0.0    33700.0
NH2+NO2=N2O+H2O           1.620E+16    -1.44     270.0
NH2+NO2=H2NO+NO           6.480E+16    -1.44     270.0
NH+O=NO+H              7.000E+13     0.0        0.0
NH+O=N+OH              7.000E+12     0.0        0.0
NH+OH=HNO+H             2.000E+13     0.0        0.0
NH+OH=N+H2O             2.000E+09     1.2        0.0
NH+OH=NO+H2             2.000E+13     0.0        0.0
NH+HO2=HNO+OH            1.000E+13     0.0     2000.0
NH+O2=HNO+O             4.000E+13     0.0    17880.0
NH+O2=NO+OH             4.500E+08     0.79    1190.0
NH+H2O=HNO+H2            2.000E+13     0.0    13850.0
NH+N2O=N2+HNO            2.000E+12     0.0     6000.0
NNH+O=NH+NO             2.000E+14     0.0     4000.0
NH+NO=N2+OH             6.100E+13    -0.50     120.0
N2H4+O=N2H2+H2O           8.500E+13     0.0     1200.0
N2H4+O=N2H3+OH           2.500E+12     0.0     1200.0
N2H4+OH=N2H3+H2O          3.000E+10     0.68    1290.0
N2H4+OH=NH3+H2NO          3.670E+13     0.0        0.0
N2H4+HO2=N2H3+H2O2         4.000E+13     0.0     2000.0
N2H3+O=N2H2+OH           2.000E+13     0.0     1000.0
N2H3+O=NNH+H2O           3.160E+11     0.5        0.0
N2H3+O=NH2+HNO           1.000E+13     0.0        0.0
N2H3+OH=N2H2+H2O          3.000E+10     0.68    1290.0
N2H3+OH=NH3+HNO          1.000E+12     0.0    15000.0
N2H3+O2=N2H2+HO2          3.000E+12     0.0        0.0
N2H3+HO2=N2H2+H2O2         1.000E+13     0.0     2000.0
N2H3+HO2=N2H4+O2          8.000E+12     0.0        0.0
N2H3+NO=HNO+N2H2          1.000E+12     0.0        0.0
N2H2+O=NH2+NO            1.000E+13     0.0        0.0
N2H2+O=NNH+OH            2.000E+13     0.0     1000.0
N2H2+OH=NNH+H2O           5.920E+01     3.4    -1360.0
N2H2+HO2=NNH+H2O2          1.000E+13     0.0     2000.0
N2H2+NO=N2O+NH2           3.000E+10     0.0        0.0
NNH+O=N2+OH             1.700E+16    -1.23     500.0
NNH+OH=N2+H2O            2.400E+22    -2.88    2444.0
NNH+O2=N2+HO2            1.200E+12    -0.34     150.0
NNH+O2=N2O+OH            2.900E+11    -0.34     150.0
NNH+HO2=N2+H2O2           1.000E+13     0.0     2000.0
```

```
NNH+NO=N2+HNO                 5.000E+13     0.0       0.0
!KD-> NH2OH+OH=HNOH+H2O             2.500E+13     0.0     4250.0
H2NO+M=H2+NO+M                7.830E+27    -4.29   60300.0
H2O/10.0/
H2NO+M=HNO+H+M                2.800E+24    -2.83   64915.0
H2O/10.0/
H2NO+M=HNOH+M                 1.100E+29    -3.99   43980.0
H2O/10.0/
H2NO+H=HNO+H2                 3.000E+07     2.0     2000.0
H2NO+H=NH2+OH                 5.000E+13     0.0       0.0
H2NO+O=HNO+OH                 3.000E+07     2.0     2000.0
H2NO+OH=HNO+H2O               2.000E+07     2.0     1000.0
H2NO+HO2=HNO+H2O2             2.900E+04     2.69   -1600.0
H2NO+NH2=HNO+NH3              3.000E+12     0.0     1000.0
H2NO+O2=HNO+HO2               3.000E+12     0.0    25000.0
H2NO+NO=HNO+HNO               2.000E+07     2.0    13000.0
H2NO+NO2=HONO+HNO             6.000E+11     0.0     2000.0
HNOH+M=HNO+H+M                2.000E+24    -2.84   58935.0
H2O/10.0/
HNOH+H=HNO+H2                 4.800E+08     1.5      380.0
HNOH+H=NH2+OH                 4.000E+13     0.0       0.0
HNOH+O=HNO+OH                 7.000E+13     0.0       0.0
DUPLICATE
HNOH+O=HNO+OH                 3.300E+08     1.5     -360.0
DUPLICATE
HNOH+OH=HNO+H2O               2.400E+06     2.0    -1190.0
HNOH+HO2=HNO+H2O2             2.900E+04     2.69   -1600.0
HNOH+NH2=HNO+NH3              1.800E+06     1.94   -1150.0
HNOH+NO2=HONO+HNO             6.000E+11     0.0     2000.0
HNOH+O2=HNO+HO2               3.000E+12     0.0    25000.0
!KD-> HNOH+HNO=NH2OH+NO            1.000E+12     0.0     3000.0
!END
CO+HO2=CO2+OH                 1.500E+14     0.0    23650.0
CO+OH=CO2+H                   1.170E+07     1.354   -725.0
CO+O+M=CO2+M                  6.160E+14     0.0     3000.0
!KD->  H2/2.5/ H2O/6.2/ CO/1.875/ CO2/3.75/ AR/0.88/
H2/2.5/ H2O/6.2/ CO/1.875/ CO2/3.75/
CH4/3.2/ CH3OH/7.5/
CO+O2=CO2+O                   2.500E+12     0.0    47800.0
HCO+M=H+CO+M                  1.560E+14     0.0    15760.0
!KD->  H2/2.5/ H2O/6.2/ CO/1.875/ CO2/3.75/ AR/1.0/
H2/2.5/ H2O/6.2/ CO/1.875/ CO2/3.75/
CH4/3.2/ CH3OH/7.5/
HCO+OH=CO+H2O                 1.000E+14     0.0       0.0
HCO+O=CO+OH                   3.000E+13     0.0       0.0
HCO+O=CO2+H                   3.000E+13     0.0       0.0
HCO+H=CO+H2                   9.000E+13     0.0       0.0
HCO+O2=CO+HO2                 2.700E+13     0.0     1190.0
HCO+CH3=CO+CH4                1.200E+14     0.0       0.0
HCO+HO2=CO2+OH+H              3.000E+13     0.0       0.0
HCO+HCO=CH2O+CO               3.000E+13     0.0       0.0
```

```
HCO+HCO=H2+CO+CO             2.200E+13     0.0       0.0
CH4(+M)=CH3+H(+M)            2.400E+16     0.0    104913.0
LOW /4.5E+17 0.0 90800/
TROE /1.0 10.0 1350.0 7830.0/
CH4/0.0/ H2/2.0/ CO/2.0/ CO2/3.0/ H2O/5.0/
CH4(+CH4)=CH3+H(+CH4)        2.400E+16     0.0    104913.0
LOW /8.4E+18 0.0 90800/
TROE /0.31 2210.0 90/
CH4+HO2=CH3+H2O2             9.000E+12     0.0     24641.0
CH4+OH=CH3+H2O               1.548E+07     1.83     2774.0
CH4+O=CH3+OH                 7.200E+08     1.56     8485.0
CH4+H=CH3+H2                 1.300E+04     3.0      8050.0
CH4+CH2=CH3+CH3              4.300E+12     0.0     10038.0
CH4+O2=CH3+HO2               4.000E+13     0.0     56900.0
CH3+M=CH2+H+M                2.720E+36    -5.31   117100.0
!KD->  H2/2.5/ H2O/6.2/ CO/1.875/ CO2/3.75/ AR/1.0/
H2/2.5/ H2O/6.2/ CO/1.875/ CO2/3.75/
CH4/3.2/ CH3OH/7.5/
CH3+M=CH+H2+M                1.000E+16     0.0     85240.0
!KD->  H2/2.5/ H2O/6.2/ CO/1.875/ CO2/3.75/ AR/0.88/
H2/2.5/ H2O/6.2/ CO/1.875/ CO2/3.75/
CH4/3.2/ CH3OH/7.5/
CH3+HO2=CH3O+OH              1.800E+13     0.0       0.0
CH3+OH=CH2OH+H               2.640E+19    -1.8      8068.0
CH3+OH=CH3O+H                5.740E+12    -0.23    13931.0
CH3+OH=CH2+H2O               8.900E+18    -1.8      8067.0
CH3+OH=CH2O+H2               3.190E+12    -0.53    10810.0
CH3+O=H+CH2O                 8.430E+13     0.0       0.0
CH3+O2=CH2O+OH               3.400E+11     0.0      8940.0
CH3+O2=CH3O+O                1.320E+14     0.0     31400.0
CH3+CH3=C2H5+H               5.000E+12     0.099   10600.0
CH3+CH3(+M)=C2H6(+M)         9.210E+16    -1.174     636.0
LOW /1.13E+36 -5.246 1705/
TROE /0.405 1120.0 69.6/
H2/2.0/ CO/2.0/ CO2/3.0/ H2O/5.0/
CH3+CH3O=CH4+CH2O            2.409E+13     0.0       0.0
CH3+CH2OH=CH4+CH2O           8.500E+13     0.0       0.0
CH3+H=SCH2+H2                6.000E+13     0.0     15100.0
CH3+O2(+M)=CH3O2(+M)         7.800E+08     1.2       0.0
LOW/5.8E+25 -3.30 0.0/
TROE /0.495 2325.5 10/
CH3+CH3=C2H4+H2              1.000E+14     0.0     32000.0
CH3+OH=SCH2+H2O              7.200E+13     0.0      2780.0
CH2+OH=CH2O+H                2.500E+13     0.0       0.0
CH2+O=CO+H2                  4.800E+13     0.0       0.0
CH2+O=CO+H+H                 7.200E+13     0.0       0.0
CH2+O=CH+OH                  3.000E+14     0.0     11920.0
CH2+O=HCO+H                  3.000E+13     0.0       0.0
CH2+H=CH+H2                  3.120E+13     0.0     -1340.0
CH2+O2=HCO+OH                4.300E+10     0.0      -500.0
CH2+O2=CO2+H2                6.900E+11     0.0       500.0
```

```
CH2+O2=CO2+H+H          1.600E+12   0.0    1000.0
CH2+O2=CO+H2O           1.900E+10   0.0   -1000.0
CH2+O2=CO+OH+H          8.600E+10   0.0    -500.0
CH2+O2=CH2O+O           5.000E+13   0.0    9000.0
CH2+CO2=CH2O+CO         1.100E+11   0.0    1000.0
CH2+CH2=C2H2+H2         1.580E+15   0.0   11950.0
CH2+CH2=C2H2+H+H        2.000E+14   0.0   11000.0
CH2+CH2=CH3+CH          2.400E+14   0.0    9940.0
CH2+CH2=C2H3+H          2.000E+13   0.0       0.0
CH2+CH3=C2H4+H          4.200E+13   0.0       0.0
CH2+CH=C2H2+H           4.000E+13   0.0       0.0
!KD-> CH2+C=CH+CH           1.620E+12   0.67  46800.0
!KD-> CH2+M=C+H2+M          1.600E+14   0.0   64000.0
CH2+M=CH+H+M            5.600E+15   0.0   89600.0
SCH2+M=CH2+M            6.000E+12   0.0       0.0
!KD->  H2/2.5/ H2O/5.0/ CO/1.875/ CO2/3.75/ AR/0.6/ CH4/1.2/
H2/2.5/ H2O/5.0/ CO/1.875/ CO2/3.75/      CH4/1.2/
C2H2/8.0/ C2H4/4.0/ C2H6/3.6/ H/33.3/
SCH2+O2=CO+OH+H         3.000E+13   0.0       0.0
SCH2+H=CH+H2            3.000E+13   0.0       0.0
SCH2+O=CO+H+H           1.500E+13   0.0       0.0
SCH2+O=CO+H2            1.500E+13   0.0       0.0
SCH2+OH=CH2O+H          3.000E+13   0.0       0.0
SCH2+HO2=CH2O+OH        3.000E+13   0.0       0.0
SCH2+H2O2=CH3O+OH       3.000E+13   0.0       0.0
SCH2+H2O=>CH3OH         1.800E+13   0.0       0.0
SCH2+CH2O=CH3+HCO       1.200E+12   0.0       0.0
SCH2+HCO=CH3+CO         1.800E+13   0.0       0.0
SCH2+CH3=C2H4+H         1.800E+13   0.0       0.0
SCH2+CH4=CH3+CH3        4.000E+13   0.0       0.0
SCH2+C2H6=CH3+C2H5      1.200E+14   0.0       0.0
SCH2+CO2=CH2O+CO        3.000E+12   0.0       0.0
SCH2+CH2CO=C2H4+CO      1.600E+14   0.0       0.0
CH+OH=HCO+H             3.000E+13   0.0       0.0
CH+O=CO+H               4.000E+13   0.0       0.0
!KD-> CH+O=C+OH             1.520E+13   0.0    4730.0
!KD-> H2O+C=CH+OH           7.800E+11   0.67  39300.0
CH+O2=HCO+O             4.900E+13   0.0       0.0
CH+O2=CO+OH             4.900E+13   0.0       0.0
CH+CO2=HCO+CO           3.220E-02   4.44  -3530.0
CH+CH4=C2H4+H           3.900E+14  -0.4       0.0
CH+CH3=C2H3+H           3.000E+13   0.0       0.0
CH2+OH=CH+H2O           1.130E+07   2.0    3000.0
!KD-> CH+H=C+H2             7.900E+13   0.0     160.0
CH+H2O=CH2O+H           1.170E+15  -0.75      0.0
CH+H2O=CH2OH            5.700E+12   0.0    -760.0
CH+CH2O=CH2CO+H         1.000E+14   0.0    -515.0
CH3O+M=CH2O+H+M         5.400E+13   0.0   13500.0
!KD->  H2/2.5/ H2O/6.2/ CO/1.875/ CO2/3.75/ AR/0.88/
H2/2.5/ H2O/6.2/ CO/1.875/ CO2/3.75/
CH4/3.2/ CH3OH/7.5/
```

```
CH3O+HO2=CH2O+H2O2          3.000E+11     0.0       0.0
CH3O+OH=CH2O+H2O            1.800E+13     0.0       0.0
CH3O+O=CH2O+OH              1.800E+12     0.0       0.0
CH3O+H=CH2O+H2              1.800E+13     0.0       0.0
CH3O+O2=CH2O+HO2            2.200E+10     0.0    1750.0
CH3O+CH2O=CH3OH+HCO         1.000E+11     0.0    2980.0
CH3O+CO=CH3+CO2             6.810E-18     9.2   -2850.0
CH3O+HCO=CH3OH+CO           9.000E+13     0.0       0.0
CH3O+C2H5=CH2O+C2H6         2.410E+13     0.0       0.0
CH3O+C2H3=CH2O+C2H4         2.410E+13     0.0       0.0
CH3O+C2H4=CH2O+C2H5         1.200E+11     0.0    6750.0
CH3O+H=CH2OH+H              3.400E+06     1.6       0.0
CH3O+H=SCH2+H2O             1.000E+12     0.0       0.0
CH2O+M=HCO+H+M              5.000E+35    -5.54  96680.0
!KD->  H2/2.5/ H2O/6.2/ CO/1.875/ CO2/3.75/ AR/1.0/
H2/2.5/ H2O/6.2/ CO/1.875/ CO2/3.75/
CH4/3.2/ CH3OH/7.5/
CH2O+M=CO+H2+M              1.100E+36    -5.54  96680.0
!KD->  H2/2.5/ H2O/6.2/ CO/1.875/ CO2/3.75/ AR/1.0/
H2/2.5/ H2O/6.2/ CO/1.875/ CO2/3.75/
CH4/3.2/ CH3OH/7.5/
CH2O+HO2=HCO+H2O2           4.110E+04     2.5   10210.0
CH2O+OH=HCO+H2O             3.433E+09     1.18   -447.0
CH2O+O=HCO+OH               4.100E+11     0.57   2760.0
CH2O+H=HCO+H2               1.260E+08     1.62   2166.0
CH2O+O2=HCO+HO2             6.000E+13     0.0   40650.0
CH2O+CH3=HCO+CH4            7.800E-08     6.1    1970.0
C2H6(+M)=C2H5+H(+M)         8.850E+20    -1.228 102210.0
LOW /6.90E+42 -6.431 107175.0/
SRI /47.61 16182.0 3371.0/
!KD->  H2/2.0/ H2O/6.0/ CH4/2.0/ CO/1.5/ CO2/2.0/ C2H6/3.0/ AR/0.7/
H2/2.0/ H2O/6.0/ CH4/2.0/ CO/1.5/ CO2/2.0/ C2H6/3.0/
C2H6+HO2=C2H5+H2O2          1.330E+13     0.0   20535.0
C2H6+OH=C2H5+H2O            7.200E+06     2.0     870.0
C2H6+O=C2H5+OH              1.000E+09     1.5    5800.0
C2H6+H=C2H5+H2              1.400E+09     1.5    7400.0
C2H6+H=CH3+CH4              5.400E+04     0.0   11630.0
C2H6+O2=C2H5+HO2            6.000E+13     0.0   52000.0
C2H6+CH3=C2H5+CH4           1.470E-07     6.0    6060.0
C2H6+CH2=CH3+C2H5           6.500E+12     0.0    7911.0
C2H6+C2H3=C2H4+C2H5         8.566E-02     4.14   2543.0
C2H6+HCO=CH2O+C2H5          4.700E+04     2.72  18235.0
C2H5(+M)=C2H4+H(+M)         1.110E+10     1.037  36767.0
LOW /4.0E+33 -4.99 40000.0/
TROE /0.832 10 1203.0/
!KD->  H2/2.0/ CO/2.0/ CO2/3.0/ H2O/5.0/ CH4/2.0/ C2H6/0.0/ AR/0.7/
H2/2.0/ CO/2.0/ CO2/3.0/ H2O/5.0/ CH4/2.0/ C2H6/0.0/
C2H5(+C2H6)=C2H4+H(+C2H6)   8.200E+13     0.0   39880.0
LOW /1.0E+18 0.0 33380.0/
TROE /0.75 97.0 1379.0/
C2H5+HO2=C2H4+H2O2          1.800E+12     0.0       0.0
```

```
C2H5+OH=C2H4+H2O              2.409E+13    0.0       0.0
C2H5+OH=>CH3+CH2O+H           2.409E+13    0.0       0.0
C2H5+O=CH2O+CH3               4.240E+13    0.0       0.0
C2H5+O=CH3HCO+H               5.300E+13    0.0       0.0
C2H5+O=C2H4+OH                3.460E+13    0.0       0.0
C2H5+H=C2H4+H2                1.700E+12    0.0       0.0
C2H5+O2=C2H4+HO2              2.560E+19   -2.77   1980.0
C2H5+CH3=C2H4+CH4             1.100E+12    0.0       0.0
C2H5+C2H5=C2H4+C2H6           1.400E+12    0.0       0.0
C2H5+HO2=C2H5O+OH             3.000E+13    0.0       0.0
C2H4+M=C2H2+H2+M              3.500E+16    0.0   71530.0
!KD->   H2/2.5/ H2O/6.2/ CO/1.875/ CO2/3.75/ AR/1.0/
H2/2.5/ H2O/6.2/ CO/1.875/ CO2/3.75/
CH4/3.2/ CH3OH/7.5/
C2H4+M=C2H3+H+M               2.600E+17    0.0   96570.0
!KD->   H2/2.5/ H2O/6.2/ CO/1.875/ CO2/3.75/ AR/1.0/
H2/2.5/ H2O/6.2/ CO/1.875/ CO2/3.75/
CH4/3.2/ CH3OH/7.5/
C2H4+OH=C2H3+H2O              5.530E+05    2.31   2900.0
C2H4+O=CH3+HCO                8.100E+06    1.88    180.0
C2H4+H=C2H3+H2                4.490E+07    2.12  13366.0
C2H4+O2=C2H3+HO2              4.000E+13    0.0   61500.0
C2H4+C2H4=C2H5+C2H3           1.860E+14    0.0   64200.0
C2H4+CH3=C2H3+CH4             4.200E+12    0.0   11100.0
C2H4+O=CH2HCO+H               4.700E+06    1.88    180.0
C2H4+O=CH2O+CH2               3.000E+04    1.88    180.0
C2H4+O=CH2CO+H2               6.700E+05    1.88    180.0
C2H4+O=C2H3+OH                1.510E+07    1.91   3790.0
C2H4+OH=CH2O+CH3              2.000E+12    0.0     960.0
C2H4+OH(+M)=PC2H5O(+M)        5.420E+12    0.0       0.0
LOW /1.19E+27 -3.1 0.0/
C2H4+HO2=C2H3+H2O2            1.120E+13    0.0   30400.0
C2H4+CH3O=C2H3+CH3OH          1.000E+11    0.0   10000.0
C2H3(+M)=C2H2+H(+M)           2.100E+14    0.0   39740.0
LOW /4.15E+41 -7.5 45500.0/
TROE /0.65 100000 10/
!KD->  H2/2.0/ CO/2.0/ CO2/3.0/ H2O/5.0/ CH4/2.0/ C2H6/3.0/ AR/0.7/
H2/2.0/ CO/2.0/ CO2/3.0/ H2O/5.0/ CH4/2.0/ C2H6/3.0/
C2H3+HO2=>CH3+CO+OH           3.000E+13    0.0       0.0
C2H3+OH=C2H2+H2O              3.000E+13    0.0       0.0
C2H3+H=C2H2+H2                1.200E+13    0.0       0.0
C2H3+O=CH3+CO                 1.000E+13    0.0       0.0
C2H3+O2=CH2O+HCO              1.700E+29   -5.312  6500.0
C2H3+CH=CH2+C2H2              5.000E+13    0.0       0.0
C2H3+CH3=C2H2+CH4             2.050E+13    0.0       0.0
C2H3+C2H=C2H2+C2H2            3.000E+13    0.0       0.0
C2H3+HCO=C2H4+CO              9.034E+13    0.0       0.0
C2H3+CH2O=C2H4+HCO            5.420E+03    2.81   5862.0
C2H3+C2H3=C2H2+C2H4           1.450E+13    0.0       0.0
C2H3+O=C2H2+OH                1.000E+13    0.0       0.0
C2H3+O=CH2+HCO                1.000E+13    0.0       0.0
```

```
C2H3+O=CH2CO+H              1.000E+13     0.0        0.0
C2H3+OH=CH3HCO              3.000E+13     0.0        0.0
C2H3+O2=C2H2+HO2            5.190E+15    -1.26     3310.0
DUPLICATE
C2H3+O2=C2H2+HO2            2.120E-06     6.0     9484.0
DUPLICATE
C2H3+O2=CH2HCO+O            3.500E+14    -0.61     5260.0
C2H3+CH2=C2H2+CH3           3.000E+13     0.0        0.0
C2H2=C2H+H               2.373E+32    -5.28   130688.0
C2H2+O2=HCCO+OH             2.000E+08     1.5    30100.0
C2H2+O2=C2H+HO2             1.200E+13     0.0    74520.0
C2H2+OH=C2H+H2O             3.385E+07     2.0    14000.0
C2H2+OH=CH2CO+H             1.100E+13     0.0     7170.0
C2H2+O=CH2+CO              1.200E+06     2.1     1570.0
C2H2+O=HCCO+H              5.000E+06     2.1     1570.0
C2H2+CH3=C2H+CH4            1.800E+11     0.0    17290.0
C2H2+O=C2H+OH              3.000E+14     0.0    25000.0
C2H2+OH=CH3+CO              4.830E-04     4.0    -2000.0
C2H2+HO2=CH2CO+OH            6.100E+09     0.0     7950.0
C2H2+O2=HCO+HCO             4.000E+12     0.0    28000.0
C2H+OH=HCCO+H              2.000E+13     0.0        0.0
!KD-> C2H+OH=C2+H2O              4.000E+07     2.0     8000.0
C2H+O=CO+CH                1.450E+13     0.0      460.0
C2H+O2=HCO+CO              9.000E+12     0.0        0.0
C2H+H2=C2H2+H              7.880E+05     2.39      346.0
C2H+O2=CO+CO+H              9.000E+12     0.0        0.0
C2H+O2=HCCO+O              6.000E+11     0.0        0.0
CH2CO(+M)=CH2+CO(+M)         3.000E+14     0.0    71000.0
LOW /2.300E+15   0.0  57600.0/
!KD->     H2/2.5/ H2O/6.2/ CO/1.875/ CO2/3.75/ AR/1.0/
H2/2.5/ H2O/6.2/ CO/1.875/ CO2/3.75/
CH4/3.2/ CH3OH/7.5/
CH2CO+O2=CH2O+CO2            2.000E+13     0.0    61500.0
CH2CO+HO2=>CH2O+CO+OH         6.000E+11     0.0    12738.0
CH2CO+O=HCCO+OH             1.000E+13     0.0     8000.0
CH2CO+OH=CH2OH+CO            1.000E+13     0.0        0.0
CH2CO+H=CH3+CO              3.280E+10    0.851    2840.0
CH2CO+CH3=C2H5+CO            2.400E+12     0.0     8000.0
CH2CO+CH2=C2H4+CO            2.900E+12     0.0     3800.0
CH2CO+CH2=HCCO+CH3           3.600E+13     0.0    11000.0
CH2CO+CH3=HCCO+CH4           7.500E+12     0.0    13000.0
CH2CO+OH=CH2O+HCO            2.800E+13     0.0        0.0
CH2CO+H=HCCO+H2             1.800E+14     0.0     8600.0
CH2CO+O=HCO+HCO             7.500E+11     0.0     1350.0
CH2CO+O=HCO+CO+H             7.500E+11     0.0     1350.0
CH2CO+O=CH2O+CO             7.500E+11     0.0     1350.0
CH2CO+OH=HCCO+H2O            7.500E+12     0.0     2000.0
HCCO+M=CH+CO+M              6.000E+15     0.0    58821.0
!KD->     H2/2.5/ H2O/6.2/ CO/1.875/ CO2/3.75/ AR/0.88/
H2/2.5/ H2O/6.2/ CO/1.875/ CO2/3.75/
CH4/3.2/ CH3OH/7.5/
```

```
HCCO+OH=HCO+CO+H              1.000E+13     0.0        0.0
!KD-> HCCO+OH=C2O+H2O              3.000E+13     0.0        0.0
HCCO+O=CO+CO+H              1.000E+14     0.0        0.0
HCCO+O=CH+CO2              2.950E+13     0.0     1110.0
HCCO+H=CH2+CO              1.500E+14     0.0        0.0
HCCO+O2=CO2+CO+H             5.400E+11     0.0      850.0
HCCO+CH2=C2H+CH2O            1.000E+13     0.0     2000.0
HCCO+CH2=C2H3+CO            3.000E+13     0.0        0.0
HCCO+CH3=C2H4+CO            2.000E+12     0.0        0.0
HCCO+CH=CO+C2H2             5.000E+13     0.0        0.0
HCCO+HCCO=CO+C2H2+CO         1.000E+13     0.0        0.0
HCCO+OH=HCO+HCO             1.000E+13     0.0        0.0
HCCO+O2=CO+CO+OH             5.400E+11     0.0      850.0
HCCO+O2=CO2+HCO             5.400E+11     0.0      850.0
CH3OH(+M)=CH3+OH(+M)         1.700E+16     0.0    90885.0
LOW /6.60E+16 0.0 65730.0/
TROE /0.82 200.0 1438.0/
CH3OH+HO2=CH2OH+H2O2         9.640E+10     0.0    12580.0
CH3OH+OH=CH2OH+H2O           1.440E+06     2.0     -840.0
CH3OH+OH=CH3O+H2O           1.000E+13     0.0     1700.0
CH3OH+O=CH2OH+OH            1.630E+13     0.0     5030.0
CH3OH+H=CH2OH+H2            1.640E+07     2.0     4520.0
CH3OH+CH3=CH2OH+CH4          3.190E+01     3.17     7172.0
CH3OH+CH3=CH3O+CH4           1.450E+01     3.1     6935.0
CH3OH+C2H5=C2H6+CH3O         1.440E+01     3.1     8942.0
CH3OH+H=CH3+H2O             2.000E+14     0.0     5300.0
CH3OH+O=CH3O+OH             1.000E+13     0.0     4680.0
CH3OH+CH3=C2H6+OH            2.000E+12     0.0    15000.0
CH3OH+CH3O=CH2OH+CH3OH       3.000E+11     0.0     4070.0
CH3OH(+M)=CH2OH+H(+M)        1.380E+16     0.0    95950.0
LOW /5.35E+16 0.0 70800.0/
TROE /0.82 200.0 1438.0/
CH3OH+H=H2+CH3O             4.000E+13     0.0     6095.0
CH3OH+O2=CH2OH+HO2           2.050E+13     0.0    44900.0
CH3OH+C2H5=C2H6+CH2OH        3.190E+01     3.2     9161.0
CH2OH+M=CH2O+H+M            1.140E+43    -8.0    43000.0
H2O/16.0/ CH4/3.0/ CO2/3.75/  CO/1.875/  H2/2.5/   CH3OH/6.0/
CH2OH+H=CH2O+H2             1.000E+13     0.0        0.0
CH2OH+O2=CH2O+HO2            1.500E+15    -1.0        0.0
DUPLICATE
CH2OH+O2=CH2O+HO2            7.200E+13     0.0     3570.0
DUPLICATE
H+CH2OH=SCH2+H2O            1.000E+12     0.0        0.0
CH2OH+O=CH2O+OH             9.000E+13     0.0        0.0
CH2OH+OH=CH2O+H2O           1.000E+13     0.0        0.0
CH2OH+HO2=CH2O+H2O2          1.210E+13     0.0        0.0
CH2OH+CH2OH=CH3OH+CH2O       4.820E+12     0.0        0.0
CH2OH+CH2OH=CH2O+CH2O+H2     1.000E+15    -0.7        0.0
CH2OH+HCO=CH3OH+CO           1.210E+14     0.0        0.0
CH2OH+CH2O=CH3OH+HCO         5.490E+03     2.8     5900.0
CH2OH+CH3O=CH3OH+CH2O        2.400E+13     0.0        0.0
```

```
CH3O+CH3O=CH3OH+CH2O          2.320E+13     0.0        0.0
CH3HCO=CH3+HCO              7.100E+15     0.0    81790.0
CH3HCO+HO2=CH3CO+H2O2         3.000E+12     0.0    12000.0
CH3HCO+OH=CH3CO+H2O          2.300E+10     0.73   -1100.0
CH3HCO+O=CH3CO+OH            5.800E+12     0.0     1800.0
CH3HCO+H=CH3CO+H2            4.100E+09     1.16    2400.0
CH3HCO+O2=CH3CO+HO2          3.000E+13     0.0    39200.0
CH3HCO+CH3=CH3CO+CH4         7.600E+00     3.4     3740.0
CH3HCO+H=CH2HCO+H2           7.000E+08     1.5     7400.0
CH3HCO+O=CH2HCO+OH           5.000E+08     1.5     5800.0
CH3HCO+OH=CH2HCO+H2O         2.000E+14     0.0     6000.0
CH3HCO+HO2=CH2HCO+H2O2        3.000E+13     0.0    15000.0
CH3HCO+CH2=CH3CO+CH3         1.660E+12     0.0     3510.0
CH3HCO+CH3=CH2HCO+CH4        1.580E+00     4.0     7720.0
CH3HCO+CH3O=CH3CO+CH3OH       5.000E+12     0.0        0.0
CH3HCO+C2H5=CH3CO+C2H6        1.260E+12     0.0     8500.0
CH3HCO+C2H3=CH3CO+C2H4        8.130E+10     0.0     3680.0
CH2HCO=CH3CO               1.600E+11     0.0    21600.0
CH3HCO+CH2HCO=CH3CO+CH3HCO    3.000E+12     0.0    11200.0
CH3CO(+M)=CH3+CO(+M)         2.800E+13     0.0    17150.0
LOW /6.0E+15 0.0 14070.0/
TROE /0.5 100000 10/
!KD->    H2/2.5/ H2O/6.2/ CO/1.875/ CO2/3.75/ AR/0.88/
H2/2.5/ H2O/6.2/ CO/1.875/ CO2/3.75/
CH4/3.2/ CH3OH/7.5/
CH3CO+H=CH2CO+H2            1.150E+13     0.0        0.0
CH3CO+H=CH3+HCO             2.150E+13     0.0        0.0
CH3CO+O=CH2CO+OH            4.000E+13     0.0        0.0
CH3CO+O=CH3+CO2             1.500E+14     0.0        0.0
CH3CO+CH3=C2H6+CO           3.300E+13     0.0        0.0
CH3CO+CH3=CH4+CH2CO          6.100E+12     0.0        0.0
CH2HCO+H=CH2CO+H2           2.000E+13     0.0        0.0
CH2HCO+O2=CH2O+OH+CO         1.800E+10     0.0        0.0
CH2HCO+O2=CH2CO+HO2          1.500E+11     0.0        0.0
CH2HCO=CH2CO+H              1.580E+13     0.0    35200.0
C2H5O=CH3+CH2O              1.000E+15     0.0    21600.0
C2H5O+O2=CH3HCO+HO2          3.600E+10     0.0     1090.0
C2H5O=CH3HCO+H              2.000E+14     0.0    23300.0
C2H5O+OH=CH3HCO+H2O          1.000E+14     0.0        0.0
C2H5O+H=CH3HCO+H2            1.000E+14     0.0        0.0
C2H5O+O=CH3HCO+OH            1.210E+14     0.0        0.0
C2H5O+HO2=CH3HCO+H2O2         1.000E+14     0.0        0.0
C2H5O+C2H5O=C2H5OH+CH3HCO     5.000E+13     0.0        0.0
C2H5O+PC2H5O=C2H5OH+CH3HCO    5.000E+13     0.0        0.0
C2H5O+SC2H5O=C2H5OH+CH3HCO    5.000E+13     0.0        0.0
SC2H5O+M=CH3HCO+H+M          5.000E+13     0.0    21860.0
SC2H5O+H=CH3HCO+H2           2.000E+13     0.0        0.0
SC2H5O+OH=CH3HCO+H2O         1.500E+13     0.0        0.0
SC2H5O+O=CH3HCO+OH           9.040E+13     0.0        0.0
SC2H5O+O2=CH3HCO+HO2         8.400E+15    -1.20       0.0
DUPLICATE
```

```
SC2H5O+O2=CH3HCO+HO2          4.800E+14     0.0     5000.0
DUPLICATE
SC2H5O+HO2=CH3HCO+H2O2        1.000E+13     0.0        0.0
SC2H5O+SC2H5O=C2H5OH+CH3HCO   3.500E+13     0.0        0.0
SC2H5O+PC2H5O=C2H5OH+CH3HCO   5.000E+13     0.0        0.0
PC2H5O=SC2H5O                 1.000E+11     0.0    27000.0
PC2H5O+PC2H5O=C2H5OH+CH3HCO   3.400E+13     0.0        0.0
C2H5OH=CH2OH+CH3              3.100E+15     0.0    80600.0
C2H5OH+OH=SC2H5O+H2O          3.000E+13     0.0     5960.0
C2H5OH+OH=C2H5O+H2O           1.138E+06     2.0      914.0
C2H5OH+OH=PC2H5O+H2O          2.563E+06     2.06     860.0
C2H5OH+O=SC2H5O+OH            6.000E+05     2.46    1850.0
C2H5OH+O=C2H5O+OH             4.820E+13     0.0     6856.0
C2H5OH+O=PC2H5O+OH            5.000E+12     0.0     4411.0
C2H5OH+H=C2H5+H2O             5.900E+11     0.0     3450.0
C2H5OH+H=SC2H5O+H2            4.400E+12     0.0     4570.0
C2H5OH+HO2=SC2H5O+H2O2        2.000E+13     0.0    17000.0
C2H5OH+CH3=SC2H5O+CH4         4.000E+11     0.0     9700.0
C2H5OH+CH3=PC2H5O+CH4         3.000E+00     4.0    10480.0
C2H5OH+CH3=C2H5O+CH4          8.000E+10     0.0     9400.0
C2H5OH+CH3O=SC2H5O+CH3OH      2.000E+11     0.0     7000.0
C2H5OH+CH2O=C2H5O+CH3O        1.500E+12     0.0    79500.0
C2H5OH+C2H5O=C2H5OH+SC2H5O    2.000E+11     0.0     7000.0
C2H5OH=C2H5+OH                5.000E+16     0.0    91212.0
C2H5OH=C2H4+H2O               1.000E+14     0.0    76706.0
C2H5OH+O2=PC2H5O+HO2          4.000E+13     0.0    50900.0
C2H5OH+O2=SC2H5O+HO2          4.000E+13     0.0    51200.0
C2H5OH+O2=C2H5O+HO2           2.000E+13     0.0    56000.0
C2H5OH+H=PC2H5O+H2            2.000E+12     0.0     9500.0
C2H5OH+H=C2H5O+H2             1.760E+12     0.0     4570.0
C2H5OH+HO2=H2O2+C2H5O         1.000E+11     0.0    15500.0
C2H5OH+HO2=H2O2+PC2H5O        1.000E+11     0.0    12500.0
C2H5OH+C2H5=PC2H5O+C2H6       1.500E+12     0.0    11700.0
C2H5OH+C2H5=SC2H5O+C2H6       4.000E+13     0.0    10000.0
C2H5OH+CH2OH=SC2H5O+CH3OH     4.000E+11     0.0     9700.0
!KD-> C+OH=CO+H               5.000E+13     0.0        0.0
!KD-> C+O2=CO+O               1.200E+14     0.0     4000.0
!KD-> C+CH3=C2H2+H            5.000E+13     0.0        0.0
!KD-> C+CH2=C2H+H             5.000E+13     0.0        0.0
!KD-> CH2O+CH3O2=HCO+CH3O2H          2.000E+12     0.0    11660.0
CH3O2+H=CH3O+OH               9.600E+13     0.0        0.0
CH3O2+OH=CH3OH+O2             6.000E+13     0.0        0.0
CH3O2+CH3=CH3O+CH3O           2.400E+13     0.0        0.0
CH3O2+CH3O2=>CH2O+CH3OH+O2    2.700E+10     0.0     -780.0
CH3O2+CH3O2=>CH3O+CH3O+O2     2.800E+10     0.0     -780.0
!KD-> CH3O2+H2O2=CH3O2H+HO2          2.400E+12     0.0    10000.0
!KD-> CH3O2H=CH3O+OH                 6.000E+14     0.0    42300.0
!KD-> CH3O2+HO2=CH3O2H+O2            2.290E+11     0.0    -1550.0
!KD-> CH3O2H+OH=CH3O2+H2O            1.150E+12     0.0     -380.0
!KD-> CH4+CH3O2=CH3+CH3O2H           1.810E+11     0.0    18600.0
!KD-> C2H6+CH3O2=C2H5+CH3O2H         2.950E+11     0.0    14940.0
```

```
!KD-> CH3OH+CH3O2=CH2OH+CH3O2H      1.810E+12     0.0    13800.0
!KD-> CH3O2H+O=OH+CH3O2            2.000E+13     0.0     4750.0
!KD-> CH3CO+O2=CH3CO3              1.000E+10     0.0    -2700.0
!KD-> CH3HCO+CH3CO3=CH3CO+CH3CO3H    1.200E+11     0.0     4900.0
!KD-> CH3HCO+C2H5O2=CH3CO+C2H5O2H    1.150E+11     0.0    10000.0
!KD-> C2H5+O2(+M)=C2H5O2(+M)        2.200E+10     0.772   -570.0
!KD->     LOW /7.10E+42 -8.24 4270.0 /
!KD-> C2H5O2=C2H4+HO2              5.620E+11     0.0    28900.0
!KD-> C2H5O2+HO2=C2H5O2H+O2         3.400E+11     0.0    -1300.0
!KD-> C2H5O2H=C2H5O+OH             4.000E+15     0.0    43000.0
!KD-> C2H5O2H+O=OH+C2H5O2          2.000E+13     0.0     4750.0
!KD-> C2H5O2H+OH=C2H5O2+H2O         2.000E+12     0.0     -370.0
!KD-> CH4+C2H5O2=CH3+C2H5O2H        1.140E+13     0.0    20460.0
!KD-> CH4+CH3CO3=CH3+CH3CO3H        1.140E+13     0.0    20460.0
!KD-> C2H4+C2H5O2=C2H3+C2H5O2H      1.000E+12     0.0    25000.0
!KD-> C2H4+CH3CO3=C2H3+CH3CO3H      3.000E+12     0.0    29000.0
!KD-> CH3CO3+HO2=CH3CO3H+O2         1.000E+12     0.0        0.0
!KD-> CH3CO3H=>CH3CO2+OH           1.150E+13     0.0    32550.0
!KD-> CH3CO3H=>CH3+CO2+OH          2.000E+14     0.0    40150.0
!KD-> CH3CO3+CH3O2=>CH3CO2+CH3O+O2   1.080E+15     0.0     3600.0
!KD-> CH3CO3+CH3O2=>CH3CO2H+CH2O+O2  2.470E+09     0.0    -4200.0
!KD-> CH3CO3+HO2=>CH3CO2+OH+O2      2.590E+11     0.0    -2080.0
!KD-> CH3CO3+CH3CO3=>CH3CO2+CH3CO2+O2  1.690E+12   0.0    -1060.0
!KD-> CH3CO2+M=>CH3+CO2+M           8.700E+15     0.0    14400.0
!KD-> CH3CO2H=CH4+CO2              7.080E+13     0.0    74600.0
!KD-> CH3CO2H=CH2CO+H2O            4.470E+14     0.0    79800.0
!KD-> CH3CO2H+OH=CH3CO2+H2O         2.400E+11     0.0     -400.0
!KD-> CH3OH+C2H5O2=CH2OH+C2H5O2H    6.300E+12     0.0    19360.0
!KD-> CH3OH+CH3CO3=CH2OH+CH3CO3H    6.300E+12     0.0    19360.0
!KD-> CH2O+C2H5O2=HCO+C2H5O2H       1.300E+11     0.0     9000.0
!KD-> CH2O+CH3CO3=HCO+CH3CO3H       1.000E+12     0.0    10560.0
!KD-> C2H4+CH3O2=C2H3+CH3O2H        1.000E+13     0.0    25000.0
!KD-> CH3HCO+CH3O2=CH3CO+CH3O2H     1.150E+11     0.0    10000.0
!KD-> C2H5OH+CH3O2=SC2H5O+CH3O2H    1.000E+13     0.0    10000.0
C2H5+CH3O2=C2H5O+CH3O         2.410E+13     0.0        0.0
!KD-> C2H4+HO2=C2H4O+OH            2.200E+12     0.0    17200.0
!KD-> C2H4+CH3O=C2H4O+CH3          1.000E+11     0.0    14500.0
!KD-> C2H4+CH3O2=C2H4O+CH3O         7.000E+11     0.0    14500.0
!KD-> C2H4O=>CH3HCOW               1.600E+13     0.0    54300.0
!KD-> CH3HCOW+M=>CH3HCO+M          1.000E+14     0.0        0.0
!KD-> CH3HCOW=>CH3+HCO             5.000E+08     0.0        0.0
!KD-> C2H4O+H=H2+C2H3O             8.000E+13     0.0     9740.0
!KD-> C2H4O+H=H2O+C2H3             5.000E+09     0.0     5030.0
!KD-> C2H4O+H=C2H4+OH              9.510E+10     0.0     5030.0
!KD-> C2H4O+CH2HCO=CH3HCO+C2H3O     1.000E+11     0.0    14000.0
!KD-> C2H4O+CH3=CH4+C2H3O          1.070E+12     0.0    11900.0
!KD-> C2H4O+O=OH+C2H3O             1.910E+12     0.0     5300.0
!KD-> C2H4O+OH=H2O+C2H3O           1.780E+13     0.0     3600.0
!KD-> C2H3O=>CH2CHOW               1.000E+11     0.0    10000.0
!KD-> C2H3O=>CH3+CO                8.000E+11     0.0    10000.0
!KD-> C2H3O+H+M=>C2H4O+M           4.000E+15     0.0        0.0
```

```
!KD-> CH2CHOW+M=>CH2HCO+M          1.000E+14     0.0        0.0
!KD-> CH2CHOW=>CH3+CO              1.000E+08     0.0        0.0
!KD-> CH2CHOW=>OH+C2H2             1.000E+11     0.0     17000.0
!KD-> CH2CHOW=>CH2CO+H             1.000E+08     0.0        0.0
!KD-> C2H4O+O2=HO2+C2H3O           1.000E+14     0.0     52000.0
!KD-> C2H4O+HO2=H2O2+C2H3O         5.000E+13     0.0     18000.0
!KD-> CH3HCOW+O2=>HO2+CH3CO        1.000E+14     0.0        0.0
!KD-> CH2CHOW+O2=>HO2+CH2CO        1.000E+14     0.0        0.0
CH2+C2H2=H+C3H3              1.200E+13     0.0     6620.0
CH2+C2H4=C3H6                3.160E+12     0.0     5280.0
SCH2+C2H4=>C3H6              1.000E+14     0.0        0.0
CH2+C3H8=CH3+IC3H7           1.500E+00     3.46    7470.0
CH2+C3H8=CH3+NC3H7           9.000E-01     3.65    7150.0
SCH2+C2H2=C3H3+H             1.800E+14     0.0        0.0
C2H3+CH2=C3H4+H              3.000E+13     0.0        0.0
C2H3+C2H2=C4H4+H             1.930E+12     0.0     6000.0
C2H3+C2H3=C4H6               7.230E+13     0.0        0.0
C2H2+CH3=SC3H5               1.610E+40    -8.58   20331.0
C2H2+CH3=C3H5                2.610E+46    -9.82   36951.0
C2H2+CH3=C3H4+H              6.740E+19    -2.08   31591.0
CH2CO+C2H3=C3H5+CO           1.000E+12     0.0     3000.0
HCCO+C2H2=C3H3+CO            1.000E+11     0.0     3000.0
C3H8(+M)=C2H5+CH3(+M)        1.100E+17     0.0    84400.0
LOW /7.83E+18 0.0 65000.0/
C3H8+O2=NC3H7+HO2            4.000E+13     0.0    50870.0
C3H8+O2=IC3H7+HO2            4.000E+13     0.0    47690.0
C3H8+HO2=NC3H7+H2O2          4.760E+04     2.55   16490.0
C3H8+HO2=IC3H7+H2O2          9.640E+03     2.6    13910.0
C3H8+OH=NC3H7+H2O            3.160E+07     1.80     934.0
C3H8+OH=IC3H7+H2O            7.060E+06     1.90    -159.0
C3H8+O=NC3H7+OH              3.715E+06     2.4     5505.0
C3H8+O=IC3H7+OH              5.495E+05     2.5     3140.0
C3H8+H=NC3H7+H2              1.336E+06     2.54    6756.0
C3H8+H=IC3H7+H2              1.300E+06     2.4     4470.0
C3H8+CH3=NC3H7+CH4           9.000E-01     3.65    7150.0
C3H8+CH3=IC3H7+CH4           1.500E+00     3.46    5480.0
C3H8+C2H5=NC3H7+C2H6         9.000E-01     3.65    9140.0
C3H8+C2H5=IC3H7+C2H6         1.200E+00     3.46    7470.0
C3H8+C2H3=NC3H7+C2H4         6.000E+02     3.3    10502.0
C3H8+C2H3=IC3H7+C2H4         1.000E+03     3.1     8829.0
C3H8+IC3H7=NC3H7+C3H8        8.440E-03     4.2     8720.0
C3H8+C3H5=NC3H7+C3H6         2.350E+02     3.3    19800.0
C3H8+C3H5=IC3H7+C3H6         7.840E+01     3.3    18200.0
C3H8+CH3O=NC3H7+CH3OH        4.340E+11     0.0     6460.0
C3H8+CH3O=IC3H7+CH3OH        1.450E+11     0.0     4570.0
NC3H7=C2H4+CH3               1.260E+13     0.0    30404.0
NC3H7+O2=C3H6+HO2            1.000E+12     0.0     5000.0
IC3H7=C2H4+CH3               1.000E+12     0.0    34500.0
IC3H7+O2=C3H6+HO2            2.754E+10     0.0    -2151.0
C3H6=C3H5+H                  4.570E+14     0.0    88900.0
C3H6=SC3H5+H                 7.590E+14     0.0   101300.0
```

```
C3H6=TC3H5+H                1.450E+15     0.0    98060.0
C3H6=C2H3+CH3               1.100E+21    -1.2    97720.0
!KD-> C3H6+HO2=C3H6O+OH            1.050E+12     0.0    14210.0
C3H6+HO2=C3H5+H2O2          9.640E+03     2.6    13910.0
C3H6+HO2=SC3H5+H2O2         7.500E+09     0.0    12570.0
C3H6+HO2=TC3H5+H2O2         3.000E+09     0.0     9930.0
C3H6+OH=C3H5+H2O            3.120E+06     2.0     -300.0
C3H6+OH=SC3H5+H2O           2.140E+06     2.0     2780.0
C3H6+OH=TC3H5+H2O           1.110E+06     2.0     1450.0
C3H6+O=C2H5+HCO             6.833E+06     1.57    -628.0
C3H6+O=CH3+CH3CO            9.111E+06     1.57    -628.0
C3H6+O=C2H4+CH2O            4.555E+06     1.57    -628.0
NC3H7=C3H6+H                1.000E+14     0.0    37286.0
C3H6+H=IC3H7                5.704E+09     1.16     874.0
C3H6+H=C3H5+H2              6.457E+12     0.0     4445.0
C3H6+H=SC3H5+H2             7.810E+05     2.5    12280.0
C3H6+O2=SC3H5+HO2           1.950E+12     0.0    39000.0
C3H6+O2=TC3H5+HO2           1.950E+12     0.0    39000.0
C3H6+O2=C3H5+HO2            1.950E+12     0.0    39000.0
C3H6+CH3=C3H5+CH4           2.210E+00     3.5     5680.0
C3H6+CH3=SC3H5+CH4          1.350E+00     3.5    12850.0
C3H6+CH3=TC3H5+CH4          8.400E-01     3.5    11660.0
C3H6+C2H5=C3H5+C2H6         2.230E+00     3.5     6640.0
!KD-> C3H6O=C2H5+HCO              2.450E+13     0.0    58500.0
!KD-> C3H6O=C2H5CHO               1.820E+14     0.0    58500.0
!KD-> C3H6O=CH3+CH3CO             4.540E+13     0.0    59900.0
!KD-> C3H6O=CH3+CH2HCO            2.450E+13     0.0    58820.0
!KD-> C3H6O=CH3+C2H3O             8.000E+15     0.0    92010.0
!KD-> C2H5CHO=C2H5+HCO            2.450E+16     0.0    73000.0
!KD-> C2H5CHO+O=C2H5CO+OH          5.680E+12     0.0     1540.0
!KD-> C2H5CHO+OH=C2H5CO+H2O        1.210E+13     0.0        0.0
!KD-> C2H5CHO+HO2=C2H5CO+H2O2      1.520E+09     0.0        0.0
!KD-> C2H5CHO+C2H5=C2H5CO+C2H6     5.000E+10     0.0     6290.0
!KD-> C2H5CO=C2H5+CO              5.890E+12     0.0    14400.0
C3H5+O2=>CH2O+CH2HCO        5.000E+12     0.0    19190.0
C3H5+H=C3H4+H2              1.800E+13     0.0        0.0
C3H5+O=>C2H4+CO+H           1.807E+14     0.0        0.0
C3H5+CH3=C3H4+CH4           3.000E+12    -0.32    -130.0
C3H5+C2H5=C3H4+C2H6         9.640E+11     0.0     -130.0
C3H5+C2H3=C3H4+C2H4         2.400E+12     0.0        0.0
C3H5+C2H3=C3H6+C2H2         4.800E+12     0.0        0.0
SC3H5+O2=CH3HCO+HCO         4.340E+12     0.0        0.0
SC3H5+HO2=>CH2CO+CH3+OH     4.500E+12     0.0        0.0
SC3H5+H=C3H4+H2             3.333E+12     0.0        0.0
SC3H5+O=>CH2CO+CH3          1.807E+14     0.0        0.0
SC3H5+CH3=C3H4+CH4          1.000E+11     0.0        0.0
SC3H5+C2H5=C3H4+C2H6        1.000E+11     0.0        0.0
SC3H5+C2H3=C3H4+C2H4        1.000E+11     0.0        0.0
TC3H5+O2=CH3CO+CH2O         4.335E+11     0.0        0.0
TC3H5+HO2=>CH2CO+CH3+OH     4.500E+12     0.0        0.0
TC3H5+H=C3H4+H2             3.333E+12     0.0        0.0
```

```
TC3H5+O=>HCCO+CH3+H          1.807E+14     0.0       0.0
TC3H5+CH3=C3H4+CH4           1.000E+11     0.0       0.0
TC3H5+C2H5=C3H4+C2H6         1.000E+11     0.0       0.0
TC3H5+C2H3=C3H4+C2H4         1.000E+11     0.0       0.0
C3H4+M=C3H3+H+M              2.000E+18     0.0    80000.0
H2O/16.0/ CO2/3.75/ CO/1.875/ H2/2.5/ CH4/3.0/ C3H6/16.0/ C2H4/16.0/ C3H8/16.0/
C3H4(+M)=PC3H4(+M)           1.070E+14     0.0    64300.0
LOW /3.48E+17 0.0 48390.0/
C3H4+O2=C3H3+HO2             4.000E+13     0.0    61500.0
C3H4+HO2=>CH2CO+CH2+OH       8.000E+12     0.0    19000.0
C3H4+OH=CH2CO+CH3            3.120E+12     0.0     -397.0
C3H4+OH=C3H3+H2O             2.000E+07     2.0     1000.0
C3H4+O=C2H3+HCO              1.100E-02     4.613  -4243.0
C3H4+H=C3H5                  1.200E+11     0.69    3000.0
C3H4+H=TC3H5                 8.500E+12     0.0     2000.0
C3H4+H=C3H3+H2               2.000E+07     2.0     5000.0
C3H4+CH3=C3H3+CH4            2.000E+11     0.0     7700.0
PC3H4+M=C3H3+H+M             4.700E+18     0.0    80000.0
H2O/16.0/ CO2/3.75/ CO/1.875/ H2/2.5/ CH4/3.0/ C3H6/16.0/ C2H4/16.0/ C3H8/16.0/
PC3H4+O2=>HCCO+OH+CH2        2.000E+08     1.5    30100.0
PC3H4+O2=C3H3+HO2            5.000E+12     0.0    51000.0
PC3H4+HO2=>C2H4+CO+OH        3.000E+12     0.0    19000.0
PC3H4+OH=C3H3+H2O            2.000E+07     2.0     1000.0
PC3H4+OH=CH2CO+CH3           5.000E-04     4.5    -1000.0
PC3H4+O=CH2CO+CH2            6.400E+12     0.0     2010.0
PC3H4+O=C2H3+HCO             3.200E+12     0.0     2010.0
PC3H4+O=HCCO+CH3             6.300E+12     0.0     2010.0
PC3H4+O=>HCCO+CH2+H          3.200E+11     0.0     2010.0
PC3H4+H=TC3H5                6.500E+12     0.0     2000.0
PC3H4+H=C3H3+H2              2.000E+07     2.0     5000.0
PC3H4+H=C2H2+CH3             1.300E+05     2.5     1000.0
PC3H4+CH3=C3H3+CH4           1.500E+00     3.5     5600.0
PC3H4+C2H3=C3H3+C2H4         1.000E+12     0.0     7700.0
PC3H4+C3H5=C3H3+C3H6         1.000E+12     0.0     7700.0
!KD-> C3H3+H=C3H2+H2         5.000E+13     0.0     3000.0
C3H3+O=>C2H+HCO+H            7.000E+13     0.0       0.0
C3H3+O=>C2H2+CO+H            7.000E+13     0.0       0.0
!KD-> C3H3+OH=C3H2+H2O       1.000E+13     0.0       0.0
C3H3+O2=CH2CO+HCO            3.010E+10     0.0     2870.0
C3H3+CH=IC4H3+H              7.000E+13     0.0       0.0
!KD-> C3H3+CH=NC4H3+H        7.000E+13     0.0       0.0
C3H3+CH2=C4H4+H              4.000E+13     0.0       0.0
!KD-> C3H3+C3H3=C6H5+H       2.000E+12     0.0       0.0
!KD-> CH+C2H2=C3H2+H         1.000E+14     0.0       0.0
!KD-> C3H2+O2=HCCO+CO+H      1.000E+14     0.0     3000.0
!KD-> C3H2+OH=C2H2+HCO       5.000E+13     0.0       0.0
!KD-> C3H2+CH2=IC4H3+H       3.000E+13     0.0       0.0
C4H8=IC4H7+H                 4.078E+18    -1.0    97350.0
!KD-> C4H8=C2C4H8            4.000E+11     0.0    60000.0
!KD-> C4H8=T2C4H8            4.000E+11     0.0    60000.0
C4H8=C3H5+CH3                1.000E+16     0.0    73000.0
```

```
C4H8=C2H3+C2H5               1.000E+19     -1.0     96770.0
C4H8+O2=IC4H7+HO2             4.000E+12      0.0    33200.0
C4H8+HO2=IC4H7+H2O2           1.000E+11      0.0    17060.0
C4H8+OH=NC3H7+CH2O            6.500E+12      0.0        0.0
C4H8+OH=CH3HCO+C2H5           1.000E+11      0.0        0.0
C4H8+OH=C2H6+CH3CO            1.000E+10      0.0        0.0
C4H8+OH=IC4H7+H2O             2.250E+13      0.0     2217.0
C4H8+O=C3H6+CH2O              2.505E+12      0.0        0.0
C4H8+O=CH3HCO+C2H4            1.250E+12      0.0      850.0
C4H8+O=C2H5+CH3CO             1.625E+13      0.0      850.0
C4H8+O=IC4H7+OH               9.600E+12      0.0     1970.0
C4H8+O=NC3H7+HCO              1.800E+05      2.5    -1029.0
C4H8+H=IC4H7+H2               5.000E+13      0.0     3900.0
C4H8+CH3=IC4H7+CH4            1.000E+11      0.0     7300.0
C4H8+C2H5=IC4H7+C2H6          1.000E+11      0.0     8000.0
C4H8+C3H5=IC4H7+C3H6          7.900E+10      0.0    12400.0
C4H8+SC3H5=IC4H7+C3H6         8.000E+10      0.0    12400.0
C4H8+TC3H5=IC4H7+C3H6         8.000E+10      0.0    12400.0
!KD-> C2C4H8=T2C4H8               4.000E+13      0.0    62000.0
!KD-> C2C4H8=C4H6+H2              1.000E+13      0.0    65500.0
!KD-> C2C4H8=IC4H7+H              4.074E+18     -1.0    97350.0
!KD-> C2C4H8=SC3H5+CH3            2.000E+16      0.0    95000.0
!KD-> C2C4H8+OH=IC4H7+H2O         1.250E+14      0.0     3060.0
!KD-> C2C4H8+OH=CH3HCO+C2H5       1.400E+13      0.0        0.0
!KD-> C2C4H8+O=IC3H7+HCO          6.030E+12      0.0        0.0
!KD-> C2C4H8+O=CH3HCO+C2H4        1.000E+12      0.0        0.0
!KD-> C2C4H8+H=IC4H7+H2           1.000E+13      0.0     3500.0
!KD-> C2C4H8+CH3=IC4H7+CH4        1.000E+11      0.0     8200.0
!KD-> T2C4H8=IC4H7+H              4.074E+18     -1.0    97350.0
!KD-> T2C4H8=SC3H5+CH3            2.000E+16      0.0    96000.0
!KD-> T2C4H8+OH=IC4H7+H2O         1.000E+14      0.0     3060.0
!KD-> T2C4H8+OH=CH3HCO+C2H5       1.500E+13      0.0        0.0
!KD-> T2C4H8+O=IC3H7+HCO          6.030E+12      0.0        0.0
!KD-> T2C4H8+O=CH3HCO+C2H4        1.000E+12      0.0        0.0
!KD-> T2C4H8+H=IC4H7+H2           5.000E+12      0.0     3500.0
!KD-> T2C4H8+CH3=IC4H7+CH4        1.000E+11      0.0     8200.0
IC4H7=C4H6+H                  1.200E+14      0.0    49300.0
IC4H7=C2H4+C2H3               1.000E+14      0.0    49000.0
IC4H7+H=C4H6+H2               3.160E+12      0.0        0.0
IC4H7+O2=C4H6+HO2             1.000E+11      0.0        0.0
IC4H7+CH3=C4H6+CH4            1.000E+13      0.0        0.0
IC4H7+C2H3=C4H6+C2H4          4.000E+12      0.0        0.0
IC4H7+C2H5=C4H6+C2H6          4.000E+12      0.0        0.0
IC4H7+C2H5=C4H8+C2H4          5.000E+11      0.0        0.0
!KD-> IC4H7+C2H5=T2C4H8+C2H4      5.000E+11      0.0        0.0
!KD-> IC4H7+C2H5=C2C4H8+C2H4      5.000E+11      0.0        0.0
IC4H7+C3H5=C4H6+C3H6          4.000E+13      0.0        0.0
IC4H7+IC4H7=C4H6+C4H8         3.160E+12      0.0        0.0
C2H3+C2H4=C4H6+H              3.000E+12      0.0     1000.0
!KD-> C4H6+H=NC4H5+H2             3.000E+07      2.0    13000.0
C4H6+H=IC4H5+H2               3.000E+07      2.0     6000.0
```

```
!KD-> C4H6+OH=NC4H5+H2O           2.000E+07     2.0     5000.0
C4H6+OH=IC4H5+H2O           2.000E+07     2.0     2000.0
C4H6+O=C2H4+CH2CO           1.000E+12     0.0        0.0
C4H6+O=PC3H4+CH2O           1.000E+12     0.0        0.0
!KD-> C2H2+NC4H5=C6H6+H           2.800E+03     2.9     1400.0
!KD-> NC4H5+OH=C4H4+H2O           2.000E+07     2.0     1000.0
!KD-> NC4H5+H=C4H4+H2             3.000E+07     2.0     1000.0
!KD-> NC4H5+H=IC4H5+H             1.000E+14     0.0        0.0
IC4H5=C4H4+H                2.000E+15     0.0    45000.0
!KD-> NC4H5=C4H4+H                1.600E+14     0.0    41400.0
C4H4+OH=IC4H3+H2O           1.000E+07     2.0     2000.0
!KD-> C4H4+OH=NC4H3+H2O           7.500E+06     2.0     5000.0
!KD-> C4H4+H=NC4H3+H2             2.000E+07     2.0    15000.0
!KD-> NC4H3+H=IC4H3+H             1.000E+14     0.0        0.0
IC4H3+CH2=C3H4+C2H          2.000E+13     0.0        0.0
IC4H3+O2=CH2CO+HCCO         1.000E+12     0.0        0.0
!KD-> IC4H3+OH=C4H2+H2O           3.000E+13     0.0        0.0
IC4H3+O=CH2CO+C2H           2.000E+13     0.0        0.0
!KD-> IC4H3+H=C4H2+H2             5.000E+13     0.0        0.0
!KD-> NC4H3+C2H2=C6H5             2.800E+03     2.9     1400.0
!KD-> NC4H3+M=C4H2+H+M            1.000E+16     0.0    59700.0
!KD->   H2O/16.0/   CO2/3.75/   CO/1.875/   H2/2.5/   CH4/3.0/   C3H6/16.0/   C2H4/16.0/
C3H8/16.0/
!KD-> IC4H3+M=C4H2+H+M            4.460E+15     0.0    46516.0
!KD->   H2O/16.0/   CO2/3.75/   CO/1.875/   H2/2.5/   CH4/3.0/   C3H6/16.0/   C2H4/16.0/
C3H8/16.0/
!KD-> IC4H3+O=H2C4O+H             2.000E+13     0.0        0.0
!KD-> H2C4O+H=C2H2+HCCO           5.000E+13     0.0     3000.0
!KD-> H2C4O+OH=CH2CO+HCCO         1.000E+07     2.0     2000.0
!KD-> C4H2+OH=H2C4O+H             6.660E+12     0.0     -410.0
C2H2+C2H2=IC4H3+H           2.200E+12     0.0    64060.0
!KD-> C2H2+C2H2=NC4H3+H           1.000E+12     0.0    66000.0
C2H2+C2H2=C4H4              5.500E+12     0.0    37000.0
!KD-> C4H2(+M)=C4H+H(+M)          2.200E+14     0.0   116740.0
!KD->       LOW /3.50E+17  0.0  80065.0/
!KD->       H2O /16.0/ H2 /2.5/ CO /1.875/ CO2 /3.75/ CH4 /3.0/
!KD->       C3H6 /16.0/ C2H4 /16.0/ C3H8 /16.0/
!KD-> C4H2+O=C3H2+CO              2.700E+13     0.0     1720.0
!KD-> C2H2+C2H=C4H2+H             1.820E+14     0.0      467.0
!KD-> C2H2+C2H=NC4H3              1.000E+13     0.0        0.0
!KD-> C4H+O2=C2H+CO+CO            1.000E+14     0.0        0.0
!KD-> C2O+H=CH+CO                 1.320E+13     0.0        0.0
!KD-> C2O+O=CO+CO                 5.200E+13     0.0        0.0
!KD-> C2O+OH=CO+CO+H              2.000E+13     0.0        0.0
!KD-> C2O+O2=CO+CO+O              2.000E+13     0.0        0.0
!KD-> C2O+O2=CO+CO2               2.000E+13     0.0        0.0
!KD-> C2+H2=C2H+H                 6.600E+13     0.0     7950.0
!KD-> C2+O=C+CO                   3.600E+14     0.0        0.0
!KD-> C2+O2=CO+CO                 9.000E+12     0.0      980.0
!KD-> C2+OH=C2O+H                 5.000E+13     0.0        0.0
!KD-> C6H5+OH=C6H5O+H             5.000E+13     0.0        0.0
```

```
!KD-> C6H5+O2=C6H5O+O              2.600E+13     0.0     6120.0
!KD-> C6H5+HO2=C6H5O+OH            5.000E+13     0.0     1000.0
!KD-> C6H6+H=C6H5+H2               3.000E+12     0.0     8100.0
!KD-> C6H6+OH=C6H5+H2O             1.680E+08     1.42    1450.0
!KD-> C6H6+O=C6H5O+H               2.780E+13     0.0     4910.0
!KD-> C6H6+O2=C6H5O+OH             4.000E+13     0.0    34000.0
!KD-> H+C6H5=C6H6                  7.800E+13     0.0        0.0
C3H3+O=>C2H3+CO              3.800E+13     0.0        0.0
C3H3+O=CH2O+C2H              2.000E+13     0.0        0.0
C3H3+O2=>HCCO+CH2O           6.000E+12     0.0        0.0
C3H3+CH3=C2H5+C2H            1.000E+13     0.0    37500.0
C3H3+CH3=C4H6                5.000E+12     0.0        0.0
C3H6+C2H3=C3H5+C2H4          2.210E+00     3.5     4680.0
C3H6+C2H3=SC3H5+C2H4         1.350E+00     3.5    10860.0
C3H6+C2H3=TC3H5+C2H4         8.400E-01     3.5     9670.0
C3H6+CH3O=C3H5+CH3OH         9.000E+01     2.95   12000.0
CH2+C2H2=C3H4                1.200E+13     0.0     6620.0
C3H4+C3H4=C3H5+C3H3          5.000E+14     0.0    64700.0
C3H4+OH=CH2O+C2H3            1.700E+12     0.0     -300.0
C3H4+OH=HCO+C2H4             1.700E+12     0.0     -300.0
C3H4+O=CH2O+C2H2             1.000E+12     0.0        0.0
C3H4+O=>CO+C2H4              7.800E+12     0.0     1600.0
C3H4+C3H5=C3H3+C3H6          2.000E+12     0.0     7700.0
C3H4+C2H=C3H3+C2H2           1.000E+13     0.0        0.0
PC3H4=C2H+CH3                4.200E+16     0.0   100000.0
PC3H4+C2H=C3H3+C2H2          1.000E+13     0.0        0.0
!KD-> C3H2+O2=HCO+HCCO             1.000E+13     0.0        0.0
!KD-> C2H2+C2H3=NC4H5              2.510E+05     1.9     2100.0
C2H3+C2H3=IC4H5+H            4.000E+13     0.0        0.0
IC4H5+H=C4H4+H2              3.000E+07     2.0     1000.0
!KD-> C4H2+H=C4H+H2                1.000E+14     0.0    35000.0
C4H6+OH=C3H5+CH2O            7.230E+12     0.0     -994.0
!KD-> C4H8+IC4H7=IC4H7+C2C4H8      3.980E+10     0.0    12400.0
!KD-> C4H8+IC4H7=IC4H7+T2C4H8      3.980E+10     0.0    12400.0
!KD-> C3H3+C3H3=C6H6               3.000E+11     0.0        0.0
!KD-> C3H3+C3H4=C6H6+H             1.400E+12     0.0    10000.0
C3H5+C2H5=C3H6+C2H4          2.600E+12     0.0     -130.0
C3H6+OH=C2H5+CH2O            8.000E+12     0.0        0.0
C3H6+OH=CH3+CH3HCO           3.400E+11     0.0        0.0
C3H5+O2=C3H4+HO2             1.200E+12     0.0    13550.0
CH2O+C3H5=HCO+C3H6           8.000E+10     0.0    12400.0
CH3HCO+C3H5=CH3CO+C3H6       3.800E+11     0.0     7200.0
!KD-> C3H8+CH3O2=NC3H7+CH3O2H      6.030E+12     0.0    19380.0
!KD-> C3H8+CH3O2=IC3H7+CH3O2H      1.990E+12     0.0    17050.0
!KD-> C3H8+C2H5O2=NC3H7+C2H5O2H    6.030E+12     0.0    19380.0
!KD-> C3H8+C2H5O2=IC3H7+C2H5O2H    1.990E+12     0.0    17050.0
!KD-> C3H8+IC3H7O2=NC3H7+IC3H7O2H  6.030E+12     0.0    19380.0
!KD-> C3H8+IC3H7O2=IC3H7+IC3H7O2H  1.990E+12     0.0    17050.0
!KD-> C3H8+NC3H7O2=NC3H7+NC3H7O2H  6.030E+12     0.0    19380.0
!KD-> C3H8+NC3H7O2=IC3H7+NC3H7O2H  1.990E+12     0.0    17050.0
!KD-> NC3H7+O2=NC3H7O2             4.820E+12     0.0        0.0
```

```
!KD-> IC3H7+O2=IC3H7O2              6.620E+12     0.0        0.0
!KD-> NC3H7+HO2=NC3H7O+OH           3.200E+13     0.0        0.0
!KD-> IC3H7+HO2=IC3H7O+OH           3.200E+13     0.0        0.0
!KD-> NC3H7+CH3O2=NC3H7O+CH3O       3.800E+12     0.0    -1200.0
!KD-> IC3H7+CH3O2=IC3H7O+CH3O       3.800E+12     0.0    -1200.0
!KD-> NC3H7+NC3H7O2=NC3H7O+NC3H7O    3.800E+12     0.0    -1200.0
!KD-> IC3H7+NC3H7O2=IC3H7O+NC3H7O    3.800E+12     0.0    -1200.0
!KD-> NC3H7+IC3H7O2=NC3H7O+IC3H7O    3.800E+12     0.0    -1200.0
!KD-> IC3H7+IC3H7O2=IC3H7O+IC3H7O    3.800E+12     0.0    -1200.0
!KD-> NC3H7O2+HO2=NC3H7O2H+O2       4.600E+10     0.0    -2600.0
!KD-> IC3H7O2+HO2=IC3H7O2H+O2       4.600E+10     0.0    -2600.0
!KD-> CH3+NC3H7O2=CH3O+NC3H7O       3.800E+12     0.0    -1200.0
!KD-> CH3+IC3H7O2=CH3O+IC3H7O       3.800E+12     0.0    -1200.0
!KD-> NC3H7O2H=NC3H7O+OH            4.000E+15     0.0    43000.0
!KD-> IC3H7O2H=IC3H7O+OH            4.000E+15     0.0    43000.0
!KD-> NC3H7O=C2H5+CH2O              5.000E+13     0.0    15700.0
!KD-> IC3H7O=CH3+CH3HCO             4.000E+14     0.0    17200.0
!KD-> C3H6+OH(+M)=C3H6OH(+M)        1.810E+13     0.0        0.0
!KD->     LOW /1.33E+30  -3.5  0.0/
!KD-> C3H6OH=>C2H5+CH2O             1.400E+09     0.0    17200.0
!KD-> C3H6OH=>CH3+CH3HCO            1.000E+09     0.0    17200.0
!KD-> C3H6OH+O2=O2C3H6OH            1.000E+12     0.0    -1100.0
!KD-> O2C3H6OH=>CH3HCO+CH2O+OH      1.000E+16     0.0    25000.0
!KD-> C3H6+CH3O2=C3H5+CH3O2H        2.000E+12     0.0    17000.0
!KD-> C3H6+CH3O2=C3H6O+CH3O         4.000E+11     0.0    11720.0
!KD-> C3H6+C2H5O2=C3H5+C2H5O2H      3.200E+11     0.0    14900.0
!KD-> C3H6+C3H5O2=C3H5+C3H5O2H      3.200E+11     0.0    14900.0
!KD-> C3H6+C3H5O2=C3H6O+C3H5O       1.050E+11     0.0    14200.0
!KD-> C3H6+CH3CO3=C3H5+CH3CO3H      3.200E+11     0.0    14900.0
!KD-> C3H6+NC3H7O2=C3H5+NC3H7O2H    3.200E+11     0.0    14900.0
!KD-> C3H6+IC3H7O2=C3H5+IC3H7O2H    3.200E+11     0.0    14900.0
!KD-> C3H6+NC3H7O2=C3H6O+NC3H7O     1.700E+07     0.0        0.0
!KD-> C3H5+O2=C3H5O2                1.200E+10     0.0    -2300.0
C3H5+HO2=C3H5O+OH             9.000E+12     0.0        0.0
C3H5+CH3O2=C3H5O+CH3O         3.800E+11     0.0    -1200.0
!KD-> C3H5O2+CH3=C3H5O+CH3O         3.800E+11     0.0    -1200.0
!KD-> C3H5O2+C3H5=C3H5O+C3H5O       3.800E+11     0.0    -1200.0
!KD-> C3H5O2+HO2=C3H5O2H+O2         4.600E+10     0.0    -2600.0
!KD-> C3H5O2+HO2=>C3H5O+OH+O2       1.000E+12     0.0        0.0
!KD-> C3H5O2+CH3O2=>C3H5O+CH3O+O2    1.700E+11     0.0    -1000.0
!KD-> C3H5O2+C3H5O2=>C3H5O+C3H5O+O2  3.700E+12     0.0     2200.0
C3H5O=CH2O+C2H3               1.000E+14     0.0    21600.0
!KD-> C3H5O2H=C3H5O+OH              4.000E+15     0.0    43000.0
!KD-> CH2O+C3H5O2=HCO+C3H5O2H       1.300E+11     0.0    10500.0
!KD-> CH2O+NC3H7O2=HCO+NC3H7O2H     1.300E+11     0.0     9000.0
!KD-> CH2O+IC3H7O2=HCO+IC3H7O2H     1.300E+11     0.0     9000.0
!KD-> C2H4+NC3H7O2=C2H3+NC3H7O2H    7.100E+11     0.0    25000.0
!KD-> C2H4+IC3H7O2=C2H3+IC3H7O2H    7.100E+11     0.0    25000.0
!KD-> CH4+C3H5O2=CH3+C3H5O2H        1.140E+13     0.0    20460.0
!KD-> CH4+NC3H7O2=CH3+NC3H7O2H      1.140E+13     0.0    20460.0
!KD-> CH4+IC3H7O2=CH3+IC3H7O2H      1.140E+13     0.0    20460.0
```

```
!KD-> CH3OH+NC3H7O2=CH2OH+NC3H7O2H   6.300E+12     0.0    19360.0
!KD-> CH3OH+IC3H7O2=CH2OH+IC3H7O2H   6.300E+12     0.0    19360.0
!KD-> CH3HCO+C3H5O2=CH3CO+C3H5O2H    1.150E+11     0.0    10000.0
!KD-> CH3HCO+NC3H7O2=CH3CO+NC3H7O2H  1.150E+11     0.0    10000.0
!KD-> CH3HCO+IC3H7O2=CH3CO+IC3H7O2H  1.150E+11     0.0    10000.0
!KD-> C+N2+M=CNN+M                   1.120E+15     0.0        0.0
C2H+NO=HCN+CO                  6.000E+13     0.0      570.0
C2H+HCN=CN+C2H2                3.200E+12     0.0     1530.0
CH2+NO=HCN+OH                  5.000E+11     0.0     2870.0
HCN+M=H+CN+M                   3.570E+26    -2.6   124900.0
!KD-> C2N2+M=CN+CN+M                 3.200E+16     0.0    94400.0
!KD-> CH+N2(+M)=HCNN(+M)             3.100E+12     0.15       0.0
!KD->      LOW / 1.30E+25 -3.16 740.0 /
!KD->      TROE /0.667 235.0 2117.0 4536.0 /
!KD->      H2O/10.0/ O2/2.0/ AR/0.75/ H2/2.0/
!KD-> HCNN+H=H2+CNN                  5.000E+13     0.0        0.0
!KD-> HCNN+H=>CH2+N2                 2.000E+13     0.0     3000.0
!KD-> HCNN+O=OH+CNN                  2.000E+13     0.0    20000.0
!KD-> HCNN+O=CO+H+N2                 5.000E+13     0.0    15000.0
!KD-> HCNN+O=HCN+NO                  5.000E+13     0.0    15000.0
!KD-> HCNN+OH=H2O+CNN                1.000E+13     0.0     8000.0
!KD-> HCNN+OH=H+HCO+N2               1.000E+13     0.0    16000.0
!KD-> HCNN+O2=HO2+CNN                1.000E+12     0.0     4000.0
!KD-> HCNN+O2=>H+CO2+N2              4.000E+12     0.0        0.0
!KD-> HCNN+O2=HCO+N2O                4.000E+12     0.0        0.0
!KD-> CNN+O=CO+N2                    1.000E+13     0.0        0.0
!KD-> CNN+O=CN+NO                    1.000E+14     0.0    20000.0
!KD-> CNN+OH=H+CO+N2                 1.000E+13     0.0     1000.0
!KD-> CNN+H=NH+CN                    5.000E+14     0.0    40000.0
!KD-> CNN+OH=HCN+NO                  1.000E+12     0.0     1000.0
!KD-> CNN+H=HCN+N                    5.000E+13     0.0    25000.0
!KD-> CNN+O2=NO+NCO                  1.000E+13     0.0     5000.0
HNO+CH3=NO+CH4                 8.200E+05     1.87      954.0
HONO+CH3=NO2+CH4               8.100E+05     1.87     5504.0
H2NO+CH3=CH3O+NH2              2.000E+13     0.0        0.0
H2NO+CH3=HNO+CH4               1.600E+06     1.87     2960.0
HNOH+CH3=HNO+CH4               1.600E+06     1.87     2096.0
!KD-> NH2OH+CH3=HNOH+CH4             1.600E+06     1.87     6350.0
!KD-> NH2OH+CH3=H2NO+CH4             8.200E+05     1.87     5500.0
N2H2+CH3=NNH+CH4               1.600E+06     1.87     2970.0
N2H3+CH3=N2H2+CH4              8.200E+05     1.87     1818.0
N2H4+CH3=N2H3+CH4              3.300E+06     1.87     5325.0
CH4+NH=CH3+NH2                 9.000E+13     0.0    20080.0
CH4+NH2=CH3+NH3                1.200E+13     0.0    15150.0
CH3+NH2=CH2+NH3                1.600E+06     1.87     7570.0
C2H6+NH=C2H5+NH2               7.000E+13     0.0    16700.0
C2H6+NH2=C2H5+NH3              9.700E+12     0.0    11470.0
C3H8+NH2=NC3H7+NH3             1.700E+13     0.0    10660.0
C3H8+NH2=IC3H7+NH3             4.500E+11     0.0     6150.0
!KD-> CH3+NO(+M)=CH3NO(+M)           1.000E+13     0.0        0.0
!KD->     LOW /1.90E+18 0.0 0.0/
```

```
!KD->    SRI /0.03 -790.0 1.0/
!KD-> CH3NO+H=H2CNO+H2            4.400E+08     1.5      377.0
!KD-> CH3NO+H=CH3+HNO             1.800E+13     0.0     2800.0
!KD-> CH3NO+O=H2CNO+OH            3.300E+08     1.5     3615.0
!KD-> CH3NO+O=CH3+NO2             1.700E+06     2.08       0.0
!KD-> CH3NO+OH=H2CNO+H2O          3.600E+06     2.0    -1192.0
!KD-> CH3NO+OH=CH3+HONO           2.500E+12     0.0     1000.0
!KD-> CH3NO+CH3=H2CNO+CH4         7.900E+05     1.87    5415.0
!KD-> CH3NO+NH2=H2CNO+NH3         2.800E+06     1.94    1073.0
!KD-> H2CNO=HNCO+H                2.300E+42    -9.11   53840.0
!KD-> H2CNO+O2=CH2O+NO2           2.900E+12    -0.31   17700.0
!KD-> H2CNO+H=CH3+NO              4.000E+13     0.0        0.0
!KD-> H2CNO+H=HCNO+H2             4.800E+08     1.5     -894.0
!KD-> H2CNO+O=HCNO+OH             3.300E+08     1.5     -894.0
!KD-> H2CNO+O=CH2O+NO             7.000E+13     0.0        0.0
!KD-> H2CNO+OH=CH2OH+NO           4.000E+13     0.0        0.0
!KD-> H2CNO+OH=HCNO+H2O           2.400E+06     2.0    -1192.0
!KD-> H2CNO+CH3=C2H5+NO           3.000E+13     0.0        0.0
!KD-> H2CNO+CH3=HCNO+CH4          1.600E+06     1.87   -1113.0
!KD-> H2CNO+NH2=HCNO+NH3          1.800E+06     1.94   -1152.0
CH3+NO2=CH3O+NO             1.400E+13     0.0        0.0
CH+NO2=HCO+NO               1.200E+14     0.0        0.0
CH2+NO2=CH2O+NO             4.200E+13     0.0        0.0
CN+NO=N2+CO                 1.000E+11     0.0        0.0
HNCO+M=H+NCO+M              5.000E+15     0.0   120000.0
HNCO+N=NH+NCO               4.000E+13     0.0    36000.0
CH3O+HNO=CH3OH+NO           3.160E+13     0.0        0.0
NCO+HO2=HNCO+O2             2.000E+13     0.0        0.0
N2O+CO=CO2+N2               2.510E+14     0.0    46000.0
N2O+CH2=CH2O+N2             1.000E+12     0.0        0.0
N2O+CH3=CH3O+N2             9.000E+09     0.0        0.0
N2O+HCO=CO2+H+N2            1.700E+14     0.0    20000.0
N2O+HCCO=CO+HCO+N2          1.700E+14     0.0    25500.0
N2O+C2H2=HCCO+H+N2          6.590E+16     0.0    61200.0
N2O+C2H3=CH2HCO+N2          1.000E+11     0.0        0.0
HOCN+O=NCO+OH               1.500E+04     2.64    4000.0
HOCN+H=NCO+H2               2.000E+07     2.0     2000.0
HOCN+H=NH2+CO               1.200E+08     0.61    2080.0
HOCN+OH=NCO+H2O             6.380E+05     2.0     2560.0
HOCN+CH3=NCO+CH4            8.200E+05     1.87    6620.0
HOCN+NH2=NCO+NH3            9.200E+05     1.94    3645.0
CN+NO2=CO+N2O               4.930E+14    -0.752    344.0
CN+NO2=CO2+N2               3.700E+14    -0.752    344.0
CN+CO2=NCO+CO               3.670E+06     2.16    26900.0
CN+NH3=HCN+NH2              9.200E+12     0.0     -357.0
HNCO+CN=HCN+NCO             1.500E+13     0.0        0.0
HONO+NCO=HNCO+NO2           3.600E+12     0.0        0.0
NCO+CH2O=HNCO+HCO           6.000E+12     0.0        0.0
!CH+N2=HCN+N                3.680E+07     1.42    20723.0
!KD-> NH2+C=CH+NH                 5.800E+11     0.67   20900.0
!KD-> C+N2=CN+N                   5.200E+13     0.0    44700.0
```

```
CH2+N2=HCN+NH               4.800E+12     0.0    35850.0
!KD-> C2+N2=CN+CN               1.500E+13     0.0    41700.0
H2CN+N=N2+CH2               6.000E+13     0.0      400.0
H2CN+H=HCN+H2               2.400E+08     1.5     -894.0
H2CN+O=HCN+OH               1.700E+08     1.5     -894.0
H2CN+O=HNCO+H               6.000E+13     0.0        0.0
H2CN+O=HCNO+H               2.000E+13     0.0        0.0
H2CN+M=HCN+H+M              3.000E+14     0.0    22000.0
H2CN+HO2=HCN+H2O2           1.400E+04     2.69   -1610.0
H2CN+O2=CH2O+NO             3.000E+12     0.0     6000.0
H2CN+CH3=HCN+CH4            8.100E+05     1.87   -1113.0
H2CN+OH=HCN+H2O             1.200E+06     2.0    -1192.0
H2CN+NH2=HCN+NH3            9.200E+05     1.94   -1152.0
!KD-> C+NO=CN+O                 2.000E+13     0.0        0.0
CH+NO=HCN+O                 8.690E+13     0.0        0.0
CH+NO=CN+OH                 1.680E+12     0.0        0.0
CH+NO=CO+NH                 9.840E+12     0.0        0.0
CH+NO=NCO+H                 1.670E+13     0.0        0.0
CH2+NO=HNCO+H               2.500E+12     0.0     5970.0
CH2+NO=HCNO+H               3.800E+13    -0.36     576.0
CH2+NO=NH2+CO               2.300E+16    -1.43    1331.0
CH2+NO=H2CN+O               8.100E+07     1.42    4110.0
CH3+NO=HCN+H2O              2.400E+12     0.0    15700.0
CH3+NO=H2CN+OH              5.200E+12     0.0    24240.0
HCCO+NO=HCNO+CO             4.640E+13     0.0      700.0
HCCO+NO=HCN+CO2             1.390E+13     0.0      700.0
SCH2+NO=HCN+OH              1.000E+14     0.0        0.0
HCNO=HCN+O                  4.200E+31    -6.12   61210.0
HCNO+H=HCN+OH               1.000E+14     0.0    12000.0
HCNO+H=HNCO+H               2.100E+15    -0.69    2850.0
HCNO+H=HOCN+H               1.400E+11    -0.19    2484.0
HCNO+H=NH2+CO               1.700E+14    -0.75    2890.0
HCNO+O=HCO+NO               7.000E+13     0.0        0.0
CH2+N=HCN+H                 5.000E+13     0.0        0.0
CH2+N=NH+CH                 6.000E+11     0.67   40500.0
CH+N=CN+H                   1.670E+14    -0.09       0.0
!KD-> CH+N=C+NH                 4.500E+11     0.65    2400.0
N+CO2=NO+CO                 1.900E+11     0.0     3400.0
N+HCCO=HCN+CO               5.000E+13     0.0        0.0
CH3+N=H2CN+H                7.100E+13     0.0        0.0
!KD-> CH3+N=HCNH+H              1.200E+11     0.52     367.6
!KD-> HCNH=HCN+H                6.100E+28    -5.69   24270.0
!KD-> HCNH+H=H2CN+H             2.000E+13     0.0        0.0
!KD-> HCNH+H=HCN+H2             2.400E+08     1.5     -894.0
!KD-> HCNH+O=HNCO+H             7.000E+13     0.0        0.0
!KD-> HCNH+O=HCN+OH             1.700E+08     1.5     -894.0
!KD-> HCNH+OH=HCN+H2O           1.200E+06     2.0    -1192.0
!KD-> HCNH+CH3=HCN+CH4          8.200E+05     1.87   -1113.0
C2H3+N=HCN+CH2              2.000E+13     0.0        0.0
CN+H2O=HCN+OH               4.000E+12     0.0     7400.0
CN+H2O=HOCN+H               4.000E+12     0.0     7400.0
```

```
OH+HCN=HOCN+H              3.200E+04     2.45    12120.0
OH+HCN=HNCO+H              5.600E-06     4.71     -490.0
OH+HCN=NH2+CO              6.440E+10     0.0     11700.0
HOCN+H=HNCO+H              1.000E+13     0.0         0.0
HCN+O=NCO+H                1.380E+04     2.64     4980.0
HCN+O=NH+CO                3.450E+03     2.64     4980.0
HCN+O=CN+OH                2.700E+09     1.58    26600.0
CN+H2=HCN+H                2.000E+04     2.87     1600.0
CN+O=CO+N                  1.900E+12     0.46      720.0
CN+O2=NCO+O                7.200E+12     0.0      -400.0
CN+OH=NCO+H                4.000E+13     0.0         0.0
!KD-> CN+HCN=C2N2+H              1.510E+07     1.71     1530.0
CN+NO2=NCO+NO              5.320E+15    -0.752     344.0
CN+N2O=NCO+N2              6.000E+12     0.0     15360.0
!KD-> C2N2+O=NCO+CN              4.570E+12     0.0      8880.0
!KD-> C2N2+OH=HNCO+CN            1.860E+11     0.0      2900.0
!KD-> C2N2+OH=HOCN+CN            2.000E+12     0.0     19000.0
HNCO+H=H2+NCO              1.760E+05     2.41    12300.0
HNCO+H=NH2+CO              3.600E+04     2.49     2340.0
HNCO+M=NH+CO+M             1.100E+16     0.0     86000.0
N2/1.5/ O2/1.5/ H2O/18.6/
HNCO+O=NCO+OH              2.200E+06     2.11    11430.0
HNCO+O=NH+CO2              9.800E+07     1.41     8530.0
HNCO+O=HNO+CO              1.500E+08     1.57    44012.0
HNCO+OH=NCO+H2O            3.450E+07     1.5      3600.0
HNCO+OH=NH2+CO2            6.300E+10    -0.06    11645.0
HNCO+HO2=NCO+H2O2          3.000E+11     0.0     29000.0
HNCO+O2=HNO+CO2            1.000E+12     0.0     35000.0
HNCO+NH2=NCO+NH3           5.000E+12     0.0      6200.0
HNCO+NH=NCO+NH2            1.040E+15     0.0     39390.0
NCO+H=NH+CO                5.360E+13     0.0         0.0
NCO+O=NO+CO                4.200E+13     0.0         0.0
NCO+O=N+CO2                8.000E+12     0.0      2500.0
NCO+N=N2+CO                2.000E+13     0.0         0.0
NCO+OH=NO+HCO              5.000E+12     0.0     15000.0
NCO+M=N+CO+M               2.200E+14     0.0     54050.0
NCO+NO=N2O+CO              4.600E+18    -2.01      934.0
NCO+NO=N2+CO2              5.800E+18    -2.01      934.0
NCO+O2=NO+CO2              2.000E+12     0.0     20000.0
NCO+HCO=HNCO+CO            3.600E+13     0.0         0.0
NCO+NO2=CO+NO+NO           2.830E+13    -0.646    -326.0
NCO+NO2=CO2+N2O            3.570E+14    -0.646    -326.0
NCO+HNO=HNCO+NO            1.800E+13     0.0         0.0
NCO+NCO=CO+CO+N2           3.000E+12     0.0         0.0
NO+HCO=CO+HNO              7.240E+13    -0.4        0.0
NO2+CO=CO2+NO              9.000E+13     0.0     33800.0
NO2+HCO=H+CO2+NO           8.400E+15    -0.75     1930.0
CH3O+NO2=HONO+CH2O         3.000E+12     0.0         0.0
CH3O+NO=CH2O+HNO           1.300E+14    -0.7        0.0
NO2+CH2O=HONO+HCO          1.000E+10     0.0     15100.0
NO+CH2O=HNO+HCO            1.000E+13     0.0     40820.0
```

```
NO2+HCO=HONO+CO            1.000E+13     0.0       0.0
NO2+HCO=OH+NO+CO            1.000E+14     0.0       0.0
NCO+N=NO+CN              2.700E+18    -0.995   17200.0
CN+CH4=HCN+CH3             9.000E+04     2.64    -300.0
!KD-> C+NO=CO+N             2.800E+13     0.0       0.0
NH+CO2=HNO+CO              1.000E+13     0.0    14350.0
NCO+CH4=HNCO+CH3            1.000E+13     0.0     8130.0
!KD-> C+N2O=CN+NO             4.800E+12     0.0       0.0
CH+NH2=HCN+H+H              3.000E+13     0.0       0.0
CH+NH=HCN+H               5.000E+13     0.0       0.0
CH2+NH=HCN+H+H              3.000E+13     0.0       0.0
CH3+N=HCN+H+H              2.000E+11     0.0       0.0
CH3+N=HCN+H2              7.100E+12     0.0       0.0
CH4+N=NH+CH3              1.000E+13     0.0    24000.0
C3H3+N=HCN+C2H2             1.000E+13     0.0       0.0
CH+N2O=HCN+NO              1.340E+13     0.0     -510.0
CH+N2O=CO+H+N2              5.200E+12     0.0     -510.0
!KD-> C2O+N2=>NCO+CN              7.000E+11     0.0    17000.0
END
```

Mech.3

```
ELEM H C O N AR
END
SPECIES
H H2 O O2 OH
HO2 H2O H2O2 CO CO2
HCO CH3 CH4 C2H6 CH2O
C2H5 CH2 CH3O CH2OH CH
C2H2 C2H4 C2H3 CH3OH CH3HCO
C2H CH2CO HCCO SCH2 CH3CO
CH3O2 C2H5O CH2HCO CN H2CN
N NH HCN NO HCNO
HOCN HNCO NCO N2O NH2
HNO NO2 NNH NH3 N2H2
N2H3 N2H4 H2NO C3H6 NC3H7
C3H3 PC3H4 C3H5 C3H4 N2
END
```

REACTIONS, A_i ((cm^3/mol)$^{(r-1)}$/s), β_i, E_i (cal/mol)

```
H+H+M=H2+M               7.000E+17    -1.0       0.0
H2/0.0/ N2/0.0/ H/0.0/ H2O/14.3/ CO/3.0/ CO2/3.0/
H+H+H2=H2+H2              1.000E+17    -0.6       0.0
H+H+N2=H2+N2              5.400E+18    -1.3       0.0
H+H+H=H2+H              3.200E+15     0.0       0.0
```

```
O+O+M=O2+M                  1.000E+17     -1.0        0.0
O/71.0/ O2/20.0/ NO/5.0/ N2/5.0/ N/5.0/ H2O/5.0/
O+H+M=OH+M                  6.200E+16     -0.6        0.0
H2O/5.0/
H2+O2=OH+OH                 2.500E+12      0.0    39000.0
O+H2=OH+H                  5.060E+04      2.67     6290.0
H+O2=OH+O                  9.750E+13      0.0    14850.0
H+O2(+M)=HO2(+M)             1.480E+12      0.6        0.0
LOW /3.50E+16 -0.41 -1116.0/
TROE /0.5 100000 10/
!KD->  AR/0.0/ H2O/10.6/ H2/1.5/ CO2/2.4/
H2O/10.6/ H2/1.5/ CO2/2.4/
!KD-> H+O2(+AR)=HO2(+AR)           1.480E+12      0.6        0.0
!KD->     LOW /7.00E+17 -0.8  0.0/
!KD->     TROE /0.45 10 100000/
H+OH+M=H2O+M                 2.200E+22     -2.0        0.0
!KD->  H2O/6.4/ AR/0.38/ CO2/1.9/
H2O/6.4/        CO2/1.9/
H2+OH=H2O+H                 1.000E+08      1.6     3300.0
OH+OH=H2O+O                 1.500E+09      1.14     100.0
HO2+OH=H2O+O2                2.890E+13      0.0     -500.0
HO2+O=OH+O2                 1.630E+13      0.0     -445.0
H+HO2=H2+O2                4.280E+13      0.0     1411.0
H+HO2=OH+OH                 1.700E+14      0.0      875.0
H+HO2=H2O+O                 3.000E+13      0.0     1720.0
HO2+HO2=H2O2+O2              4.200E+14      0.0    12000.0
DUPLICATE
HO2+HO2=H2O2+O2              1.300E+11      0.0    -1640.0
DUPLICATE
OH+OH(+M)=H2O2(+M)           7.200E+13     -0.37       0.0
LOW /2.2E+19 -0.76 0.0/
TROE /0.5 100000 10/
H2O/0.0/
OH+OH(+H2O)=H2O2(+H2O)        7.200E+13     -0.37       0.0
LOW /1.45E+18 0.0 0.0/
H2O2+OH=HO2+H2O              1.000E+12      0.0        0.0
DUPLICATE
H2O2+OH=HO2+H2O              5.800E+14      0.0     9560.0
DUPLICATE
H2O2+H=HO2+H2               1.700E+12      0.0     3755.0
H2O2+H=H2O+OH               1.000E+13      0.0     3575.0
H2O2+O=HO2+OH               2.800E+13      0.0     6400.0
N2+O=NO+N                  1.800E+14      0.0    76100.0
N+O2=NO+O                  9.000E+09      1.0     6500.0
NO+M=N+O+M                  9.640E+14      0.0   148300.0
N2 /1.5/ NO /3.0/ CO2/2.5/
NO+NO=N2+O2                 3.000E+11      0.0    65000.0
N2O(+M)=N2+O(+M)             1.260E+12      0.0    62620.0
LOW / 4.000E+14 0.0 56640.0/
O2/1.4/ N2/1.7/ H2O/12.0/ NO/3.0/ N2O/3.5/
N2O+O=N2+O2                 1.000E+14      0.0    28200.0
```

```
N2O+O=NO+NO                 6.920E+13     0.0    26630.0
N2O+N=N2+NO                 1.000E+13     0.0    20000.0
N2O+NO=N2+NO2                 2.750E+14     0.0    50000.0
NO+O(+M)=NO2(+M)              1.300E+15    -0.75       0.0
LOW /4.72E+24 -2.87 1551.0/
TROE /0.962 10.0 7962.0 /
!KD->    AR /0.6/ NO2 /6.2/ NO /1.8/ O2 /0.8/ N2O /4.4/ CO2/0/
NO2 /6.2/ NO /1.8/ O2 /0.8/ N2O /4.4/ CO2/0/
H2O /10.0/
NO+O(+CO2)=NO2(+CO2)          1.300E+15    -0.75       0.0
LOW /4.0E+22 -2.16 1051.0/
TROE /0.962 10.0 7962.0 /
NO2+O=NO+O2                 3.910E+12     0.0     -238.0
NO2+N=N2O+O                 8.400E+11     0.0        0.0
NO2+N=NO+NO                 1.000E+12     0.0        0.0
NO2+NO=N2O+O2                 1.000E+12     0.0    60000.0
NO2+NO2=NO+NO+O2              3.950E+12     0.0    27590.0
!KD-> NO2+NO2=NO3+NO              1.130E+04     2.58    22720.0
!KD-> NO2+O(+M)=NO3(+M)            1.330E+13     0.0        0.0
!KD->    LOW / 1.49E+28 -4.08 2467.0 /
!KD->    TROE /0.86 10.0 2800.0 /
!KD->    H2O/10.0/ O2/0.8/ H2/2.0/ CO2 /0/
!KD-> NO2+O(+CO2)=NO3(+CO2)        1.330E+13     0.0        0.0
!KD->    LOW / 1.34E+28 -3.94 2277.0 /
!KD->    TROE /0.86 10.0 2800.0 /
!KD-> NO3=NO+O2                   2.500E+06     0.0    12120.0
!KD-> NO3+NO2=NO+NO2+O2            1.200E+11     0.0     3200.0
!KD-> NO3+O=NO2+O2                1.020E+13     0.0        0.0
!KD-> NO3+NO3=NO2+NO2+O2           5.120E+11     0.0     4870.0
!KD-> N2O4(+M)=NO2+NO2(+M)         4.050E+18    -1.1    12840.0
!KD->     LOW /1.96E+28  -3.8  12840./
!KD->     AR/0.8/ N2O4/2.0/ NO2/2.0/
!KD-> N2O4+O=N2O3+O2              1.210E+12     0.0        0.0
!KD-> NO2+NO(+M)=N2O3(+M)          1.600E+09     1.4        0.0
!KD->     LOW /1.0E+33  -7.7  0.0/
!KD->     N2/1.36/
!KD-> N2O3+O=NO2+NO2              2.710E+11     0.0        0.0
N2+M=N+N+M                  1.000E+28    -3.33   225000.0
N/5/ O/2.2/
NH+M=N+H+M                  2.650E+14     0.0    75500.0
NH+H=N+H2                 3.200E+13     0.0      325.0
NH+N=N2+H                 9.000E+11     0.5        0.0
NH+NH=NNH+H                 5.100E+13     0.0        0.0
NH+NH=NH2+N                 5.950E+02     2.89    -2030.0
NH+NH=N2+H2                 1.000E+08     1.0        0.0
NH2+M=NH+H+M                  3.160E+23    -2.0    91400.0
NH+H2=NH2+H                 1.000E+14     0.0    20070.0
NH2+N=N2+H+H                 6.900E+13     0.0        0.0
NH2+NH=N2H2+H                 1.500E+15    -0.5        0.0
NH2+NH=NH3+N                 1.000E+13     0.0     2000.0
NH3+NH=NH2+NH2                 3.160E+14     0.0    26770.0
```

```
NH2+NH2=N2H2+H2              1.000E+13     0.0     1500.0
N2H3+H=NH2+NH2               5.000E+13     0.0     2000.0
NH3+M=NH2+H+M                2.200E+16     0.0    93470.0
NH3+M=NH+H2+M                6.300E+14     0.0    93390.0
NH3+H=NH2+H2                 5.420E+05     2.4     9920.0
NH3+NH2=N2H3+H2              1.000E+11     0.5    21600.0
NNH=N2+H                     3.000E+08     0.0        0.0
!    DUPLICATE
NNH+M=N2+H+M                 1.000E+13     0.5     3060.0
!    DUPLICATE
NNH+H=N2+H2                  1.000E+14     0.0        0.0
NNH+N=NH+N2                  3.000E+13     0.0     2000.0
NNH+NH=N2+NH2                2.000E+11     0.5     2000.0
NNH+NH2=N2+NH3               1.000E+13     0.0        0.0
NNH+NNH=N2H2+N2              1.000E+13     0.0     4000.0
N2H2+M=NNH+H+M               5.000E+16     0.0    50000.0
H2O/15.0/ O2/2.0/ N2/2.0/ H2/2.0/
N2H2+M=NH+NH+M               3.160E+16     0.0    99400.0
H2O/15.0/ O2/2.0/ N2/2.0/ H2/2.0/
N2H2+H=NNH+H2                8.500E+04     2.63    -230.0
N2H2+N=NNH+NH                1.000E+06     2.0        0.0
N2H2+NH=NNH+NH2              1.000E+13     0.0     6000.0
N2H2+NH2=NH3+NNH             8.800E-02     4.05   -1610.0
N2H3+NH=N2H2+NH2             2.000E+13     0.0        0.0
N2H3+NNH=N2H2+N2H2           1.000E+13     0.0     4000.0
N2H3+M=NH2+NH+M              5.000E+16     0.0    60000.0
N2H3+M=N2H2+H+M              1.000E+16     0.0    37000.0
N2H3+H=N2H2+H2               1.000E+13     0.0        0.0
N2H3+H=NH+NH3                1.000E+11     0.0        0.0
N2H3+N=N2H2+NH               1.000E+06     2.0        0.0
N2H3+NH2=NH3+N2H2            1.000E+11     0.5        0.0
N2H3+N2H2=N2H4+NNH           1.000E+13     0.0     6000.0
N2H3+N2H3=NH3+NH3+N2         3.000E+12     0.0        0.0
N2H3+N2H3=N2H4+N2H2          1.200E+13     0.0        0.0
N2H4(+M)=NH2+NH2(+M)         5.000E+14     0.0    60000.0
LOW/1.50E+15 0.0 39000.0 /
N2/2.4/ NH3/3.0/ N2H4/4.0/
N2H4+M=N2H3+H+M              1.000E+15     0.0    63600.0
N2/2.4/ NH3/3.0/ N2H4/4.0/
N2H4+H=N2H3+H2               7.000E+12     0.0     2500.0
N2H4+H=NH2+NH3               2.400E+09     0.0     3100.0
N2H4+N=N2H3+NH               1.000E+10     1.0     2000.0
N2H4+NH=NH2+N2H3             1.000E+09     1.5     2000.0
N2H4+NH2=N2H3+NH3            1.800E+06     1.71   -1380.0
N+OH=NO+H                    2.800E+13     0.0        0.0
N2O+H=N2+OH                  2.200E+14     0.0    16750.0
N2O+H=NH+NO                  6.700E+22    -2.16   37155.0
N2O+H=NNH+O                  5.500E+18    -1.06   47290.0
!KD-> N2O+H=HNNO             8.000E+24    -4.39   10530.0
N2O+OH=N2+HO2                1.000E+14     0.0    30000.0
HNO+NO=N2O+OH                8.500E+12     0.0    29580.0
```

```
!KD-> HNNO+NO+NO=HNNO+NO2          1.600E+11     0.0     2090.0
!KD-> NH+NO+M=HNNO+M               1.630E+23    -2.6     1820.0
!KD-> HNNO+H=N2O+H2                2.000E+13     0.0        0.0
!KD-> HNNO+H=NH2+NO                1.000E+12     0.0        0.0
!KD-> HNNO+O=N2O+OH                2.000E+13     0.0        0.0
!KD-> HNNO+OH=H2O+N2O              2.000E+13     0.0        0.0
!KD-> HNNO+OH=HNOH+NO              1.000E+12     0.0        0.0
!KD-> HNNO+NO=N2+HONO              2.600E+11     0.0     1610.0
!KD-> HNNO+NO=NNH+NO2              3.200E+12     0.0      540.0
!KD-> HNNO+NO=N2O+HNO              1.000E+12     0.0        0.0
!KD-> HNNO+NO2=N2O+HONO            1.000E+12     0.0        0.0
!KD-> HNNO+NO2=NNH+NO3             1.000E+13     0.0    17000.0
NO2+H=NO+OH                  1.320E+14     0.0      362.0
NO2+OH=HO2+NO                1.810E+13     0.0     6676.0
!KD-> NO2+HO2=HONO+O2              4.640E+11     0.0     -479.0
!KD-> NO2+H2=HONO+H                7.330E+11     0.0    28800.0
NO2+NH=N2O+OH                8.650E+10     0.0    -2270.0
NO2+NH=NO+HNO                1.245E+11     0.0    -2270.0
!KD-> NO3+H=NO2+OH                 6.620E+13     0.0        0.0
!KD-> NO3+OH=NO2+HO2               1.210E+13     0.0        0.0
!KD-> NO3+HO2=HNO3+O2              5.550E+11     0.0        0.0
!KD-> NO3+HO2=NO2+OH+O2            1.510E+12     0.0        0.0
!KD-> N2O4+H2O=HONO+HNO3           2.520E+14     0.0    11590.0
!KD-> N2O3+H2O=HONO+HONO           3.790E+13     0.0     8880.0
H+NO(+M)=HNO(+M)             1.520E+15    -0.41       0.0
LOW /4.00E+20 -1.75 0.0 /
!KD->    H2O/10.0/ O2/1.5/ AR/0.75/ H2/2.0/ CO2/3.0/
H2O/10.0/ O2/1.5/         H2/2.0/ CO2/3.0/
HNO+H=NO+H2                  4.460E+11     0.72     655.0
HNO+OH=NO+H2O                1.300E+07     1.88    -956.0
HNO+O=OH+NO                  5.000E+11     0.5     2000.0
HNO+O=NO2+H                  5.000E+10     0.0     2000.0
HNO+O2=NO+HO2                2.200E+10     0.0     9140.0
HNO+N=NO+NH                  1.000E+11     0.5     2000.0
HNO+N=H+N2O                  5.000E+10     0.5     3000.0
HNO+NH=NH2+NO                5.000E+11     0.5        0.0
HNO+NH2=NH3+NO               2.000E+13     0.0     1000.0
HNO+HNO=N2O+H2O              3.630E-03     3.98    1190.0
!KD-> HNO+HNO=HNOH+NO              2.000E+08     0.0     4170.0
!KD-> HNO+NO2=HONO+NO              6.020E+11     0.0     2000.0
!KD-> NO+OH(+M)=HONO(+M)           2.000E+12    -0.05    -721.0
!KD->    LOW / 5.08E+23 -2.51 -67.6 /
!KD->    TROE /0.62 10.0 100000.0 /
!KD->    H2O/10.0/ O2/2.0/ AR/0.75/ H2/2.0/ CO2/0.0/
!KD-> NO+OH(+CO2)=HONO(+CO2)       2.000E+12    -0.05    -721.0
!KD->    LOW / 1.70E+23 -2.3 -246.0 /
!KD->    TROE /0.62 10.0 100000.0 /
!KD-> NO2+H+M=HONO+M               1.400E+18    -1.5      900.0
!KD-> HONO+H=HNO+OH                5.640E+10     0.86    4970.0
!KD-> HONO+H=NO+H2O                8.120E+06     1.89    3840.0
!KD-> HONO+O=OH+NO2                1.200E+13     0.0     5960.0
```

```
!KD-> HONO+OH=H2O+NO2               1.690E+12     0.0     -517.0
!KD-> HONO+NH=NH2+NO2               1.000E+13     0.0        0.0
!KD-> HONO+HONO=H2O+NO2+NO          1.000E+13     0.0     8540.0
!KD-> HONO+NH2=NO2+NH3              5.000E+12     0.0        0.0
!KD-> NO2+OH(+M)=HNO3(+M)           2.410E+13     0.0        0.0
!KD->     LOW / 6.42E+32 -5.49 2350.0 /
!KD->     TROE /1.0 10.0 1168.0 /
!KD->     H2O/10.0/ O2/2.0/ AR/0.75/ H2/2.0/ CO2/0.0/
!KD-> NO2+OH(+CO2)=HNO3(+CO2)       2.410E+13     0.0        0.0
!KD->     LOW / 5.80E+32 -5.4 2186.0 /
!KD->     TROE /1.0 10.0 1168.0 /
!KD-> NO+HO2+M=HNO3+M               1.500E+24    -3.5     2200.0
!KD-> HNO3+H=H2+NO3                 5.560E+08     1.53   16400.0
!KD-> HNO3+H=H2O+NO2                6.080E+01     3.29    6290.0
!KD-> HNO3+H=OH+HONO                3.820E+05     2.3     6980.0
!KD-> HNO3+OH=NO3+H2O               1.030E+10     0.0    -1240.0
NH3+O=NH2+OH                  1.100E+06     2.1     5210.0
NH3+OH=NH2+H2O                5.000E+07     1.6      950.0
NH3+HO2=NH2+H2O2              3.000E+11     0.0    22000.0
NH2+HO2=NH3+O2                1.650E+04     1.55    2027.0
NH2+O=H2+NO                   5.000E+12     0.0        0.0
NH2+O=HNO+H                   4.500E+13     0.0        0.0
NH2+O=NH+OH                   7.000E+12     0.0        0.0
NH2+OH=NH+H2O                 9.000E+07     1.5     -460.0
!KD-> NH2+OH=NH2OH                  1.790E+13     0.2        0.0
NH2+HO2=HNO+H2O               5.680E+15    -1.12     707.0
NH2+HO2=H2NO+OH               2.910E+17    -1.32    1248.0
NH2+O2=HNO+OH                 1.000E+13     0.0    26290.0
NH2+O2=H2NO+O                 6.000E+13     0.0    29880.0
NH2+NO=NNH+OH                 2.290E+10     0.425   -814.0
NH2+NO=N2+H2O                 2.770E+20    -2.65    1258.0
NH2+NO=H2+N2O                 1.000E+13     0.0    33700.0
NH2+NO2=N2O+H2O               1.620E+16    -1.44     270.0
NH2+NO2=H2NO+NO               6.480E+16    -1.44     270.0
NH+O=NO+H                     7.000E+13     0.0        0.0
NH+O=N+OH                     7.000E+12     0.0        0.0
NH+OH=HNO+H                   2.000E+13     0.0        0.0
NH+OH=N+H2O                   2.000E+09     1.2        0.0
NH+OH=NO+H2                   2.000E+13     0.0        0.0
NH+HO2=HNO+OH                 1.000E+13     0.0     2000.0
NH+O2=HNO+O                   4.000E+13     0.0    17880.0
NH+O2=NO+OH                   4.500E+08     0.79    1190.0
NH+H2O=HNO+H2                 2.000E+13     0.0    13850.0
NH+N2O=N2+HNO                 2.000E+12     0.0     6000.0
NNH+O=NH+NO                   2.000E+14     0.0     4000.0
NH+NO=N2+OH                   6.100E+13    -0.50     120.0
N2H4+O=N2H2+H2O               8.500E+13     0.0     1200.0
N2H4+O=N2H3+OH                2.500E+12     0.0     1200.0
N2H4+OH=N2H3+H2O              3.000E+10     0.68    1290.0
N2H4+OH=NH3+H2NO              3.670E+13     0.0        0.0
N2H4+HO2=N2H3+H2O2            4.000E+13     0.0     2000.0
```

```
N2H3+O=N2H2+OH              2.000E+13     0.0     1000.0
N2H3+O=NNH+H2O              3.160E+11     0.5        0.0
N2H3+O=NH2+HNO              1.000E+13     0.0        0.0
N2H3+OH=N2H2+H2O            3.000E+10     0.68    1290.0
N2H3+OH=NH3+HNO             1.000E+12     0.0    15000.0
N2H3+O2=N2H2+HO2            3.000E+12     0.0        0.0
N2H3+HO2=N2H2+H2O2          1.000E+13     0.0     2000.0
N2H3+HO2=N2H4+O2            8.000E+12     0.0        0.0
N2H3+NO=HNO+N2H2            1.000E+12     0.0        0.0
N2H2+O=NH2+NO               1.000E+13     0.0        0.0
N2H2+O=NNH+OH               2.000E+13     0.0     1000.0
N2H2+OH=NNH+H2O             5.920E+01     3.4    -1360.0
N2H2+HO2=NNH+H2O2           1.000E+13     0.0     2000.0
N2H2+NO=N2O+NH2             3.000E+10     0.0        0.0
NNH+O=N2+OH                 1.700E+16    -1.23     500.0
NNH+OH=N2+H2O               2.400E+22    -2.88    2444.0
NNH+O2=N2+HO2               1.200E+12    -0.34     150.0
NNH+O2=N2O+OH               2.900E+11    -0.34     150.0
NNH+HO2=N2+H2O2             1.000E+13     0.0     2000.0
NNH+NO=N2+HNO               5.000E+13     0.0        0.0
!KD-> NH2OH+OH=HNOH+H2O           2.500E+13     0.0     4250.0
H2NO+M=H2+NO+M              7.830E+27    -4.29   60300.0
H2O/10.0/
H2NO+M=HNO+H+M              2.800E+24    -2.83   64915.0
H2O/10.0/
!KD-> H2NO+M=HNOH+M               1.100E+29    -3.99   43980.0
!KD->   H2O/10.0/
H2NO+H=HNO+H2               3.000E+07     2.0     2000.0
H2NO+H=NH2+OH               5.000E+13     0.0        0.0
H2NO+O=HNO+OH               3.000E+07     2.0     2000.0
H2NO+OH=HNO+H2O             2.000E+07     2.0     1000.0
H2NO+HO2=HNO+H2O2           2.900E+04     2.69   -1600.0
H2NO+NH2=HNO+NH3            3.000E+12     0.0     1000.0
H2NO+O2=HNO+HO2             3.000E+12     0.0    25000.0
H2NO+NO=HNO+HNO             2.000E+07     2.0    13000.0
!KD-> H2NO+NO2=HONO+HNO           6.000E+11     0.0     2000.0
!KD-> HNOH+M=HNO+H+M              2.000E+24    -2.84   58935.0
!KD->    H2O/10.0/
!KD-> HNOH+H=HNO+H2               4.800E+08     1.5      380.0
!KD-> HNOH+H=NH2+OH               4.000E+13     0.0        0.0
!KD-> HNOH+O=HNO+OH               7.000E+13     0.0        0.0
!KD->    DUPLICATE
!KD-> HNOH+O=HNO+OH               3.300E+08     1.5     -360.0
!KD->    DUPLICATE
!KD-> HNOH+OH=HNO+H2O             2.400E+06     2.0    -1190.0
!KD-> HNOH+HO2=HNO+H2O2           2.900E+04     2.69   -1600.0
!KD-> HNOH+NH2=HNO+NH3            1.800E+06     1.94   -1150.0
!KD-> HNOH+NO2=HONO+HNO           6.000E+11     0.0     2000.0
!KD-> HNOH+O2=HNO+HO2             3.000E+12     0.0    25000.0
!KD-> HNOH+HNO=NH2OH+NO           1.000E+12     0.0     3000.0
!END
```

```
CO+HO2=CO2+OH               1.500E+14     0.0     23650.0
CO+OH=CO2+H                 1.170E+07     1.354   -725.0
CO+O+M=CO2+M                6.160E+14     0.0      3000.0
!KD->  H2/2.5/ H2O/6.2/ CO/1.875/ CO2/3.75/ AR/0.88/
H2/2.5/ H2O/6.2/ CO/1.875/ CO2/3.75/
CH4/3.2/ CH3OH/7.5/
CO+O2=CO2+O                 2.500E+12     0.0     47800.0
HCO+M=H+CO+M                1.560E+14     0.0     15760.0
!KD->  H2/2.5/ H2O/6.2/ CO/1.875/ CO2/3.75/ AR/1.0/
H2/2.5/ H2O/6.2/ CO/1.875/ CO2/3.75/
CH4/3.2/ CH3OH/7.5/
HCO+OH=CO+H2O               1.000E+14     0.0         0.0
HCO+O=CO+OH                 3.000E+13     0.0         0.0
HCO+O=CO2+H                 3.000E+13     0.0         0.0
HCO+H=CO+H2                 9.000E+13     0.0         0.0
HCO+O2=CO+HO2               2.700E+13     0.0      1190.0
HCO+CH3=CO+CH4              1.200E+14     0.0         0.0
HCO+HO2=CO2+OH+H            3.000E+13     0.0         0.0
HCO+HCO=CH2O+CO             3.000E+13     0.0         0.0
HCO+HCO=H2+CO+CO            2.200E+13     0.0         0.0
CH4(+M)=CH3+H(+M)           2.400E+16     0.0    104913.0
LOW /4.5E+17 0.0 90800/
TROE /1.0 10.0 1350.0 7830.0/
CH4/0.0/ H2/2.0/ CO/2.0/ CO2/3.0/ H2O/5.0/
CH4(+CH4)=CH3+H(+CH4)       2.400E+16     0.0    104913.0
LOW /8.4E+18 0.0 90800/
TROE /0.31 2210.0 90/
CH4+HO2=CH3+H2O2            9.000E+12     0.0     24641.0
CH4+OH=CH3+H2O              1.548E+07     1.83     2774.0
CH4+O=CH3+OH                7.200E+08     1.56     8485.0
CH4+H=CH3+H2                1.300E+04     3.0      8050.0
CH4+CH2=CH3+CH3             4.300E+12     0.0     10038.0
CH4+O2=CH3+HO2              4.000E+13     0.0     56900.0
CH3+M=CH2+H+M               2.720E+36    -5.31   117100.0
!KD->  H2/2.5/ H2O/6.2/ CO/1.875/ CO2/3.75/ AR/1.0/
H2/2.5/ H2O/6.2/ CO/1.875/ CO2/3.75/
CH4/3.2/ CH3OH/7.5/
CH3+M=CH+H2+M               1.000E+16     0.0     85240.0
!KD->  H2/2.5/ H2O/6.2/ CO/1.875/ CO2/3.75/ AR/0.88/
H2/2.5/ H2O/6.2/ CO/1.875/ CO2/3.75/
CH4/3.2/ CH3OH/7.5/
CH3+HO2=CH3O+OH             1.800E+13     0.0         0.0
CH3+OH=CH2OH+H              2.640E+19    -1.8      8068.0
CH3+OH=CH3O+H               5.740E+12    -0.23    13931.0
CH3+OH=CH2+H2O              8.900E+18    -1.8      8067.0
CH3+OH=CH2O+H2              3.190E+12    -0.53    10810.0
CH3+O=H+CH2O                8.430E+13     0.0         0.0
CH3+O2=CH2O+OH              3.400E+11     0.0      8940.0
CH3+O2=CH3O+O               1.320E+14     0.0     31400.0
CH3+CH3=C2H5+H              5.000E+12     0.099   10600.0
CH3+CH3(+M)=C2H6(+M)        9.210E+16    -1.174     636.0
```

```
LOW /1.13E+36 -5.246 1705/
TROE /0.405 1120.0 69.6/
H2/2.0/ CO/2.0/ CO2/3.0/ H2O/5.0/
CH3+CH3O=CH4+CH2O            2.409E+13     0.0        0.0
CH3+CH2OH=CH4+CH2O           8.500E+13     0.0        0.0
CH3+H=SCH2+H2                6.000E+13     0.0    15100.0
CH3+O2(+M)=CH3O2(+M)         7.800E+08     1.2        0.0
LOW/5.8E+25 -3.30 0.0/
TROE /0.495 2325.5 10/
CH3+CH3=C2H4+H2              1.000E+14     0.0    32000.0
CH3+OH=SCH2+H2O              7.200E+13     0.0     2780.0
CH2+OH=CH2O+H                2.500E+13     0.0        0.0
CH2+O=CO+H2                  4.800E+13     0.0        0.0
CH2+O=CO+H+H                 7.200E+13     0.0        0.0
CH2+O=CH+OH                  3.000E+14     0.0    11920.0
CH2+O=HCO+H                  3.000E+13     0.0        0.0
CH2+H=CH+H2                  3.120E+13     0.0    -1340.0
CH2+O2=HCO+OH                4.300E+10     0.0     -500.0
CH2+O2=CO2+H2                6.900E+11     0.0      500.0
CH2+O2=CO2+H+H               1.600E+12     0.0     1000.0
CH2+O2=CO+H2O                1.900E+10     0.0    -1000.0
CH2+O2=CO+OH+H               8.600E+10     0.0     -500.0
CH2+O2=CH2O+O                5.000E+13     0.0     9000.0
CH2+CO2=CH2O+CO              1.100E+11     0.0     1000.0
CH2+CH2=C2H2+H2              1.580E+15     0.0    11950.0
CH2+CH2=C2H2+H+H             2.000E+14     0.0    11000.0
CH2+CH2=CH3+CH               2.400E+14     0.0     9940.0
CH2+CH2=C2H3+H               2.000E+13     0.0        0.0
CH2+CH3=C2H4+H               4.200E+13     0.0        0.0
CH2+CH=C2H2+H                4.000E+13     0.0        0.0
!KD-> CH2+C=CH+CH                 1.620E+12     0.67   46800.0
!KD-> CH2+M=C+H2+M                1.600E+14     0.0    64000.0
CH2+M=CH+H+M                 5.600E+15     0.0    89600.0
SCH2+M=CH2+M                 6.000E+12     0.0        0.0
!KD->  H2/2.5/ H2O/5.0/ CO/1.875/ CO2/3.75/ AR/0.6/ CH4/1.2/
H2/2.5/ H2O/5.0/ CO/1.875/ CO2/3.75/        CH4/1.2/
C2H2/8.0/ C2H4/4.0/ C2H6/3.6/ H/33.3/
SCH2+O2=CO+OH+H              3.000E+13     0.0        0.0
SCH2+H=CH+H2                 3.000E+13     0.0        0.0
SCH2+O=CO+H+H                1.500E+13     0.0        0.0
SCH2+O=CO+H2                 1.500E+13     0.0        0.0
SCH2+OH=CH2O+H               3.000E+13     0.0        0.0
SCH2+HO2=CH2O+OH             3.000E+13     0.0        0.0
SCH2+H2O2=CH3O+OH            3.000E+13     0.0        0.0
SCH2+H2O=>CH3OH              1.800E+13     0.0        0.0
SCH2+CH2O=CH3+HCO            1.200E+12     0.0        0.0
SCH2+HCO=CH3+CO              1.800E+13     0.0        0.0
SCH2+CH3=C2H4+H              1.800E+13     0.0        0.0
SCH2+CH4=CH3+CH3             4.000E+13     0.0        0.0
SCH2+C2H6=CH3+C2H5           1.200E+14     0.0        0.0
SCH2+CO2=CH2O+CO             3.000E+12     0.0        0.0
```

```
SCH2+CH2CO=C2H4+CO           1.600E+14     0.0       0.0
CH+OH=HCO+H                  3.000E+13     0.0       0.0
CH+O=CO+H                    4.000E+13     0.0       0.0
!KD-> CH+O=C+OH                   1.520E+13     0.0     4730.0
!KD-> H2O+C=CH+OH                 7.800E+11     0.67   39300.0
CH+O2=HCO+O                  4.900E+13     0.0       0.0
CH+O2=CO+OH                  4.900E+13     0.0       0.0
CH+CO2=HCO+CO                3.220E-02     4.44    -3530.0
CH+CH4=C2H4+H                3.900E+14    -0.4       0.0
CH+CH3=C2H3+H                3.000E+13     0.0       0.0
CH2+OH=CH+H2O                1.130E+07     2.0     3000.0
!KD-> CH+H=C+H2                   7.900E+13     0.0      160.0
CH+H2O=CH2O+H                1.170E+15    -0.75      0.0
CH+H2O=CH2OH                 5.700E+12     0.0     -760.0
CH+CH2O=CH2CO+H              1.000E+14     0.0     -515.0
CH3O+M=CH2O+H+M              5.400E+13     0.0    13500.0
!KD->  H2/2.5/ H2O/6.2/ CO/1.875/ CO2/3.75/ AR/0.88/
H2/2.5/ H2O/6.2/ CO/1.875/ CO2/3.75/
CH4/3.2/ CH3OH/7.5/
CH3O+HO2=CH2O+H2O2           3.000E+11     0.0       0.0
CH3O+OH=CH2O+H2O             1.800E+13     0.0       0.0
CH3O+O=CH2O+OH               1.800E+12     0.0       0.0
CH3O+H=CH2O+H2               1.800E+13     0.0       0.0
CH3O+O2=CH2O+HO2             2.200E+10     0.0     1750.0
CH3O+CH2O=CH3OH+HCO          1.000E+11     0.0     2980.0
CH3O+CO=CH3+CO2              6.810E-18     9.2    -2850.0
CH3O+HCO=CH3OH+CO            9.000E+13     0.0       0.0
CH3O+C2H5=CH2O+C2H6          2.410E+13     0.0       0.0
CH3O+C2H3=CH2O+C2H4          2.410E+13     0.0       0.0
CH3O+C2H4=CH2O+C2H5          1.200E+11     0.0     6750.0
CH3O+H=CH2OH+H               3.400E+06     1.6       0.0
CH3O+H=SCH2+H2O              1.000E+12     0.0       0.0
CH2O+M=HCO+H+M               5.000E+35    -5.54   96680.0
!KD->  H2/2.5/ H2O/6.2/ CO/1.875/ CO2/3.75/ AR/1.0/
H2/2.5/ H2O/6.2/ CO/1.875/ CO2/3.75/
CH4/3.2/ CH3OH/7.5/
CH2O+M=CO+H2+M               1.100E+36    -5.54   96680.0
!KD->  H2/2.5/ H2O/6.2/ CO/1.875/ CO2/3.75/ AR/1.0/
H2/2.5/ H2O/6.2/ CO/1.875/ CO2/3.75/
CH4/3.2/ CH3OH/7.5/
CH2O+HO2=HCO+H2O2            4.110E+04     2.5    10210.0
CH2O+OH=HCO+H2O              3.433E+09     1.18    -447.0
CH2O+O=HCO+OH                4.100E+11     0.57    2760.0
CH2O+H=HCO+H2                1.260E+08     1.62    2166.0
CH2O+O2=HCO+HO2              6.000E+13     0.0    40650.0
CH2O+CH3=HCO+CH4             7.800E-08     6.1     1970.0
C2H6(+M)=C2H5+H(+M)          8.850E+20    -1.228  102210.0
LOW /6.90E+42 -6.431 107175.0/
SRI /47.61 16182.0 3371.0/
!KD->  H2/2.0/ H2O/6.0/ CH4/2.0/ CO/1.5/ CO2/2.0/ C2H6/3.0/ AR/0.7/
H2/2.0/ H2O/6.0/ CH4/2.0/ CO/1.5/ CO2/2.0/ C2H6/3.0/
```

```
C2H6+HO2=C2H5+H2O2           1.330E+13     0.0     20535.0
C2H6+OH=C2H5+H2O             7.200E+06     2.0       870.0
C2H6+O=C2H5+OH               1.000E+09     1.5      5800.0
C2H6+H=C2H5+H2               1.400E+09     1.5      7400.0
C2H6+H=CH3+CH4               5.400E+04     0.0     11630.0
C2H6+O2=C2H5+HO2             6.000E+13     0.0     52000.0
C2H6+CH3=C2H5+CH4            1.470E-07     6.0      6060.0
C2H6+CH2=CH3+C2H5            6.500E+12     0.0      7911.0
C2H6+C2H3=C2H4+C2H5          8.566E-02     4.14     2543.0
C2H6+HCO=CH2O+C2H5           4.700E+04     2.72    18235.0
C2H5(+M)=C2H4+H(+M)          1.110E+10     1.037   36767.0
LOW /4.0E+33 -4.99 40000.0/
TROE /0.832 10 1203.0/
!KD->  H2/2.0/ CO/2.0/ CO2/3.0/ H2O/5.0/ CH4/2.0/ C2H6/0.0/ AR/0.7/
H2/2.0/ CO/2.0/ CO2/3.0/ H2O/5.0/ CH4/2.0/ C2H6/0.0/
C2H5(+C2H6)=C2H4+H(+C2H6)     8.200E+13     0.0     39880.0
LOW /1.0E+18 0.0 33380.0/
TROE /0.75 97.0 1379.0/
C2H5+HO2=C2H4+H2O2           1.800E+12     0.0        0.0
C2H5+OH=C2H4+H2O             2.409E+13     0.0        0.0
C2H5+OH=>CH3+CH2O+H          2.409E+13     0.0        0.0
C2H5+O=CH2O+CH3              4.240E+13     0.0        0.0
C2H5+O=CH3HCO+H              5.300E+13     0.0        0.0
C2H5+O=C2H4+OH               3.460E+13     0.0        0.0
C2H5+H=C2H4+H2               1.700E+12     0.0        0.0
C2H5+O2=C2H4+HO2             2.560E+19    -2.77     1980.0
C2H5+CH3=C2H4+CH4            1.100E+12     0.0        0.0
C2H5+C2H5=C2H4+C2H6          1.400E+12     0.0        0.0
C2H5+HO2=C2H5O+OH            3.000E+13     0.0        0.0
C2H4+M=C2H2+H2+M             3.500E+16     0.0     71530.0
!KD->    H2/2.5/ H2O/6.2/ CO/1.875/ CO2/3.75/ AR/1.0/
H2/2.5/ H2O/6.2/ CO/1.875/ CO2/3.75/
CH4/3.2/ CH3OH/7.5/
C2H4+M=C2H3+H+M              2.600E+17     0.0     96570.0
!KD->    H2/2.5/ H2O/6.2/ CO/1.875/ CO2/3.75/ AR/1.0/
H2/2.5/ H2O/6.2/ CO/1.875/ CO2/3.75/
CH4/3.2/ CH3OH/7.5/
C2H4+OH=C2H3+H2O             5.530E+05     2.31     2900.0
C2H4+O=CH3+HCO               8.100E+06     1.88      180.0
C2H4+H=C2H3+H2               4.490E+07     2.12    13366.0
C2H4+O2=C2H3+HO2             4.000E+13     0.0     61500.0
C2H4+C2H4=C2H5+C2H3          1.860E+14     0.0     64200.0
C2H4+CH3=C2H3+CH4            4.200E+12     0.0     11100.0
C2H4+O=CH2HCO+H              4.700E+06     1.88      180.0
C2H4+O=CH2O+CH2              3.000E+04     1.88      180.0
C2H4+O=CH2CO+H2              6.700E+05     1.88      180.0
C2H4+O=C2H3+OH               1.510E+07     1.91     3790.0
C2H4+OH=CH2O+CH3             2.000E+12     0.0       960.0
!KD-> C2H4+OH(+M)=PC2H5O(+M)        5.420E+12     0.0        0.0
!KD->      LOW /1.19E+27 -3.1 0.0/
C2H4+HO2=C2H3+H2O2           1.120E+13     0.0     30400.0
```

```
C2H4+CH3O=C2H3+CH3OH          1.000E+11     0.0     10000.0
C2H3(+M)=C2H2+H(+M)           2.100E+14     0.0     39740.0
LOW /4.15E+41 -7.5 45500.0/
TROE /0.65 100000 10/
!KD->  H2/2.0/ CO/2.0/ CO2/3.0/ H2O/5.0/ CH4/2.0/ C2H6/3.0/ AR/0.7/
H2/2.0/ CO/2.0/ CO2/3.0/ H2O/5.0/ CH4/2.0/ C2H6/3.0/
C2H3+HO2=>CH3+CO+OH           3.000E+13     0.0        0.0
C2H3+OH=C2H2+H2O              3.000E+13     0.0        0.0
C2H3+H=C2H2+H2                1.200E+13     0.0        0.0
C2H3+O=CH3+CO                 1.000E+13     0.0        0.0
C2H3+O2=CH2O+HCO              1.700E+29    -5.312    6500.0
C2H3+CH=CH2+C2H2              5.000E+13     0.0        0.0
C2H3+CH3=C2H2+CH4             2.050E+13     0.0        0.0
C2H3+C2H=C2H2+C2H2            3.000E+13     0.0        0.0
C2H3+HCO=C2H4+CO              9.034E+13     0.0        0.0
C2H3+CH2O=C2H4+HCO            5.420E+03     2.81     5862.0
C2H3+C2H3=C2H2+C2H4           1.450E+13     0.0        0.0
C2H3+O=C2H2+OH                1.000E+13     0.0        0.0
C2H3+O=CH2+HCO                1.000E+13     0.0        0.0
C2H3+O=CH2CO+H                1.000E+13     0.0        0.0
C2H3+OH=CH3HCO                3.000E+13     0.0        0.0
C2H3+O2=C2H2+HO2              5.190E+15    -1.26     3310.0
DUPLICATE
C2H3+O2=C2H2+HO2              2.120E-06     6.0      9484.0
DUPLICATE
C2H3+O2=CH2HCO+O              3.500E+14    -0.61     5260.0
C2H3+CH2=C2H2+CH3             3.000E+13     0.0        0.0
C2H2=C2H+H                    2.373E+32    -5.28   130688.0
C2H2+O2=HCCO+OH               2.000E+08     1.5     30100.0
C2H2+O2=C2H+HO2               1.200E+13     0.0     74520.0
C2H2+OH=C2H+H2O               3.385E+07     2.0     14000.0
C2H2+OH=CH2CO+H               1.100E+13     0.0      7170.0
C2H2+O=CH2+CO                 1.200E+06     2.1      1570.0
C2H2+O=HCCO+H                 5.000E+06     2.1      1570.0
C2H2+CH3=C2H+CH4              1.800E+11     0.0     17290.0
C2H2+O=C2H+OH                 3.000E+14     0.0     25000.0
C2H2+OH=CH3+CO                4.830E-04     4.0     -2000.0
C2H2+HO2=CH2CO+OH             6.100E+09     0.0      7950.0
C2H2+O2=HCO+HCO               4.000E+12     0.0     28000.0
C2H+OH=HCCO+H                 2.000E+13     0.0        0.0
!KD-> C2H+OH=C2+H2O               4.000E+07     2.0     8000.0
C2H+O=CO+CH                   1.450E+13     0.0      460.0
C2H+O2=HCO+CO                 9.000E+12     0.0        0.0
C2H+H2=C2H2+H                 7.880E+05     2.39     346.0
C2H+O2=CO+CO+H                9.000E+12     0.0        0.0
C2H+O2=HCCO+O                 6.000E+11     0.0        0.0
CH2CO(+M)=CH2+CO(+M)          3.000E+14     0.0     71000.0
LOW /2.300E+15   0.0  57600.0/
!KD->    H2/2.5/ H2O/6.2/ CO/1.875/ CO2/3.75/ AR/1.0/
H2/2.5/ H2O/6.2/ CO/1.875/ CO2/3.75/
CH4/3.2/ CH3OH/7.5/
```

```
CH2CO+O2=CH2O+CO2            2.000E+13     0.0     61500.0
CH2CO+HO2=>CH2O+CO+OH        6.000E+11     0.0     12738.0
CH2CO+O=HCCO+OH              1.000E+13     0.0      8000.0
CH2CO+OH=CH2OH+CO            1.000E+13     0.0         0.0
CH2CO+H=CH3+CO               3.280E+10     0.851    2840.0
CH2CO+CH3=C2H5+CO            2.400E+12     0.0      8000.0
CH2CO+CH2=C2H4+CO            2.900E+12     0.0      3800.0
CH2CO+CH2=HCCO+CH3           3.600E+13     0.0     11000.0
CH2CO+CH3=HCCO+CH4           7.500E+12     0.0     13000.0
CH2CO+OH=CH2O+HCO            2.800E+13     0.0         0.0
CH2CO+H=HCCO+H2              1.800E+14     0.0      8600.0
CH2CO+O=HCO+HCO              7.500E+11     0.0      1350.0
CH2CO+O=HCO+CO+H             7.500E+11     0.0      1350.0
CH2CO+O=CH2O+CO              7.500E+11     0.0      1350.0
CH2CO+OH=HCCO+H2O            7.500E+12     0.0      2000.0
HCCO+M=CH+CO+M               6.000E+15     0.0     58821.0
!KD->    H2/2.5/ H2O/6.2/ CO/1.875/ CO2/3.75/ AR/0.88/
H2/2.5/ H2O/6.2/ CO/1.875/ CO2/3.75/
CH4/3.2/ CH3OH/7.5/
HCCO+OH=HCO+CO+H             1.000E+13     0.0         0.0
!KD-> HCCO+OH=C2O+H2O             3.000E+13     0.0         0.0
HCCO+O=CO+CO+H               1.000E+14     0.0         0.0
HCCO+O=CH+CO2                2.950E+13     0.0      1110.0
HCCO+H=CH2+CO                1.500E+14     0.0         0.0
HCCO+O2=CO2+CO+H             5.400E+11     0.0       850.0
HCCO+CH2=C2H+CH2O            1.000E+13     0.0      2000.0
HCCO+CH2=C2H3+CO             3.000E+13     0.0         0.0
HCCO+CH3=C2H4+CO             2.000E+12     0.0         0.0
HCCO+CH=CO+C2H2              5.000E+13     0.0         0.0
HCCO+HCCO=CO+C2H2+CO         1.000E+13     0.0         0.0
HCCO+OH=HCO+HCO              1.000E+13     0.0         0.0
HCCO+O2=CO+CO+OH             5.400E+11     0.0       850.0
HCCO+O2=CO2+HCO              5.400E+11     0.0       850.0
CH3OH(+M)=CH3+OH(+M)         1.700E+16     0.0     90885.0
LOW /6.60E+16 0.0 65730.0/
TROE /0.82 200.0 1438.0/
CH3OH+HO2=CH2OH+H2O2         9.640E+10     0.0     12580.0
CH3OH+OH=CH2OH+H2O           1.440E+06     2.0      -840.0
CH3OH+OH=CH3O+H2O            1.000E+13     0.0      1700.0
CH3OH+O=CH2OH+OH             1.630E+13     0.0      5030.0
CH3OH+H=CH2OH+H2             1.640E+07     2.0      4520.0
CH3OH+CH3=CH2OH+CH4          3.190E+01     3.17     7172.0
CH3OH+CH3=CH3O+CH4           1.450E+01     3.1      6935.0
CH3OH+C2H5=C2H6+CH3O         1.440E+01     3.1      8942.0
CH3OH+H=CH3+H2O              2.000E+14     0.0      5300.0
CH3OH+O=CH3O+OH              1.000E+13     0.0      4680.0
CH3OH+CH3=C2H6+OH            2.000E+12     0.0     15000.0
CH3OH+CH3O=CH2OH+CH3OH       3.000E+11     0.0      4070.0
CH3OH(+M)=CH2OH+H(+M)        1.380E+16     0.0     95950.0
LOW /5.35E+16 0.0 70800.0/
TROE /0.82 200.0 1438.0/
```

```
CH3OH+H=H2+CH3O              4.000E+13     0.0     6095.0
CH3OH+O2=CH2OH+HO2            2.050E+13     0.0    44900.0
CH3OH+C2H5=C2H6+CH2OH         3.190E+01     3.2     9161.0
CH2OH+M=CH2O+H+M              1.140E+43    -8.0    43000.0
H2O/16.0/ CH4/3.0/ CO2/3.75/  CO/1.875/  H2/2.5/   CH3OH/6.0/
CH2OH+H=CH2O+H2               1.000E+13     0.0       0.0
CH2OH+O2=CH2O+HO2             1.500E+15    -1.0       0.0
DUPLICATE
CH2OH+O2=CH2O+HO2             7.200E+13     0.0    3570.0
DUPLICATE
H+CH2OH=SCH2+H2O              1.000E+12     0.0       0.0
CH2OH+O=CH2O+OH               9.000E+13     0.0       0.0
CH2OH+OH=CH2O+H2O             1.000E+13     0.0       0.0
CH2OH+HO2=CH2O+H2O2           1.210E+13     0.0       0.0
CH2OH+CH2OH=CH3OH+CH2O        4.820E+12     0.0       0.0
CH2OH+CH2OH=CH2O+CH2O+H2      1.000E+15    -0.7       0.0
CH2OH+HCO=CH3OH+CO            1.210E+14     0.0       0.0
CH2OH+CH2O=CH3OH+HCO          5.490E+03     2.8     5900.0
CH2OH+CH3O=CH3OH+CH2O         2.400E+13     0.0       0.0
CH3O+CH3O=CH3OH+CH2O          2.320E+13     0.0       0.0
CH3HCO=CH3+HCO                7.100E+15     0.0    81790.0
CH3HCO+HO2=CH3CO+H2O2         3.000E+12     0.0    12000.0
CH3HCO+OH=CH3CO+H2O           2.300E+10     0.73   -1100.0
CH3HCO+O=CH3CO+OH             5.800E+12     0.0     1800.0
CH3HCO+H=CH3CO+H2             4.100E+09     1.16    2400.0
CH3HCO+O2=CH3CO+HO2           3.000E+13     0.0    39200.0
CH3HCO+CH3=CH3CO+CH4          7.600E+00     3.4     3740.0
CH3HCO+H=CH2HCO+H2            7.000E+08     1.5     7400.0
CH3HCO+O=CH2HCO+OH            5.000E+08     1.5     5800.0
CH3HCO+OH=CH2HCO+H2O          2.000E+14     0.0     6000.0
CH3HCO+HO2=CH2HCO+H2O2        3.000E+13     0.0    15000.0
CH3HCO+CH2=CH3CO+CH3          1.660E+12     0.0     3510.0
CH3HCO+CH3=CH2HCO+CH4         1.580E+00     4.0     7720.0
CH3HCO+CH3O=CH3CO+CH3OH       5.000E+12     0.0       0.0
CH3HCO+C2H5=CH3CO+C2H6        1.260E+12     0.0     8500.0
CH3HCO+C2H3=CH3CO+C2H4        8.130E+10     0.0     3680.0
CH2HCO=CH3CO                  1.600E+11     0.0    21600.0
CH3HCO+CH2HCO=CH3CO+CH3HCO    3.000E+12     0.0    11200.0
CH3CO(+M)=CH3+CO(+M)          2.800E+13     0.0    17150.0
LOW /6.0E+15 0.0 14070.0/
TROE /0.5 100000 10/
!KD->    H2/2.5/ H2O/6.2/ CO/1.875/ CO2/3.75/ AR/0.88/
H2/2.5/ H2O/6.2/ CO/1.875/ CO2/3.75/
CH4/3.2/ CH3OH/7.5/
CH3CO+H=CH2CO+H2              1.150E+13     0.0       0.0
CH3CO+H=CH3+HCO               2.150E+13     0.0       0.0
CH3CO+O=CH2CO+OH              4.000E+13     0.0       0.0
CH3CO+O=CH3+CO2               1.500E+14     0.0       0.0
CH3CO+CH3=C2H6+CO             3.300E+13     0.0       0.0
CH3CO+CH3=CH4+CH2CO           6.100E+12     0.0       0.0
CH2HCO+H=CH2CO+H2             2.000E+13     0.0       0.0
```

```
CH2HCO+O2=CH2O+OH+CO          1.800E+10     0.0        0.0
CH2HCO+O2=CH2CO+HO2           1.500E+11     0.0        0.0
CH2HCO=CH2CO+H                1.580E+13     0.0    35200.0
C2H5O=CH3+CH2O                1.000E+15     0.0    21600.0
C2H5O+O2=CH3HCO+HO2           3.600E+10     0.0     1090.0
C2H5O=CH3HCO+H                2.000E+14     0.0    23300.0
C2H5O+OH=CH3HCO+H2O           1.000E+14     0.0        0.0
C2H5O+H=CH3HCO+H2             1.000E+14     0.0        0.0
C2H5O+O=CH3HCO+OH             1.210E+14     0.0        0.0
C2H5O+HO2=CH3HCO+H2O2         1.000E+14     0.0        0.0
!KD-> C2H5O+C2H5O=C2H5OH+CH3HCO      5.000E+13     0.0        0.0
!KD-> C2H5O+PC2H5O=C2H5OH+CH3HCO     5.000E+13     0.0        0.0
!KD-> C2H5O+SC2H5O=C2H5OH+CH3HCO     5.000E+13     0.0        0.0
!KD-> SC2H5O+M=CH3HCO+H+M            5.000E+13     0.0    21860.0
!KD-> SC2H5O+H=CH3HCO+H2             2.000E+13     0.0        0.0
!KD-> SC2H5O+OH=CH3HCO+H2O           1.500E+13     0.0        0.0
!KD-> SC2H5O+O=CH3HCO+OH             9.040E+13     0.0        0.0
!KD-> SC2H5O+O2=CH3HCO+HO2           8.400E+15    -1.20       0.0
!KD->    DUPLICATE
!KD-> SC2H5O+O2=CH3HCO+HO2           4.800E+14     0.0     5000.0
!KD->    DUPLICATE
!KD-> SC2H5O+HO2=CH3HCO+H2O2         1.000E+13     0.0        0.0
!KD-> SC2H5O+SC2H5O=C2H5OH+CH3HCO    3.500E+13     0.0        0.0
!KD-> SC2H5O+PC2H5O=C2H5OH+CH3HCO    5.000E+13     0.0        0.0
!KD-> PC2H5O=SC2H5O                  1.000E+11     0.0    27000.0
!KD-> PC2H5O+PC2H5O=C2H5OH+CH3HCO    3.400E+13     0.0        0.0
!KD-> C2H5OH=CH2OH+CH3               3.100E+15     0.0    80600.0
!KD-> C2H5OH+OH=SC2H5O+H2O           3.000E+13     0.0     5960.0
!KD-> C2H5OH+OH=C2H5O+H2O            1.138E+06     2.0      914.0
!KD-> C2H5OH+OH=PC2H5O+H2O           2.563E+06     2.06     860.0
!KD-> C2H5OH+O=SC2H5O+OH             6.000E+05     2.46    1850.0
!KD-> C2H5OH+O=C2H5O+OH              4.820E+13     0.0     6856.0
!KD-> C2H5OH+O=PC2H5O+OH             5.000E+12     0.0     4411.0
!KD-> C2H5OH+H=C2H5+H2O              5.900E+11     0.0     3450.0
!KD-> C2H5OH+H=SC2H5O+H2             4.400E+12     0.0     4570.0
!KD-> C2H5OH+HO2=SC2H5O+H2O2         2.000E+13     0.0    17000.0
!KD-> C2H5OH+CH3=SC2H5O+CH4          4.000E+11     0.0     9700.0
!KD-> C2H5OH+CH3=PC2H5O+CH4          3.000E+00     4.0    10480.0
!KD-> C2H5OH+CH3=C2H5O+CH4           8.000E+10     0.0     9400.0
!KD-> C2H5OH+CH3O=SC2H5O+CH3OH       2.000E+11     0.0     7000.0
!KD-> C2H5OH+CH2O=C2H5O+CH3O         1.500E+12     0.0    79500.0
!KD-> C2H5OH+C2H5O=C2H5OH+SC2H5O     2.000E+11     0.0     7000.0
!KD-> C2H5OH=C2H5+OH                 5.000E+16     0.0    91212.0
!KD-> C2H5OH=C2H4+H2O                1.000E+14     0.0    76706.0
!KD-> C2H5OH+O2=PC2H5O+HO2           4.000E+13     0.0    50900.0
!KD-> C2H5OH+O2=SC2H5O+HO2           4.000E+13     0.0    51200.0
!KD-> C2H5OH+O2=C2H5O+HO2            2.000E+13     0.0    56000.0
!KD-> C2H5OH+H=PC2H5O+H2             2.000E+12     0.0     9500.0
!KD-> C2H5OH+H=C2H5O+H2              1.760E+12     0.0     4570.0
!KD-> C2H5OH+HO2=H2O2+C2H5O          1.000E+11     0.0    15500.0
!KD-> C2H5OH+HO2=H2O2+PC2H5O         1.000E+11     0.0    12500.0
```

```
!KD-> C2H5OH+C2H5=PC2H5O+C2H6       1.500E+12     0.0    11700.0
!KD-> C2H5OH+C2H5=SC2H5O+C2H6       4.000E+13     0.0    10000.0
!KD-> C2H5OH+CH2OH=SC2H5O+CH3OH     4.000E+11     0.0     9700.0
!KD-> C+OH=CO+H                   5.000E+13     0.0        0.0
!KD-> C+O2=CO+O                   1.200E+14     0.0     4000.0
!KD-> C+CH3=C2H2+H                 5.000E+13     0.0        0.0
!KD-> C+CH2=C2H+H                  5.000E+13     0.0        0.0
!KD-> CH2O+CH3O2=HCO+CH3O2H        2.000E+12     0.0    11660.0
CH3O2+H=CH3O+OH              9.600E+13     0.0        0.0
CH3O2+OH=CH3OH+O2            6.000E+13     0.0        0.0
CH3O2+CH3=CH3O+CH3O          2.400E+13     0.0        0.0
CH3O2+CH3O2=>CH2O+CH3OH+O2    2.700E+10     0.0     -780.0
CH3O2+CH3O2=>CH3O+CH3O+O2     2.800E+10     0.0     -780.0
!KD-> CH3O2+H2O2=CH3O2H+HO2        2.400E+12     0.0    10000.0
!KD-> CH3O2H=CH3O+OH              6.000E+14     0.0    42300.0
!KD-> CH3O2+HO2=CH3O2H+O2          2.290E+11     0.0    -1550.0
!KD-> CH3O2H+OH=CH3O2+H2O          1.150E+12     0.0     -380.0
!KD-> CH4+CH3O2=CH3+CH3O2H         1.810E+11     0.0    18600.0
!KD-> C2H6+CH3O2=C2H5+CH3O2H       2.950E+11     0.0    14940.0
!KD-> CH3OH+CH3O2=CH2OH+CH3O2H     1.810E+12     0.0    13800.0
!KD-> CH3O2H+O=OH+CH3O2            2.000E+13     0.0     4750.0
!KD-> CH3CO+O2=CH3CO3             1.000E+10     0.0    -2700.0
!KD-> CH3HCO+CH3CO3=CH3CO+CH3CO3H   1.200E+11     0.0     4900.0
!KD-> CH3HCO+C2H5O2=CH3CO+C2H5O2H   1.150E+11     0.0    10000.0
!KD-> C2H5+O2(+M)=C2H5O2(+M)       2.200E+10     0.772    -570.0
!KD->      LOW /7.10E+42 -8.24 4270.0 /
!KD-> C2H5O2=C2H4+HO2             5.620E+11     0.0    28900.0
!KD-> C2H5O2+HO2=C2H5O2H+O2        3.400E+11     0.0    -1300.0
!KD-> C2H5O2H=C2H5O+OH            4.000E+15     0.0    43000.0
!KD-> C2H5O2H+O=OH+C2H5O2          2.000E+13     0.0     4750.0
!KD-> C2H5O2H+OH=C2H5O2+H2O        2.000E+12     0.0     -370.0
!KD-> CH4+C2H5O2=CH3+C2H5O2H       1.140E+13     0.0    20460.0
!KD-> CH4+CH3CO3=CH3+CH3CO3H       1.140E+13     0.0    20460.0
!KD-> C2H4+C2H5O2=C2H3+C2H5O2H     1.000E+12     0.0    25000.0
!KD-> C2H4+CH3CO3=C2H3+CH3CO3H     3.000E+12     0.0    29000.0
!KD-> CH3CO3+HO2=CH3CO3H+O2        1.000E+12     0.0        0.0
!KD-> CH3CO3H=>CH3CO2+OH          1.150E+13     0.0    32550.0
!KD-> CH3CO3H=>CH3+CO2+OH         2.000E+14     0.0    40150.0
!KD-> CH3CO3+CH3O2=>CH3CO2+CH3O+O2  1.080E+15     0.0     3600.0
!KD-> CH3CO3+CH3O2=>CH3CO2H+CH2O+O2  2.470E+09     0.0    -4200.0
!KD-> CH3CO3+HO2=>CH3CO2+OH+O2     2.590E+11     0.0    -2080.0
!KD-> CH3CO3+CH3CO3=>CH3CO2+CH3CO2+O2  1.690E+12    0.0    -1060.0
!KD-> CH3CO2+M=>CH3+CO2+M          8.700E+15     0.0    14400.0
!KD-> CH3CO2H=CH4+CO2             7.080E+13     0.0    74600.0
!KD-> CH3CO2H=CH2CO+H2O           4.470E+14     0.0    79800.0
!KD-> CH3CO2H+OH=CH3CO2+H2O        2.400E+11     0.0     -400.0
!KD-> CH3OH+C2H5O2=CH2OH+C2H5O2H    6.300E+12     0.0    19360.0
!KD-> CH3OH+CH3CO3=CH2OH+CH3CO3H    6.300E+12     0.0    19360.0
!KD-> CH2O+C2H5O2=HCO+C2H5O2H      1.300E+11     0.0     9000.0
!KD-> CH2O+CH3CO3=HCO+CH3CO3H      1.000E+12     0.0    10560.0
!KD-> C2H4+CH3O2=C2H3+CH3O2H       1.000E+13     0.0    25000.0
```

```
!KD-> CH3HCO+CH3O2=CH3CO+CH3O2H     1.150E+11     0.0    10000.0
!KD-> C2H5OH+CH3O2=SC2H5O+CH3O2H    1.000E+13     0.0    10000.0
C2H5+CH3O2=C2H5O+CH3O         2.410E+13     0.0        0.0
!KD-> C2H4+HO2=C2H4O+OH             2.200E+12     0.0    17200.0
!KD-> C2H4+CH3O=C2H4O+CH3           1.000E+11     0.0    14500.0
!KD-> C2H4+CH3O2=C2H4O+CH3O         7.000E+11     0.0    14500.0
!KD-> C2H4O=>CH3HCOW                1.600E+13     0.0    54300.0
!KD-> CH3HCOW+M=>CH3HCO+M           1.000E+14     0.0        0.0
!KD-> CH3HCOW=>CH3+HCO              5.000E+08     0.0        0.0
!KD-> C2H4O+H=H2+C2H3O              8.000E+13     0.0     9740.0
!KD-> C2H4O+H=H2O+C2H3              5.000E+09     0.0     5030.0
!KD-> C2H4O+H=C2H4+OH               9.510E+10     0.0     5030.0
!KD-> C2H4O+CH2HCO=CH3HCO+C2H3O     1.000E+11     0.0    14000.0
!KD-> C2H4O+CH3=CH4+C2H3O           1.070E+12     0.0    11900.0
!KD-> C2H4O+O=OH+C2H3O              1.910E+12     0.0     5300.0
!KD-> C2H4O+OH=H2O+C2H3O            1.780E+13     0.0     3600.0
!KD-> C2H3O=>CH2CHOW                1.000E+11     0.0    10000.0
!KD-> C2H3O=>CH3+CO                 8.000E+11     0.0    10000.0
!KD-> C2H3O+H+M=>C2H4O+M            4.000E+15     0.0        0.0
!KD-> CH2CHOW+M=>CH2HCO+M           1.000E+14     0.0        0.0
!KD-> CH2CHOW=>CH3+CO               1.000E+08     0.0        0.0
!KD-> CH2CHOW=>OH+C2H2              1.000E+11     0.0    17000.0
!KD-> CH2CHOW=>CH2CO+H              1.000E+08     0.0        0.0
!KD-> C2H4O+O2=HO2+C2H3O            1.000E+14     0.0    52000.0
!KD-> C2H4O+HO2=H2O2+C2H3O          5.000E+13     0.0    18000.0
!KD-> CH3HCOW+O2=>HO2+CH3CO         1.000E+14     0.0        0.0
!KD-> CH2CHOW+O2=>HO2+CH2CO         1.000E+14     0.0        0.0
CH2+C2H2=H+C3H3               1.200E+13     0.0     6620.0
CH2+C2H4=C3H6                 3.160E+12     0.0     5280.0
SCH2+C2H4=>C3H6               1.000E+14     0.0        0.0
!KD-> CH2+C3H8=CH3+IC3H7            1.500E+00     3.46    7470.0
!KD-> CH2+C3H8=CH3+NC3H7            9.000E-01     3.65    7150.0
SCH2+C2H2=C3H3+H              1.800E+14     0.0        0.0
C2H3+CH2=C3H4+H               3.000E+13     0.0        0.0
!KD-> C2H3+C2H2=C4H4+H              1.930E+12     0.0     6000.0
!KD-> C2H3+C2H3=C4H6                7.230E+13     0.0        0.0
!KD-> C2H2+CH3=SC3H5                1.610E+40    -8.58   20331.0
C2H2+CH3=C3H5                 2.610E+46    -9.82   36951.0
C2H2+CH3=C3H4+H               6.740E+19    -2.08   31591.0
CH2CO+C2H3=C3H5+CO            1.000E+12     0.0     3000.0
HCCO+C2H2=C3H3+CO             1.000E+11     0.0     3000.0
!KD-> C3H8(+M)=C2H5+CH3(+M)         1.100E+17     0.0    84400.0
!KD->     LOW /7.83E+18 0.0 65000.0/
!KD-> C3H8+O2=NC3H7+HO2             4.000E+13     0.0    50870.0
!KD-> C3H8+O2=IC3H7+HO2             4.000E+13     0.0    47690.0
!KD-> C3H8+HO2=NC3H7+H2O2           4.760E+04     2.55   16490.0
!KD-> C3H8+HO2=IC3H7+H2O2           9.640E+03     2.6    13910.0
!KD-> C3H8+OH=NC3H7+H2O             3.160E+07     1.80     934.0
!KD-> C3H8+OH=IC3H7+H2O             7.060E+06     1.90    -159.0
!KD-> C3H8+O=NC3H7+OH               3.715E+06     2.4     5505.0
!KD-> C3H8+O=IC3H7+OH               5.495E+05     2.5     3140.0
```

```
!KD-> C3H8+H=NC3H7+H2             1.336E+06     2.54    6756.0
!KD-> C3H8+H=IC3H7+H2             1.300E+06     2.4     4470.0
!KD-> C3H8+CH3=NC3H7+CH4           9.000E-01     3.65    7150.0
!KD-> C3H8+CH3=IC3H7+CH4           1.500E+00     3.46    5480.0
!KD-> C3H8+C2H5=NC3H7+C2H6          9.000E-01     3.65    9140.0
!KD-> C3H8+C2H5=IC3H7+C2H6         1.200E+00     3.46    7470.0
!KD-> C3H8+C2H3=NC3H7+C2H4          6.000E+02     3.3    10502.0
!KD-> C3H8+C2H3=IC3H7+C2H4         1.000E+03     3.1     8829.0
!KD-> C3H8+IC3H7=NC3H7+C3H8         8.440E-03     4.2     8720.0
!KD-> C3H8+C3H5=NC3H7+C3H6          2.350E+02     3.3    19800.0
!KD-> C3H8+C3H5=IC3H7+C3H6         7.840E+01     3.3    18200.0
!KD-> C3H8+CH3O=NC3H7+CH3OH        4.340E+11     0.0     6460.0
!KD-> C3H8+CH3O=IC3H7+CH3OH        1.450E+11     0.0     4570.0
NC3H7=C2H4+CH3              1.260E+13     0.0    30404.0
NC3H7+O2=C3H6+HO2            1.000E+12     0.0     5000.0
!KD-> IC3H7=C2H4+CH3              1.000E+12     0.0    34500.0
!KD-> IC3H7+O2=C3H6+HO2            2.754E+10     0.0    -2151.0
C3H6=C3H5+H                4.570E+14     0.0    88900.0
!KD-> C3H6=SC3H5+H                7.590E+14     0.0   101300.0
!KD-> C3H6=TC3H5+H                1.450E+15     0.0    98060.0
C3H6=C2H3+CH3               1.100E+21    -1.2    97720.0
!KD-> C3H6+HO2=C3H6O+OH           1.050E+12     0.0    14210.0
C3H6+HO2=C3H5+H2O2           9.640E+03     2.6    13910.0
!KD-> C3H6+HO2=SC3H5+H2O2          7.500E+09     0.0    12570.0
!KD-> C3H6+HO2=TC3H5+H2O2          3.000E+09     0.0     9930.0
C3H6+OH=C3H5+H2O            3.120E+06     2.0     -300.0
!KD-> C3H6+OH=SC3H5+H2O           2.140E+06     2.0     2780.0
!KD-> C3H6+OH=TC3H5+H2O           1.110E+06     2.0     1450.0
C3H6+O=C2H5+HCO             6.833E+06     1.57    -628.0
C3H6+O=CH3+CH3CO            9.111E+06     1.57    -628.0
C3H6+O=C2H4+CH2O            4.555E+06     1.57    -628.0
NC3H7=C3H6+H                1.000E+14     0.0    37286.0
!KD-> C3H6+H=IC3H7                5.704E+09     1.16     874.0
C3H6+H=C3H5+H2              6.457E+12     0.0     4445.0
!KD-> C3H6+H=SC3H5+H2             7.810E+05     2.5    12280.0
!KD-> C3H6+O2=SC3H5+HO2           1.950E+12     0.0    39000.0
!KD-> C3H6+O2=TC3H5+HO2           1.950E+12     0.0    39000.0
C3H6+O2=C3H5+HO2            1.950E+12     0.0    39000.0
C3H6+CH3=C3H5+CH4           2.210E+00     3.5     5680.0
!KD-> C3H6+CH3=SC3H5+CH4          1.350E+00     3.5    12850.0
!KD-> C3H6+CH3=TC3H5+CH4          8.400E-01     3.5    11660.0
C3H6+C2H5=C3H5+C2H6          2.230E+00     3.5     6640.0
!KD-> C3H6O=C2H5+HCO             2.450E+13     0.0    58500.0
!KD-> C3H6O=C2H5CHO              1.820E+14     0.0    58500.0
!KD-> C3H6O=CH3+CH3CO             4.540E+13     0.0    59900.0
!KD-> C3H6O=CH3+CH2HCO            2.450E+13     0.0    58820.0
!KD-> C3H6O=CH3+C2H3O             8.000E+15     0.0    92010.0
!KD-> C2H5CHO=C2H5+HCO            2.450E+16     0.0    73000.0
!KD-> C2H5CHO+O=C2H5CO+OH          5.680E+12     0.0     1540.0
!KD-> C2H5CHO+OH=C2H5CO+H2O        1.210E+13     0.0       0.0
!KD-> C2H5CHO+HO2=C2H5CO+H2O2      1.520E+09     0.0       0.0
```

```
!KD-> C2H5CHO+C2H5=C2H5CO+C2H6      5.000E+10     0.0     6290.0
!KD-> C2H5CO=C2H5+CO                5.890E+12     0.0    14400.0
C3H5+O2=>CH2O+CH2HCO          5.000E+12     0.0    19190.0
C3H5+H=C3H4+H2                1.800E+13     0.0        0.0
C3H5+O=>C2H4+CO+H             1.807E+14     0.0        0.0
C3H5+CH3=C3H4+CH4             3.000E+12    -0.32    -130.0
C3H5+C2H5=C3H4+C2H6           9.640E+11     0.0     -130.0
C3H5+C2H3=C3H4+C2H4           2.400E+12     0.0        0.0
C3H5+C2H3=C3H6+C2H2           4.800E+12     0.0        0.0
!KD-> SC3H5+O2=CH3HCO+HCO           4.340E+12     0.0        0.0
!KD-> SC3H5+HO2=>CH2CO+CH3+OH       4.500E+12     0.0        0.0
!KD-> SC3H5+H=C3H4+H2               3.333E+12     0.0        0.0
!KD-> SC3H5+O=>CH2CO+CH3            1.807E+14     0.0        0.0
!KD-> SC3H5+CH3=C3H4+CH4            1.000E+11     0.0        0.0
!KD-> SC3H5+C2H5=C3H4+C2H6          1.000E+11     0.0        0.0
!KD-> SC3H5+C2H3=C3H4+C2H4          1.000E+11     0.0        0.0
!KD-> TC3H5+O2=CH3CO+CH2O           4.335E+11     0.0        0.0
!KD-> TC3H5+HO2=>CH2CO+CH3+OH       4.500E+12     0.0        0.0
!KD-> TC3H5+H=C3H4+H2               3.333E+12     0.0        0.0
!KD-> TC3H5+O=>HCCO+CH3+H           1.807E+14     0.0        0.0
!KD-> TC3H5+CH3=C3H4+CH4            1.000E+11     0.0        0.0
!KD-> TC3H5+C2H5=C3H4+C2H6          1.000E+11     0.0        0.0
!KD-> TC3H5+C2H3=C3H4+C2H4          1.000E+11     0.0        0.0
C3H4+M=C3H3+H+M               2.000E+18     0.0    80000.0
!KD->   H2O/16.0/   CO2/3.75/   CO/1.875/   H2/2.5/   CH4/3.0/   C3H6/16.0/   C2H4/16.0/
C3H8/16.0/
H2O/16.0/ CO2/3.75/ CO/1.875/ H2/2.5/ CH4/3.0/ C3H6/16.0/ C2H4/16.0/
C3H4(+M)=PC3H4(+M)            1.070E+14     0.0    64300.0
LOW /3.48E+17 0.0 48390.0/
C3H4+O2=C3H3+HO2              4.000E+13     0.0    61500.0
C3H4+HO2=>CH2CO+CH2+OH        8.000E+12     0.0    19000.0
C3H4+OH=CH2CO+CH3             3.120E+12     0.0     -397.0
C3H4+OH=C3H3+H2O              2.000E+07     2.0     1000.0
C3H4+O=C2H3+HCO               1.100E-02     4.613  -4243.0
C3H4+H=C3H5                   1.200E+11     0.69    3000.0
!KD-> C3H4+H=TC3H5                  8.500E+12     0.0     2000.0
C3H4+H=C3H3+H2                2.000E+07     2.0     5000.0
C3H4+CH3=C3H3+CH4             2.000E+11     0.0     7700.0
PC3H4+M=C3H3+H+M              4.700E+18     0.0    80000.0
!KD->   H2O/16.0/   CO2/3.75/   CO/1.875/   H2/2.5/   CH4/3.0/   C3H6/16.0/   C2H4/16.0/
C3H8/16.0/
H2O/16.0/ CO2/3.75/ CO/1.875/ H2/2.5/ CH4/3.0/ C3H6/16.0/ C2H4/16.0/
PC3H4+O2=>HCCO+OH+CH2         2.000E+08     1.5    30100.0
PC3H4+O2=C3H3+HO2             5.000E+12     0.0    51000.0
PC3H4+HO2=>C2H4+CO+OH         3.000E+12     0.0    19000.0
PC3H4+OH=C3H3+H2O             2.000E+07     2.0     1000.0
PC3H4+OH=CH2CO+CH3            5.000E-04     4.5    -1000.0
PC3H4+O=CH2CO+CH2             6.400E+12     0.0     2010.0
PC3H4+O=C2H3+HCO              3.200E+12     0.0     2010.0
PC3H4+O=HCCO+CH3              6.300E+12     0.0     2010.0
PC3H4+O=>HCCO+CH2+H           3.200E+11     0.0     2010.0
```

```
!KD-> PC3H4+H=TC3H5               6.500E+12     0.0     2000.0
PC3H4+H=C3H3+H2             2.000E+07     2.0     5000.0
PC3H4+H=C2H2+CH3            1.300E+05     2.5     1000.0
PC3H4+CH3=C3H3+CH4          1.500E+00     3.5     5600.0
PC3H4+C2H3=C3H3+C2H4        1.000E+12     0.0     7700.0
PC3H4+C3H5=C3H3+C3H6        1.000E+12     0.0     7700.0
!KD-> C3H3+H=C3H2+H2              5.000E+13     0.0     3000.0
C3H3+O=>C2H+HCO+H           7.000E+13     0.0       0.0
C3H3+O=>C2H2+CO+H           7.000E+13     0.0       0.0
!KD-> C3H3+OH=C3H2+H2O            1.000E+13     0.0       0.0
C3H3+O2=CH2CO+HCO           3.010E+10     0.0     2870.0
!KD-> C3H3+CH=IC4H3+H             7.000E+13     0.0       0.0
!KD-> C3H3+CH=NC4H3+H             7.000E+13     0.0       0.0
!KD-> C3H3+CH2=C4H4+H             4.000E+13     0.0       0.0
!KD-> C3H3+C3H3=C6H5+H            2.000E+12     0.0       0.0
!KD-> CH+C2H2=C3H2+H              1.000E+14     0.0       0.0
!KD-> C3H2+O2=HCCO+CO+H           1.000E+14     0.0     3000.0
!KD-> C3H2+OH=C2H2+HCO            5.000E+13     0.0       0.0
!KD-> C3H2+CH2=IC4H3+H            3.000E+13     0.0       0.0
!KD-> C4H8=IC4H7+H                4.078E+18    -1.0    97350.0
!KD-> C4H8=C2C4H8                 4.000E+11     0.0    60000.0
!KD-> C4H8=T2C4H8                 4.000E+11     0.0    60000.0
!KD-> C4H8=C3H5+CH3               1.000E+16     0.0    73000.0
!KD-> C4H8=C2H3+C2H5              1.000E+19    -1.0    96770.0
!KD-> C4H8+O2=IC4H7+HO2           4.000E+12     0.0    33200.0
!KD-> C4H8+HO2=IC4H7+H2O2         1.000E+11     0.0    17060.0
!KD-> C4H8+OH=NC3H7+CH2O          6.500E+12     0.0       0.0
!KD-> C4H8+OH=CH3HCO+C2H5         1.000E+11     0.0       0.0
!KD-> C4H8+OH=C2H6+CH3CO          1.000E+10     0.0       0.0
!KD-> C4H8+OH=IC4H7+H2O           2.250E+13     0.0     2217.0
!KD-> C4H8+O=C3H6+CH2O            2.505E+12     0.0       0.0
!KD-> C4H8+O=CH3HCO+C2H4          1.250E+12     0.0      850.0
!KD-> C4H8+O=C2H5+CH3CO           1.625E+13     0.0      850.0
!KD-> C4H8+O=IC4H7+OH             9.600E+12     0.0     1970.0
!KD-> C4H8+O=NC3H7+HCO            1.800E+05     2.5    -1029.0
!KD-> C4H8+H=IC4H7+H2             5.000E+13     0.0     3900.0
!KD-> C4H8+CH3=IC4H7+CH4          1.000E+11     0.0     7300.0
!KD-> C4H8+C2H5=IC4H7+C2H6        1.000E+11     0.0     8000.0
!KD-> C4H8+C3H5=IC4H7+C3H6        7.900E+10     0.0    12400.0
!KD-> C4H8+SC3H5=IC4H7+C3H6       8.000E+10     0.0    12400.0
!KD-> C4H8+TC3H5=IC4H7+C3H6       8.000E+10     0.0    12400.0
!KD-> C2C4H8=T2C4H8               4.000E+13     0.0    62000.0
!KD-> C2C4H8=C4H6+H2              1.000E+13     0.0    65500.0
!KD-> C2C4H8=IC4H7+H              4.074E+18    -1.0    97350.0
!KD-> C2C4H8=SC3H5+CH3            2.000E+16     0.0    95000.0
!KD-> C2C4H8+OH=IC4H7+H2O         1.250E+14     0.0     3060.0
!KD-> C2C4H8+OH=CH3HCO+C2H5       1.400E+13     0.0       0.0
!KD-> C2C4H8+O=IC3H7+HCO          6.030E+12     0.0       0.0
!KD-> C2C4H8+O=CH3HCO+C2H4        1.000E+12     0.0       0.0
!KD-> C2C4H8+H=IC4H7+H2           1.000E+13     0.0     3500.0
!KD-> C2C4H8+CH3=IC4H7+CH4        1.000E+11     0.0     8200.0
```

```
!KD-> T2C4H8=IC4H7+H               4.074E+18    -1.0    97350.0
!KD-> T2C4H8=SC3H5+CH3             2.000E+16     0.0    96000.0
!KD-> T2C4H8+OH=IC4H7+H2O          1.000E+14     0.0     3060.0
!KD-> T2C4H8+OH=CH3HCO+C2H5        1.500E+13     0.0        0.0
!KD-> T2C4H8+O=IC3H7+HCO           6.030E+12     0.0        0.0
!KD-> T2C4H8+O=CH3HCO+C2H4         1.000E+12     0.0        0.0
!KD-> T2C4H8+H=IC4H7+H2            5.000E+12     0.0     3500.0
!KD-> T2C4H8+CH3=IC4H7+CH4         1.000E+11     0.0     8200.0
!KD-> IC4H7=C4H6+H                 1.200E+14     0.0    49300.0
!KD-> IC4H7=C2H4+C2H3              1.000E+14     0.0    49000.0
!KD-> IC4H7+H=C4H6+H2              3.160E+12     0.0        0.0
!KD-> IC4H7+O2=C4H6+HO2            1.000E+11     0.0        0.0
!KD-> IC4H7+CH3=C4H6+CH4           1.000E+13     0.0        0.0
!KD-> IC4H7+C2H3=C4H6+C2H4         4.000E+12     0.0        0.0
!KD-> IC4H7+C2H5=C4H6+C2H6         4.000E+12     0.0        0.0
!KD-> IC4H7+C2H5=C4H8+C2H4         5.000E+11     0.0        0.0
!KD-> IC4H7+C2H5=T2C4H8+C2H4       5.000E+11     0.0        0.0
!KD-> IC4H7+C2H5=C2C4H8+C2H4       5.000E+11     0.0        0.0
!KD-> IC4H7+C3H5=C4H6+C3H6         4.000E+13     0.0        0.0
!KD-> IC4H7+IC4H7=C4H6+C4H8        3.160E+12     0.0        0.0
!KD-> C2H3+C2H4=C4H6+H             3.000E+12     0.0     1000.0
!KD-> C4H6+H=NC4H5+H2              3.000E+07     2.0    13000.0
!KD-> C4H6+H=IC4H5+H2              3.000E+07     2.0     6000.0
!KD-> C4H6+OH=NC4H5+H2O            2.000E+07     2.0     5000.0
!KD-> C4H6+OH=IC4H5+H2O            2.000E+07     2.0     2000.0
!KD-> C4H6+O=C2H4+CH2CO            1.000E+12     0.0        0.0
!KD-> C4H6+O=PC3H4+CH2O            1.000E+12     0.0        0.0
!KD-> C2H2+NC4H5=C6H6+H            2.800E+03     2.9     1400.0
!KD-> NC4H5+OH=C4H4+H2O            2.000E+07     2.0     1000.0
!KD-> NC4H5+H=C4H4+H2              3.000E+07     2.0     1000.0
!KD-> NC4H5+H=IC4H5+H              1.000E+14     0.0        0.0
!KD-> IC4H5=C4H4+H                 2.000E+15     0.0    45000.0
!KD-> NC4H5=C4H4+H                 1.600E+14     0.0    41400.0
!KD-> C4H4+OH=IC4H3+H2O            1.000E+07     2.0     2000.0
!KD-> C4H4+OH=NC4H3+H2O            7.500E+06     2.0     5000.0
!KD-> C4H4+H=NC4H3+H2              2.000E+07     2.0    15000.0
!KD-> NC4H3+H=IC4H3+H              1.000E+14     0.0        0.0
!KD-> IC4H3+CH2=C3H4+C2H           2.000E+13     0.0        0.0
!KD-> IC4H3+O2=CH2CO+HCCO          1.000E+12     0.0        0.0
!KD-> IC4H3+OH=C4H2+H2O            3.000E+13     0.0        0.0
!KD-> IC4H3+O=CH2CO+C2H            2.000E+13     0.0        0.0
!KD-> IC4H3+H=C4H2+H2              5.000E+13     0.0        0.0
!KD-> NC4H3+C2H2=C6H5              2.800E+03     2.9     1400.0
!KD-> NC4H3+M=C4H2+H+M             1.000E+16     0.0    59700.0
!KD->  H2O/16.0/  CO2/3.75/  CO/1.875/  H2/2.5/  CH4/3.0/  C3H6/16.0/  C2H4/16.0/
C3H8/16.0/
!KD-> IC4H3+M=C4H2+H+M             4.460E+15     0.0    46516.0
!KD->  H2O/16.0/  CO2/3.75/  CO/1.875/  H2/2.5/  CH4/3.0/  C3H6/16.0/  C2H4/16.0/
C3H8/16.0/
!KD-> IC4H3+O=H2C4O+H              2.000E+13     0.0        0.0
!KD-> H2C4O+H=C2H2+HCCO            5.000E+13     0.0     3000.0
```

```
!KD-> H2C4O+OH=CH2CO+HCCO          1.000E+07     2.0     2000.0
!KD-> C4H2+OH=H2C4O+H             6.660E+12     0.0      -410.0
!KD-> C2H2+C2H2=IC4H3+H           2.200E+12     0.0    64060.0
!KD-> C2H2+C2H2=NC4H3+H           1.000E+12     0.0    66000.0
!KD-> C2H2+C2H2=C4H4              5.500E+12     0.0    37000.0
!KD-> C4H2(+M)=C4H+H(+M)          2.200E+14     0.0   116740.0
!KD->       LOW /3.50E+17  0.0  80065.0/
!KD->      H2O /16.0/ H2 /2.5/ CO /1.875/ CO2 /3.75/ CH4 /3.0/
!KD->      C3H6 /16.0/ C2H4 /16.0/ C3H8 /16.0/
!KD-> C4H2+O=C3H2+CO              2.700E+13     0.0     1720.0
!KD-> C2H2+C2H=C4H2+H             1.820E+14     0.0      467.0
!KD-> C2H2+C2H=NC4H3              1.000E+13     0.0        0.0
!KD-> C4H+O2=C2H+CO+CO            1.000E+14     0.0        0.0
!KD-> C2O+H=CH+CO                 1.320E+13     0.0        0.0
!KD-> C2O+O=CO+CO                 5.200E+13     0.0        0.0
!KD-> C2O+OH=CO+CO+H              2.000E+13     0.0        0.0
!KD-> C2O+O2=CO+CO+O              2.000E+13     0.0        0.0
!KD-> C2O+O2=CO+CO2               2.000E+13     0.0        0.0
!KD-> C2+H2=C2H+H                 6.600E+13     0.0     7950.0
!KD-> C2+O=C+CO                   3.600E+14     0.0        0.0
!KD-> C2+O2=CO+CO                 9.000E+12     0.0      980.0
!KD-> C2+OH=C2O+H                 5.000E+13     0.0        0.0
!KD-> C6H5+OH=C6H5O+H             5.000E+13     0.0        0.0
!KD-> C6H5+O2=C6H5O+O             2.600E+13     0.0     6120.0
!KD-> C6H5+HO2=C6H5O+OH           5.000E+13     0.0     1000.0
!KD-> C6H6+H=C6H5+H2              3.000E+12     0.0     8100.0
!KD-> C6H6+OH=C6H5+H2O            1.680E+08     1.42    1450.0
!KD-> C6H6+O=C6H5O+H              2.780E+13     0.0     4910.0
!KD-> C6H6+O2=C6H5O+OH            4.000E+13     0.0    34000.0
!KD-> H+C6H5=C6H6                 7.800E+13     0.0        0.0
C3H3+O=>C2H3+CO             3.800E+13     0.0        0.0
C3H3+O=CH2O+C2H             2.000E+13     0.0        0.0
C3H3+O2=>HCCO+CH2O          6.000E+12     0.0        0.0
C3H3+CH3=C2H5+C2H           1.000E+13     0.0    37500.0
!KD-> C3H3+CH3=C4H6              5.000E+12     0.0        0.0
C3H6+C2H3=C3H5+C2H4         2.210E+00     3.5     4680.0
!KD-> C3H6+C2H3=SC3H5+C2H4       1.350E+00     3.5    10860.0
!KD-> C3H6+C2H3=TC3H5+C2H4       8.400E-01     3.5     9670.0
C3H6+CH3O=C3H5+CH3OH        9.000E+01     2.95   12000.0
CH2+C2H2=C3H4               1.200E+13     0.0     6620.0
C3H4+C3H4=C3H5+C3H3         5.000E+14     0.0    64700.0
C3H4+OH=CH2O+C2H3           1.700E+12     0.0     -300.0
C3H4+OH=HCO+C2H4            1.700E+12     0.0     -300.0
C3H4+O=CH2O+C2H2            1.000E+12     0.0        0.0
C3H4+O=>CO+C2H4             7.800E+12     0.0     1600.0
C3H4+C3H5=C3H3+C3H6         2.000E+12     0.0     7700.0
C3H4+C2H=C3H3+C2H2          1.000E+13     0.0        0.0
PC3H4=C2H+CH3               4.200E+16     0.0   100000.0
PC3H4+C2H=C3H3+C2H2         1.000E+13     0.0        0.0
!KD-> C3H2+O2=HCO+HCCO           1.000E+13     0.0        0.0
!KD-> C2H2+C2H3=NC4H5            2.510E+05     1.9     2100.0
```

```
!KD-> C2H3+C2H3=IC4H5+H            4.000E+13     0.0        0.0
!KD-> IC4H5+H=C4H4+H2              3.000E+07     2.0     1000.0
!KD-> C4H2+H=C4H+H2                1.000E+14     0.0    35000.0
!KD-> C4H6+OH=C3H5+CH2O            7.230E+12     0.0     -994.0
!KD-> C4H8+IC4H7=IC4H7+C2C4H8      3.980E+10     0.0    12400.0
!KD-> C4H8+IC4H7=IC4H7+T2C4H8      3.980E+10     0.0    12400.0
!KD-> C3H3+C3H3=C6H6               3.000E+11     0.0        0.0
!KD-> C3H3+C3H4=C6H6+H             1.400E+12     0.0    10000.0
C3H5+C2H5=C3H6+C2H4          2.600E+12     0.0     -130.0
C3H6+OH=C2H5+CH2O            8.000E+12     0.0        0.0
C3H6+OH=CH3+CH3HCO           3.400E+11     0.0        0.0
C3H5+O2=C3H4+HO2             1.200E+12     0.0    13550.0
CH2O+C3H5=HCO+C3H6           8.000E+10     0.0    12400.0
CH3HCO+C3H5=CH3CO+C3H6       3.800E+11     0.0     7200.0
!KD-> C3H8+CH3O2=NC3H7+CH3O2H      6.030E+12     0.0    19380.0
!KD-> C3H8+CH3O2=IC3H7+CH3O2H      1.990E+12     0.0    17050.0
!KD-> C3H8+C2H5O2=NC3H7+C2H5O2H    6.030E+12     0.0    19380.0
!KD-> C3H8+C2H5O2=IC3H7+C2H5O2H    1.990E+12     0.0    17050.0
!KD-> C3H8+IC3H7O2=NC3H7+IC3H7O2H   6.030E+12     0.0    19380.0
!KD-> C3H8+IC3H7O2=IC3H7+IC3H7O2H   1.990E+12     0.0    17050.0
!KD-> C3H8+NC3H7O2=NC3H7+NC3H7O2H   6.030E+12     0.0    19380.0
!KD-> C3H8+NC3H7O2=IC3H7+NC3H7O2H   1.990E+12     0.0    17050.0
!KD-> NC3H7+O2=NC3H7O2             4.820E+12     0.0        0.0
!KD-> IC3H7+O2=IC3H7O2             6.620E+12     0.0        0.0
!KD-> NC3H7+HO2=NC3H7O+OH          3.200E+13     0.0        0.0
!KD-> IC3H7+HO2=IC3H7O+OH          3.200E+13     0.0        0.0
!KD-> NC3H7+CH3O2=NC3H7O+CH3O      3.800E+12     0.0    -1200.0
!KD-> IC3H7+CH3O2=IC3H7O+CH3O      3.800E+12     0.0    -1200.0
!KD-> NC3H7+NC3H7O2=NC3H7O+NC3H7O   3.800E+12     0.0    -1200.0
!KD-> IC3H7+NC3H7O2=IC3H7O+NC3H7O   3.800E+12     0.0    -1200.0
!KD-> NC3H7+IC3H7O2=NC3H7O+IC3H7O   3.800E+12     0.0    -1200.0
!KD-> IC3H7+IC3H7O2=IC3H7O+IC3H7O   3.800E+12     0.0    -1200.0
!KD-> NC3H7O2+HO2=NC3H7O2H+O2      4.600E+10     0.0    -2600.0
!KD-> IC3H7O2+HO2=IC3H7O2H+O2      4.600E+10     0.0    -2600.0
!KD-> CH3+NC3H7O2=CH3O+NC3H7O      3.800E+12     0.0    -1200.0
!KD-> CH3+IC3H7O2=CH3O+IC3H7O      3.800E+12     0.0    -1200.0
!KD-> NC3H7O2H=NC3H7O+OH           4.000E+15     0.0    43000.0
!KD-> IC3H7O2H=IC3H7O+OH           4.000E+15     0.0    43000.0
!KD-> NC3H7O=C2H5+CH2O             5.000E+13     0.0    15700.0
!KD-> IC3H7O=CH3+CH3HCO            4.000E+14     0.0    17200.0
!KD-> C3H6+OH(+M)=C3H6OH(+M)       1.810E+13     0.0        0.0
!KD->     LOW /1.33E+30  -3.5  0.0/
!KD-> C3H6OH=>C2H5+CH2O            1.400E+09     0.0    17200.0
!KD-> C3H6OH=>CH3+CH3HCO           1.000E+09     0.0    17200.0
!KD-> C3H6OH+O2=O2C3H6OH           1.000E+12     0.0    -1100.0
!KD-> O2C3H6OH=>CH3HCO+CH2O+OH     1.000E+16     0.0    25000.0
!KD-> C3H6+CH3O2=C3H5+CH3O2H       2.000E+12     0.0    17000.0
!KD-> C3H6+CH3O2=C3H6O+CH3O        4.000E+11     0.0    11720.0
!KD-> C3H6+C2H5O2=C3H5+C2H5O2H     3.200E+11     0.0    14900.0
!KD-> C3H6+C3H5O2=C3H5+C3H5O2H     3.200E+11     0.0    14900.0
!KD-> C3H6+C3H5O2=C3H6O+C3H5O      1.050E+11     0.0    14200.0
```

```
!KD-> C3H6+CH3CO3=C3H5+CH3CO3H      3.200E+11     0.0     14900.0
!KD-> C3H6+NC3H7O2=C3H5+NC3H7O2H    3.200E+11     0.0     14900.0
!KD-> C3H6+IC3H7O2=C3H5+IC3H7O2H    3.200E+11     0.0     14900.0
!KD-> C3H6+NC3H7O2=C3H6O+NC3H7O     1.700E+07     0.0        0.0
!KD-> C3H5+O2=C3H5O2                1.200E+10     0.0     -2300.0
!KD-> C3H5+HO2=C3H5O+OH             9.000E+12     0.0        0.0
!KD-> C3H5+CH3O2=C3H5O+CH3O         3.800E+11     0.0     -1200.0
!KD-> C3H5O2+CH3=C3H5O+CH3O         3.800E+11     0.0     -1200.0
!KD-> C3H5O2+C3H5=C3H5O+C3H5O       3.800E+11     0.0     -1200.0
!KD-> C3H5O2+HO2=C3H5O2H+O2         4.600E+10     0.0     -2600.0
!KD-> C3H5O2+HO2=>C3H5O+OH+O2       1.000E+12     0.0        0.0
!KD-> C3H5O2+CH3O2=>C3H5O+CH3O+O2   1.700E+11     0.0     -1000.0
!KD-> C3H5O2+C3H5O2=>C3H5O+C3H5O+O2  3.700E+12    0.0      2200.0
!KD-> C3H5O=CH2O+C2H3               1.000E+14     0.0     21600.0
!KD-> C3H5O2H=C3H5O+OH              4.000E+15     0.0     43000.0
!KD-> CH2O+C3H5O2=HCO+C3H5O2H       1.300E+11     0.0     10500.0
!KD-> CH2O+NC3H7O2=HCO+NC3H7O2H     1.300E+11     0.0      9000.0
!KD-> CH2O+IC3H7O2=HCO+IC3H7O2H     1.300E+11     0.0      9000.0
!KD-> C2H4+NC3H7O2=C2H3+NC3H7O2H    7.100E+11     0.0     25000.0
!KD-> C2H4+IC3H7O2=C2H3+IC3H7O2H    7.100E+11     0.0     25000.0
!KD-> CH4+C3H5O2=CH3+C3H5O2H        1.140E+13     0.0     20460.0
!KD-> CH4+NC3H7O2=CH3+NC3H7O2H      1.140E+13     0.0     20460.0
!KD-> CH4+IC3H7O2=CH3+IC3H7O2H      1.140E+13     0.0     20460.0
!KD-> CH3OH+NC3H7O2=CH2OH+NC3H7O2H   6.300E+12    0.0     19360.0
!KD-> CH3OH+IC3H7O2=CH2OH+IC3H7O2H   6.300E+12    0.0     19360.0
!KD-> CH3HCO+C3H5O2=CH3CO+C3H5O2H    1.150E+11    0.0     10000.0
!KD-> CH3HCO+NC3H7O2=CH3CO+NC3H7O2H  1.150E+11    0.0     10000.0
!KD-> CH3HCO+IC3H7O2=CH3CO+IC3H7O2H  1.150E+11    0.0     10000.0
!KD-> C+N2+M=CNN+M                  1.120E+15     0.0        0.0
C2H+NO=HCN+CO                 6.000E+13     0.0       570.0
C2H+HCN=CN+C2H2               3.200E+12     0.0      1530.0
CH2+NO=HCN+OH                 5.000E+11     0.0      2870.0
HCN+M=H+CN+M                  3.570E+26    -2.6    124900.0
!KD-> C2N2+M=CN+CN+M                3.200E+16     0.0     94400.0
!KD-> CH+N2(+M)=HCNN(+M)            3.100E+12     0.15       0.0
!KD->     LOW / 1.30E+25 -3.16 740.0 /
!KD->     TROE /0.667 235.0 2117.0 4536.0 /
!KD->     H2O/10.0/ O2/2.0/ AR/0.75/ H2/2.0/
!KD-> HCNN+H=H2+CNN                 5.000E+13     0.0        0.0
!KD-> HCNN+H=>CH2+N2                2.000E+13     0.0      3000.0
!KD-> HCNN+O=OH+CNN                 2.000E+13     0.0     20000.0
!KD-> HCNN+O=CO+H+N2                5.000E+13     0.0     15000.0
!KD-> HCNN+O=HCN+NO                 5.000E+13     0.0     15000.0
!KD-> HCNN+OH=H2O+CNN               1.000E+13     0.0      8000.0
!KD-> HCNN+OH=H+HCO+N2              1.000E+13     0.0     16000.0
!KD-> HCNN+O2=HO2+CNN               1.000E+12     0.0      4000.0
!KD-> HCNN+O2=>H+CO2+N2             4.000E+12     0.0        0.0
!KD-> HCNN+O2=HCO+N2O               4.000E+12     0.0        0.0
!KD-> CNN+O=CO+N2                   1.000E+13     0.0        0.0
!KD-> CNN+O=CN+NO                   1.000E+14     0.0     20000.0
!KD-> CNN+OH=H+CO+N2                1.000E+13     0.0      1000.0
```

```
!KD-> CNN+H=NH+CN                5.000E+14     0.0    40000.0
!KD-> CNN+OH=HCN+NO               1.000E+12     0.0     1000.0
!KD-> CNN+H=HCN+N                5.000E+13     0.0    25000.0
!KD-> CNN+O2=NO+NCO               1.000E+13     0.0     5000.0
HNO+CH3=NO+CH4              8.200E+05     1.87     954.0
!KD-> HONO+CH3=NO2+CH4            8.100E+05     1.87    5504.0
H2NO+CH3=CH3O+NH2           2.000E+13     0.0       0.0
H2NO+CH3=HNO+CH4            1.600E+06     1.87    2960.0
!KD-> HNOH+CH3=HNO+CH4            1.600E+06     1.87    2096.0
!KD-> NH2OH+CH3=HNOH+CH4           1.600E+06     1.87    6350.0
!KD-> NH2OH+CH3=H2NO+CH4           8.200E+05     1.87    5500.0
N2H2+CH3=NNH+CH4            1.600E+06     1.87    2970.0
N2H3+CH3=N2H2+CH4           8.200E+05     1.87    1818.0
N2H4+CH3=N2H3+CH4           3.300E+06     1.87    5325.0
CH4+NH=CH3+NH2              9.000E+13     0.0    20080.0
CH4+NH2=CH3+NH3             1.200E+13     0.0    15150.0
CH3+NH2=CH2+NH3             1.600E+06     1.87    7570.0
C2H6+NH=C2H5+NH2            7.000E+13     0.0    16700.0
C2H6+NH2=C2H5+NH3           9.700E+12     0.0    11470.0
!KD-> C3H8+NH2=NC3H7+NH3           1.700E+13     0.0    10660.0
!KD-> C3H8+NH2=IC3H7+NH3           4.500E+11     0.0     6150.0
!KD-> CH3+NO(+M)=CH3NO(+M)          1.000E+13     0.0       0.0
!KD->     LOW /1.90E+18 0.0 0.0/
!KD->     SRI /0.03 -790.0 1.0/
!KD-> CH3NO+H=H2CNO+H2            4.400E+08     1.5      377.0
!KD-> CH3NO+H=CH3+HNO             1.800E+13     0.0     2800.0
!KD-> CH3NO+O=H2CNO+OH            3.300E+08     1.5     3615.0
!KD-> CH3NO+O=CH3+NO2             1.700E+06     2.08      0.0
!KD-> CH3NO+OH=H2CNO+H2O           3.600E+06     2.0    -1192.0
!KD-> CH3NO+OH=CH3+HONO           2.500E+12     0.0     1000.0
!KD-> CH3NO+CH3=H2CNO+CH4          7.900E+05     1.87    5415.0
!KD-> CH3NO+NH2=H2CNO+NH3          2.800E+06     1.94    1073.0
!KD-> H2CNO=HNCO+H               2.300E+42    -9.11   53840.0
!KD-> H2CNO+O2=CH2O+NO2           2.900E+12    -0.31   17700.0
!KD-> H2CNO+H=CH3+NO             4.000E+13     0.0       0.0
!KD-> H2CNO+H=HCNO+H2            4.800E+08     1.5     -894.0
!KD-> H2CNO+O=HCNO+OH            3.300E+08     1.5     -894.0
!KD-> H2CNO+O=CH2O+NO            7.000E+13     0.0       0.0
!KD-> H2CNO+OH=CH2OH+NO           4.000E+13     0.0       0.0
!KD-> H2CNO+OH=HCNO+H2O           2.400E+06     2.0    -1192.0
!KD-> H2CNO+CH3=C2H5+NO           3.000E+13     0.0       0.0
!KD-> H2CNO+CH3=HCNO+CH4          1.600E+06     1.87   -1113.0
!KD-> H2CNO+NH2=HCNO+NH3          1.800E+06     1.94   -1152.0
CH3+NO2=CH3O+NO             1.400E+13     0.0       0.0
CH+NO2=HCO+NO               1.200E+14     0.0       0.0
CH2+NO2=CH2O+NO             4.200E+13     0.0       0.0
CN+NO=N2+CO                1.000E+11     0.0       0.0
HNCO+M=H+NCO+M              5.000E+15     0.0   120000.0
HNCO+N=NH+NCO               4.000E+13     0.0    36000.0
CH3O+HNO=CH3OH+NO           3.160E+13     0.0       0.0
NCO+HO2=HNCO+O2             2.000E+13     0.0       0.0
```

```
N2O+CO=CO2+N2              2.510E+14     0.0     46000.0
N2O+CH2=CH2O+N2            1.000E+12     0.0         0.0
N2O+CH3=CH3O+N2            9.000E+09     0.0         0.0
N2O+HCO=CO2+H+N2           1.700E+14     0.0     20000.0
N2O+HCCO=CO+HCO+N2         1.700E+14     0.0     25500.0
N2O+C2H2=HCCO+H+N2         6.590E+16     0.0     61200.0
N2O+C2H3=CH2HCO+N2         1.000E+11     0.0         0.0
HOCN+O=NCO+OH              1.500E+04     2.64     4000.0
HOCN+H=NCO+H2              2.000E+07     2.0      2000.0
HOCN+H=NH2+CO              1.200E+08     0.61     2080.0
HOCN+OH=NCO+H2O            6.380E+05     2.0      2560.0
HOCN+CH3=NCO+CH4           8.200E+05     1.87     6620.0
HOCN+NH2=NCO+NH3           9.200E+05     1.94     3645.0
CN+NO2=CO+N2O              4.930E+14    -0.752     344.0
CN+NO2=CO2+N2              3.700E+14    -0.752     344.0
CN+CO2=NCO+CO              3.670E+06     2.16    26900.0
CN+NH3=HCN+NH2             9.200E+12     0.0      -357.0
HNCO+CN=HCN+NCO            1.500E+13     0.0         0.0
!KD-> HONO+NCO=HNCO+NO2          3.600E+12     0.0         0.0
NCO+CH2O=HNCO+HCO          6.000E+12     0.0         0.0
!CH+N2=HCN+N               3.680E+07     1.42    20723.0
!KD-> NH2+C=CH+NH                5.800E+11     0.67    20900.0
!KD-> C+N2=CN+N            5.200E+13     0.0     44700.0
CH2+N2=HCN+NH              4.800E+12     0.0     35850.0
!KD-> C2+N2=CN+CN          1.500E+13     0.0     41700.0
H2CN+N=N2+CH2              6.000E+13     0.0       400.0
H2CN+H=HCN+H2              2.400E+08     1.5      -894.0
H2CN+O=HCN+OH              1.700E+08     1.5      -894.0
H2CN+O=HNCO+H              6.000E+13     0.0         0.0
H2CN+O=HCNO+H              2.000E+13     0.0         0.0
H2CN+M=HCN+H+M             3.000E+14     0.0     22000.0
H2CN+HO2=HCN+H2O2          1.400E+04     2.69    -1610.0
H2CN+O2=CH2O+NO            3.000E+12     0.0      6000.0
H2CN+CH3=HCN+CH4           8.100E+05     1.87    -1113.0
H2CN+OH=HCN+H2O            1.200E+06     2.0     -1192.0
H2CN+NH2=HCN+NH3           9.200E+05     1.94    -1152.0
!KD-> C+NO=CN+O            2.000E+13     0.0         0.0
CH+NO=HCN+O                8.690E+13     0.0         0.0
CH+NO=CN+OH                1.680E+12     0.0         0.0
CH+NO=CO+NH                9.840E+12     0.0         0.0
CH+NO=NCO+H                1.670E+13     0.0         0.0
CH2+NO=HNCO+H              2.500E+12     0.0      5970.0
CH2+NO=HCNO+H              3.800E+13    -0.36      576.0
CH2+NO=NH2+CO              2.300E+16    -1.43     1331.0
CH2+NO=H2CN+O              8.100E+07     1.42     4110.0
CH3+NO=HCN+H2O             2.400E+12     0.0     15700.0
CH3+NO=H2CN+OH             5.200E+12     0.0     24240.0
HCCO+NO=HCNO+CO            4.640E+13     0.0       700.0
HCCO+NO=HCN+CO2            1.390E+13     0.0       700.0
SCH2+NO=HCN+OH             1.000E+14     0.0         0.0
HCNO=HCN+O                 4.200E+31    -6.12    61210.0
```

```
HCNO+H=HCN+OH              1.000E+14     0.0     12000.0
HCNO+H=HNCO+H              2.100E+15    -0.69     2850.0
HCNO+H=HOCN+H              1.400E+11    -0.19     2484.0
HCNO+H=NH2+CO              1.700E+14    -0.75     2890.0
HCNO+O=HCO+NO              7.000E+13     0.0        0.0
CH2+N=HCN+H              5.000E+13     0.0        0.0
CH2+N=NH+CH              6.000E+11     0.67    40500.0
CH+N=CN+H              1.670E+14    -0.09       0.0
!KD-> CH+N=C+NH              4.500E+11     0.65    2400.0
N+CO2=NO+CO              1.900E+11     0.0     3400.0
N+HCCO=HCN+CO              5.000E+13     0.0        0.0
CH3+N=H2CN+H              7.100E+13     0.0        0.0
!KD-> CH3+N=HCNH+H              1.200E+11     0.52     367.6
!KD-> HCNH=HCN+H              6.100E+28    -5.69   24270.0
!KD-> HCNH+H=H2CN+H              2.000E+13     0.0        0.0
!KD-> HCNH+H=HCN+H2              2.400E+08     1.5     -894.0
!KD-> HCNH+O=HNCO+H              7.000E+13     0.0        0.0
!KD-> HCNH+O=HCN+OH              1.700E+08     1.5     -894.0
!KD-> HCNH+OH=HCN+H2O              1.200E+06     2.0    -1192.0
!KD-> HCNH+CH3=HCN+CH4              8.200E+05     1.87    -1113.0
C2H3+N=HCN+CH2              2.000E+13     0.0        0.0
CN+H2O=HCN+OH              4.000E+12     0.0     7400.0
CN+H2O=HOCN+H              4.000E+12     0.0     7400.0
OH+HCN=HOCN+H              3.200E+04     2.45    12120.0
OH+HCN=HNCO+H              5.600E-06     4.71     -490.0
OH+HCN=NH2+CO              6.440E+10     0.0    11700.0
HOCN+H=HNCO+H              1.000E+13     0.0        0.0
HCN+O=NCO+H              1.380E+04     2.64     4980.0
HCN+O=NH+CO              3.450E+03     2.64     4980.0
HCN+O=CN+OH              2.700E+09     1.58    26600.0
CN+H2=HCN+H              2.000E+04     2.87     1600.0
CN+O=CO+N              1.900E+12     0.46      720.0
CN+O2=NCO+O              7.200E+12     0.0     -400.0
CN+OH=NCO+H              4.000E+13     0.0        0.0
!KD-> CN+HCN=C2N2+H              1.510E+07     1.71     1530.0
CN+NO2=NCO+NO              5.320E+15    -0.752     344.0
CN+N2O=NCO+N2              6.000E+12     0.0    15360.0
!KD-> C2N2+O=NCO+CN              4.570E+12     0.0     8880.0
!KD-> C2N2+OH=HNCO+CN              1.860E+11     0.0     2900.0
!KD-> C2N2+OH=HOCN+CN              2.000E+12     0.0    19000.0
HNCO+H=H2+NCO              1.760E+05     2.41    12300.0
HNCO+H=NH2+CO              3.600E+04     2.49     2340.0
HNCO+M=NH+CO+M              1.100E+16     0.0    86000.0
N2/1.5/ O2/1.5/ H2O/18.6/
HNCO+O=NCO+OH              2.200E+06     2.11    11430.0
HNCO+O=NH+CO2              9.800E+07     1.41     8530.0
HNCO+O=HNO+CO              1.500E+08     1.57    44012.0
HNCO+OH=NCO+H2O              3.450E+07     1.5      3600.0
HNCO+OH=NH2+CO2              6.300E+10    -0.06    11645.0
HNCO+HO2=NCO+H2O2              3.000E+11     0.0    29000.0
HNCO+O2=HNO+CO2              1.000E+12     0.0    35000.0
```

```
HNCO+NH2=NCO+NH3          5.000E+12     0.0     6200.0
HNCO+NH=NCO+NH2           1.040E+15     0.0    39390.0
NCO+H=NH+CO               5.360E+13     0.0        0.0
NCO+O=NO+CO               4.200E+13     0.0        0.0
NCO+O=N+CO2               8.000E+12     0.0     2500.0
NCO+N=N2+CO               2.000E+13     0.0        0.0
NCO+OH=NO+HCO             5.000E+12     0.0    15000.0
NCO+M=N+CO+M              2.200E+14     0.0    54050.0
NCO+NO=N2O+CO             4.600E+18    -2.01     934.0
NCO+NO=N2+CO2             5.800E+18    -2.01     934.0
NCO+O2=NO+CO2             2.000E+12     0.0    20000.0
NCO+HCO=HNCO+CO           3.600E+13     0.0        0.0
NCO+NO2=CO+NO+NO          2.830E+13    -0.646   -326.0
NCO+NO2=CO2+N2O           3.570E+14    -0.646   -326.0
NCO+HNO=HNCO+NO           1.800E+13     0.0        0.0
NCO+NCO=CO+CO+N2          3.000E+12     0.0        0.0
NO+HCO=CO+HNO             7.240E+13    -0.4        0.0
NO2+CO=CO2+NO             9.000E+13     0.0    33800.0
NO2+HCO=H+CO2+NO          8.400E+15    -0.75    1930.0
!KD-> CH3O+NO2=HONO+CH2O          3.000E+12     0.0        0.0
CH3O+NO=CH2O+HNO          1.300E+14    -0.7        0.0
!KD-> NO2+CH2O=HONO+HCO           1.000E+10     0.0    15100.0
NO+CH2O=HNO+HCO           1.000E+13     0.0    40820.0
!KD-> NO2+HCO=HONO+CO             1.000E+13     0.0        0.0
NO2+HCO=OH+NO+CO          1.000E+14     0.0        0.0
NCO+N=NO+CN               2.700E+18    -0.995  17200.0
CN+CH4=HCN+CH3            9.000E+04     2.64    -300.0
!KD-> C+NO=CO+N           2.800E+13     0.0        0.0
NH+CO2=HNO+CO             1.000E+13     0.0    14350.0
NCO+CH4=HNCO+CH3          1.000E+13     0.0     8130.0
!KD-> C+N2O=CN+NO             4.800E+12     0.0        0.0
CH+NH2=HCN+H+H            3.000E+13     0.0        0.0
CH+NH=HCN+H               5.000E+13     0.0        0.0
CH2+NH=HCN+H+H            3.000E+13     0.0        0.0
CH3+N=HCN+H+H             2.000E+11     0.0        0.0
CH3+N=HCN+H2              7.100E+12     0.0        0.0
CH4+N=NH+CH3              1.000E+13     0.0    24000.0
C3H3+N=HCN+C2H2           1.000E+13     0.0        0.0
CH+N2O=HCN+NO             1.340E+13     0.0     -510.0
CH+N2O=CO+H+N2            5.200E+12     0.0     -510.0
!KD-> C2O+N2=>NCO+CN            7.000E+11     0.0    17000.0
END
```

Mech.4

```
ELEM H C O N AR
END
```

```
SPECIES
!KD->  CH3HCO C2H4O C2 C2O C
!KD->  CH3CO3 CH3CO3H CH3O2H C2H5O2H C2H5O2
!KD->  CH3CO2 CH3CO2H C2H5OH C2H5O SC2H5O
!KD->  PC2H5O CN H2CN HCN HCNO
!KD->  HOCN HNCO NCO N2O3 C2N2
!KD->  HONO NO3 HNO3 CNN HCNN
!KD->  N2O4 NH2OH HNOH HNNO HCNH
!KD->  NCN HNCN H2CNO CH3NO CH2CHOW
!KD->  C2H3O CH3HCOW C3H6OH O2C3H6OH C3H5O2
!KD->  C3H5O2H C3H5O NC3H7O2 NC3H7O2H IC3H7O2
!KD->  IC3H7O2H IC3H7O NC3H7O C3H6 C3H8
!KD->  IC3H7 NC3H7 C3H2 SC3H5 TC3H5
!KD->  C3H6O C2H5CHO C2H5CO C3H5 C3H4
!KD->  IC4H7 C4H2 C4H C4H6 H2C4O
!KD->  C4H4 IC4H5 NC4H5 C4H8 T2C4H8
!KD->  C2C4H8 IC4H3 NC4H3 C6H6 C6H5O
!KD->  C6H5 AR
H H2 O O2 OH
HO2 H2O H2O2 CO CO2
HCO CH3 CH4 C2H6 CH2O
C2H5 CH2 CH3O CH2OH CH
C2H2 C2H4 C2H3 CH3OH C2H
CH2CO HCCO SCH2 CH3CO CH3O2
CH2HCO N NH NO N2O
NH2 HNO NO2 NNH NH3
N2H2 N2H3 N2H4 H2NO C3H3
PC3H4 N2
END
```

REACTIONS, A_i ((cm^3/mol)$^{(r-1)}$/s), β_i, E_i (cal/mol)

```
! CH + N2 = HCN + N      3.68E+05 1.42 20723
!KD-> CH+N2=NCN+H                 3.00E+12      0.0     22157.
!KD-> CN+N2O=NCN+NO               6.000E+13      0.0    15360.0
!KD->     DUPLICATE
!KD-> CN+N2O=NCN+NO               1.800E+10      0.0     1450.0
!KD->     DUPLICATE
!KD-> CN + NCO = NCN + CO         1.800E+13      0          0
!KD-> C2O + N2 = NCN + CO         7.00E+11      0      17000
!KD-> CH + N2 = HNCN              1.65E+21     -3.62    14196
!KD-> HNCN + M = H + NCN + M        1.79E+28     -3.44    64502
!KD-> HNCN + O = NO + HCN          1.22E+14      0.05      73.5
!KD-> HNCN + O = NH + NCO          5.60E+13      0.05      73.5
!KD-> HNCN + O = CN + HNO          9.36E+12      0.05      73.5
!KD-> HNCN + OH = NCN + H2O         8.28E+03      2.78     3135
!KD-> HNCN + O2 = HO2 + NCN         1.26E+08      1.28    24240
!KD-> NCN = N + CN                2.95E+30     -5.29   117090
!KD-> NCN = C + N2                2.66E+28     -5.32    83110
!KD-> NCN = CNN                   3.69E+29     -5.84    78410
!KD-> NCN + H = HCN +N             1.89E+14      0       8425
!KD-> NCN + O = CN + NO            2.54E+13      0.15      -34
!KD-> NCN + O = CO + N2            2.42E+02      2.32    -1135
```

```
!KD-> NCN + O = N + NCO            2.20E+09      0.42     -157
!KD-> NCN + N= N2 + CN             1.00E+13      0          0
!KD-> NCN + C = CN +CN             1.00E+13      0          0
!KD-> NCN + OH = HCN + NO           3.32E+10     -0.97     7290.
!KD->     DUPLICATE
!KD-> NCN + OH = HCN + NO           4.69E+10      0.44     4000.
!KD-> DUPLICATE
!KD-> NCN + O2 = NO + NCO           3.80E+09      0.51    24590
!KD-> NCN + CH = HCN +CN           3.21E+13      0       -860
!KD-> NCN + CN = C2N2 +N           1.25E+14      0       8020
!KD-> NCN + CH2 = H2CN + CN         7.99E+13      0       4630
H+H+M=H2+M                  7.000E+17     -1.0        0.0
H2/0.0/ N2/0.0/ H/0.0/ H2O/14.3/ CO/3.0/ CO2/3.0/
H+H+H2=H2+H2                1.000E+17     -0.6        0.0
H+H+N2=H2+N2                5.400E+18     -1.3        0.0
H+H+H=H2+H                3.200E+15      0.0        0.0
O+O+M=O2+M                  1.000E+17     -1.0        0.0
O/71.0/ O2/20.0/ NO/5.0/ N2/5.0/ N/5.0/ H2O/5.0/
O+H+M=OH+M                  6.200E+16     -0.6        0.0
H2O/5.0/
H2+O2=OH+OH                 2.500E+12      0.0    39000.0
O+H2=OH+H                 5.060E+04      2.67     6290.0
H+O2=OH+O                 9.750E+13      0.0    14850.0
H+O2(+M)=HO2(+M)            1.480E+12      0.6        0.0
LOW /3.50E+16 -0.41 -1116.0/
TROE /0.5 100000 10/
!KD->  AR/0.0/ H2O/10.6/ H2/1.5/ CO2/2.4/
H2O/10.6/ H2/1.5/ CO2/2.4/
!KD-> H+O2(+AR)=HO2(+AR)           1.480E+12      0.6        0.0
!KD->     LOW /7.00E+17 -0.8  0.0/
!KD->     TROE /0.45 10 100000/
H+OH+M=H2O+M                2.200E+22     -2.0        0.0
!KD->  H2O/6.4/ AR/0.38/ CO2/1.9/
H2O/6.4/        CO2/1.9/
H2+OH=H2O+H                 1.000E+08      1.6     3300.0
OH+OH=H2O+O                 1.500E+09      1.14      100.0
HO2+OH=H2O+O2               2.890E+13      0.0     -500.0
HO2+O=OH+O2                 1.630E+13      0.0     -445.0
H+HO2=H2+O2                 4.280E+13      0.0     1411.0
H+HO2=OH+OH                 1.700E+14      0.0      875.0
H+HO2=H2O+O                 3.000E+13      0.0     1720.0
HO2+HO2=H2O2+O2             4.200E+14      0.0    12000.0
DUPLICATE
HO2+HO2=H2O2+O2             1.300E+11      0.0    -1640.0
DUPLICATE
OH+OH(+M)=H2O2(+M)          7.200E+13     -0.37       0.0
LOW /2.2E+19 -0.76 0.0/
TROE /0.5 100000 10/
H2O/0.0/
OH+OH(+H2O)=H2O2(+H2O)       7.200E+13     -0.37       0.0
LOW /1.45E+18 0.0 0.0/
```

```
H2O2+OH=HO2+H2O              1.000E+12     0.0        0.0
DUPLICATE
H2O2+OH=HO2+H2O              5.800E+14     0.0     9560.0
DUPLICATE
H2O2+H=HO2+H2               1.700E+12     0.0     3755.0
H2O2+H=H2O+OH               1.000E+13     0.0     3575.0
H2O2+O=HO2+OH               2.800E+13     0.0     6400.0
N2+O=NO+N                  1.800E+14     0.0    76100.0
N+O2=NO+O                  9.000E+09     1.0     6500.0
NO+M=N+O+M                  9.640E+14     0.0   148300.0
N2 /1.5/ NO /3.0/ CO2/2.5/
NO+NO=N2+O2                 3.000E+11     0.0    65000.0
N2O(+M)=N2+O(+M)             1.260E+12     0.0    62620.0
LOW / 4.000E+14 0.0 56640.0/
O2/1.4/ N2/1.7/ H2O/12.0/ NO/3.0/ N2O/3.5/
N2O+O=N2+O2                 1.000E+14     0.0    28200.0
N2O+O=NO+NO                 6.920E+13     0.0    26630.0
N2O+N=N2+NO                 1.000E+13     0.0    20000.0
N2O+NO=N2+NO2                2.750E+14     0.0    50000.0
NO+O(+M)=NO2(+M)             1.300E+15    -0.75       0.0
LOW /4.72E+24 -2.87 1551.0/
TROE /0.962 10.0 7962.0 /
!KD->    AR /0.6/ NO2 /6.2/ NO /1.8/ O2 /0.8/ N2O /4.4/ CO2/0/
NO2 /6.2/ NO /1.8/ O2 /0.8/ N2O /4.4/ CO2/0/
H2O /10.0/
NO+O(+CO2)=NO2(+CO2)          1.300E+15    -0.75       0.0
LOW /4.0E+22 -2.16 1051.0/
TROE /0.962 10.0 7962.0 /
NO2+O=NO+O2                 3.910E+12     0.0     -238.0
NO2+N=N2O+O                 8.400E+11     0.0        0.0
NO2+N=NO+NO                 1.000E+12     0.0        0.0
NO2+NO=N2O+O2                1.000E+12     0.0    60000.0
NO2+NO2=NO+NO+O2              3.950E+12     0.0    27590.0
!KD-> NO2+NO2=NO3+NO              1.130E+04     2.58   22720.0
!KD-> NO2+O(+M)=NO3(+M)            1.330E+13     0.0        0.0
!KD->    LOW / 1.49E+28 -4.08 2467.0 /
!KD->    TROE /0.86 10.0 2800.0 /
!KD->    H2O/10.0/ O2/0.8/ H2/2.0/ CO2 /0/
!KD-> NO2+O(+CO2)=NO3(+CO2)         1.330E+13     0.0        0.0
!KD->    LOW / 1.34E+28 -3.94 2277.0 /
!KD->    TROE /0.86 10.0 2800.0 /
!KD-> NO3=NO+O2                   2.500E+06     0.0    12120.0
!KD-> NO3+NO2=NO+NO2+O2            1.200E+11     0.0     3200.0
!KD-> NO3+O=NO2+O2                1.020E+13     0.0        0.0
!KD-> NO3+NO3=NO2+NO2+O2           5.120E+11     0.0     4870.0
!KD-> N2O4(+M)=NO2+NO2(+M)         4.050E+18    -1.1    12840.0
!KD->     LOW /1.96E+28  -3.8  12840./
!KD->     AR/0.8/ N2O4/2.0/ NO2/2.0/
!KD-> N2O4+O=N2O3+O2              1.210E+12     0.0        0.0
!KD-> NO2+NO(+M)=N2O3(+M)          1.600E+09     1.4        0.0
!KD->     LOW /1.0E+33  -7.7  0.0/
```

```
!KD->     N2/1.36/
!KD-> N2O3+O=NO2+NO2              2.710E+11     0.0        0.0
N2+M=N+N+M                  1.000E+28    -3.33   225000.0
N/5/ O/2.2/
NH+M=N+H+M                  2.650E+14     0.0    75500.0
NH+H=N+H2                 3.200E+13     0.0      325.0
NH+N=N2+H                 9.000E+11     0.5        0.0
NH+NH=NNH+H                 5.100E+13     0.0        0.0
NH+NH=NH2+N                 5.950E+02     2.89    -2030.0
NH+NH=N2+H2                 1.000E+08     1.0        0.0
NH2+M=NH+H+M                  3.160E+23    -2.0    91400.0
NH+H2=NH2+H                 1.000E+14     0.0    20070.0
NH2+N=N2+H+H                6.900E+13     0.0        0.0
NH2+NH=N2H2+H                 1.500E+15    -0.5        0.0
NH2+NH=NH3+N                 1.000E+13     0.0     2000.0
NH3+NH=NH2+NH2                3.160E+14     0.0    26770.0
NH2+NH2=N2H2+H2               1.000E+13     0.0     1500.0
N2H3+H=NH2+NH2                5.000E+13     0.0     2000.0
NH3+M=NH2+H+M                 2.200E+16     0.0    93470.0
NH3+M=NH+H2+M                 6.300E+14     0.0    93390.0
NH3+H=NH2+H2                5.420E+05     2.4     9920.0
NH3+NH2=N2H3+H2               1.000E+11     0.5    21600.0
NNH=N2+H                  3.000E+08     0.0        0.0
!    DUPLICATE
NNH+M=N2+H+M                  1.000E+13     0.5     3060.0
!    DUPLICATE
NNH+H=N2+H2                 1.000E+14     0.0        0.0
NNH+N=NH+N2                 3.000E+13     0.0     2000.0
NNH+NH=N2+NH2                 2.000E+11     0.5     2000.0
NNH+NH2=N2+NH3                1.000E+13     0.0        0.0
NNH+NNH=N2H2+N2                1.000E+13     0.0     4000.0
N2H2+M=NNH+H+M                 5.000E+16     0.0    50000.0
H2O/15.0/ O2/2.0/ N2/2.0/ H2/2.0/
N2H2+M=NH+NH+M                 3.160E+16     0.0    99400.0
H2O/15.0/ O2/2.0/ N2/2.0/ H2/2.0/
N2H2+H=NNH+H2                8.500E+04     2.63     -230.0
N2H2+N=NNH+NH                 1.000E+06     2.0        0.0
N2H2+NH=NNH+NH2                1.000E+13     0.0     6000.0
N2H2+NH2=NH3+NNH                8.800E-02     4.05    -1610.0
N2H3+NH=N2H2+NH2               2.000E+13     0.0        0.0
N2H3+NNH=N2H2+N2H2               1.000E+13     0.0     4000.0
N2H3+M=NH2+NH+M                 5.000E+16     0.0    60000.0
N2H3+M=N2H2+H+M                 1.000E+16     0.0    37000.0
N2H3+H=N2H2+H2                1.000E+13     0.0        0.0
N2H3+H=NH+NH3                1.000E+11     0.0        0.0
N2H3+N=N2H2+NH                1.000E+06     2.0        0.0
N2H3+NH2=NH3+N2H2               1.000E+11     0.5        0.0
N2H3+N2H2=N2H4+NNH               1.000E+13     0.0     6000.0
N2H3+N2H3=NH3+NH3+N2              3.000E+12     0.0        0.0
N2H3+N2H3=N2H4+N2H2              1.200E+13     0.0        0.0
N2H4(+M)=NH2+NH2(+M)          5.000E+14     0.0    60000.0
```

```
LOW/1.50E+15 0.0 39000.0 /
N2/2.4/ NH3/3.0/ N2H4/4.0/
N2H4+M=N2H3+H+M            1.000E+15    0.0    63600.0
N2/2.4/ NH3/3.0/ N2H4/4.0/
N2H4+H=N2H3+H2             7.000E+12    0.0    2500.0
N2H4+H=NH2+NH3             2.400E+09    0.0    3100.0
N2H4+N=N2H3+NH             1.000E+10    1.0    2000.0
N2H4+NH=NH2+N2H3           1.000E+09    1.5    2000.0
N2H4+NH2=N2H3+NH3          1.800E+06    1.71   -1380.0
N+OH=NO+H                  2.800E+13    0.0    0.0
N2O+H=N2+OH                2.200E+14    0.0    16750.0
N2O+H=NH+NO                6.700E+22    -2.16  37155.0
N2O+H=NNH+O                5.500E+18    -1.06  47290.0
!KD-> N2O+H=HNNO                 8.000E+24    -4.39  10530.0
N2O+OH=N2+HO2              1.000E+14    0.0    30000.0
HNO+NO=N2O+OH              8.500E+12    0.0    29580.0
!KD-> HNO+NO+NO=HNNO+NO2         1.600E+11    0.0    2090.0
!KD-> NH+NO+M=HNNO+M             1.630E+23    -2.6   1820.0
!KD-> HNNO+H=N2O+H2              2.000E+13    0.0    0.0
!KD-> HNNO+H=NH2+NO              1.000E+12    0.0    0.0
!KD-> HNNO+O=N2O+OH              2.000E+13    0.0    0.0
!KD-> HNNO+OH=H2O+N2O            2.000E+13    0.0    0.0
!KD-> HNNO+OH=HNOH+NO            1.000E+12    0.0    0.0
!KD-> HNNO+NO=N2+HONO            2.600E+11    0.0    1610.0
!KD-> HNNO+NO=NNH+NO2            3.200E+12    0.0    540.0
!KD-> HNNO+NO=N2O+HNO            1.000E+12    0.0    0.0
!KD-> HNNO+NO2=N2O+HONO          1.000E+12    0.0    0.0
!KD-> HNNO+NO2=NNH+NO3           1.000E+13    0.0    17000.0
NO2+H=NO+OH                1.320E+14    0.0    362.0
NO2+OH=HO2+NO              1.810E+13    0.0    6676.0
!KD-> NO2+HO2=HONO+O2            4.640E+11    0.0    -479.0
!KD-> NO2+H2=HONO+H              7.330E+11    0.0    28800.0
NO2+NH=N2O+OH              8.650E+10    0.0    -2270.0
NO2+NH=NO+HNO              1.245E+11    0.0    -2270.0
!KD-> NO3+H=NO2+OH               6.620E+13    0.0    0.0
!KD-> NO3+OH=NO2+HO2             1.210E+13    0.0    0.0
!KD-> NO3+HO2=HNO3+O2            5.550E+11    0.0    0.0
!KD-> NO3+HO2=NO2+OH+O2          1.510E+12    0.0    0.0
!KD-> N2O4+H2O=HONO+HNO3         2.520E+14    0.0    11590.0
!KD-> N2O3+H2O=HONO+HONO         3.790E+13    0.0    8880.0
H+NO(+M)=HNO(+M)           1.520E+15    -0.41  0.0
LOW /4.00E+20 -1.75 0.0 /
!KD->    H2O/10.0/ O2/1.5/ AR/0.75/ H2/2.0/ CO2/3.0/
H2O/10.0/ O2/1.5/          H2/2.0/ CO2/3.0/
HNO+H=NO+H2                4.460E+11    0.72   655.0
HNO+OH=NO+H2O              1.300E+07    1.88   -956.0
HNO+O=OH+NO                5.000E+11    0.5    2000.0
HNO+O=NO2+H                5.000E+10    0.0    2000.0
HNO+O2=NO+HO2              2.200E+10    0.0    9140.0
HNO+N=NO+NH                1.000E+11    0.5    2000.0
HNO+N=H+N2O                5.000E+10    0.5    3000.0
```

```
HNO+NH=NH2+NO                5.000E+11     0.5       0.0
HNO+NH2=NH3+NO               2.000E+13     0.0     1000.0
HNO+HNO=N2O+H2O              3.630E-03     3.98    1190.0
!KD-> HNO+HNO=HNOH+NO            2.000E+08     0.0     4170.0
!KD-> HNO+NO2=HONO+NO            6.020E+11     0.0     2000.0
!KD-> NO+OH(+M)=HONO(+M)         2.000E+12    -0.05    -721.0
!KD->    LOW / 5.08E+23 -2.51 -67.6 /
!KD->    TROE /0.62 10.0 100000.0 /
!KD->    H2O/10.0/ O2/2.0/ AR/0.75/ H2/2.0/ CO2/0.0/
!KD-> NO+OH(+CO2)=HONO(+CO2)     2.000E+12    -0.05    -721.0
!KD->    LOW / 1.70E+23 -2.3 -246.0 /
!KD->    TROE /0.62 10.0 100000.0 /
!KD-> NO2+H+M=HONO+M             1.400E+18    -1.5      900.0
!KD-> HONO+H=HNO+OH              5.640E+10     0.86    4970.0
!KD-> HONO+H=NO+H2O              8.120E+06     1.89    3840.0
!KD-> HONO+O=OH+NO2              1.200E+13     0.0     5960.0
!KD-> HONO+OH=H2O+NO2            1.690E+12     0.0     -517.0
!KD-> HONO+NH=NH2+NO2            1.000E+13     0.0       0.0
!KD-> HONO+HONO=H2O+NO2+NO       1.000E+13     0.0     8540.0
!KD-> HONO+NH2=NO2+NH3           5.000E+12     0.0       0.0
!KD-> NO2+OH(+M)=HNO3(+M)        2.410E+13     0.0       0.0
!KD->    LOW / 6.42E+32 -5.49 2350.0 /
!KD->    TROE /1.0 10.0 1168.0 /
!KD->    H2O/10.0/ O2/2.0/ AR/0.75/ H2/2.0/ CO2/0.0/
!KD-> NO2+OH(+CO2)=HNO3(+CO2)    2.410E+13     0.0       0.0
!KD->    LOW / 5.80E+32 -5.4 2186.0 /
!KD->    TROE /1.0 10.0 1168.0 /
!KD-> NO+HO2+M=HNO3+M            1.500E+24    -3.5     2200.0
!KD-> HNO3+H=H2+NO3              5.560E+08     1.53   16400.0
!KD-> HNO3+H=H2O+NO2             6.080E+01     3.29    6290.0
!KD-> HNO3+H=OH+HONO             3.820E+05     2.3     6980.0
!KD-> HNO3+OH=NO3+H2O            1.030E+10     0.0    -1240.0
NH3+O=NH2+OH                 1.100E+06     2.1     5210.0
NH3+OH=NH2+H2O               5.000E+07     1.6      950.0
NH3+HO2=NH2+H2O2             3.000E+11     0.0    22000.0
NH2+HO2=NH3+O2               1.650E+04     1.55    2027.0
NH2+O=H2+NO                  5.000E+12     0.0       0.0
NH2+O=HNO+H                  4.500E+13     0.0       0.0
NH2+O=NH+OH                  7.000E+12     0.0       0.0
NH2+OH=NH+H2O                9.000E+07     1.5     -460.0
!KD-> NH2+OH=NH2OH               1.790E+13     0.2       0.0
NH2+HO2=HNO+H2O              5.680E+15    -1.12     707.0
NH2+HO2=H2NO+OH              2.910E+17    -1.32    1248.0
NH2+O2=HNO+OH                1.000E+13     0.0    26290.0
NH2+O2=H2NO+O                6.000E+13     0.0    29880.0
NH2+NO=NNH+OH                2.290E+10     0.425   -814.0
NH2+NO=N2+H2O                2.770E+20    -2.65    1258.0
NH2+NO=H2+N2O                1.000E+13     0.0    33700.0
NH2+NO2=N2O+H2O              1.620E+16    -1.44     270.0
NH2+NO2=H2NO+NO              6.480E+16    -1.44     270.0
NH+O=NO+H                    7.000E+13     0.0       0.0
```

```
NH+O=N+OH                  7.000E+12     0.0        0.0
NH+OH=HNO+H                  2.000E+13     0.0        0.0
NH+OH=N+H2O                 2.000E+09     1.2        0.0
NH+OH=NO+H2                 2.000E+13     0.0        0.0
NH+HO2=HNO+OH                 1.000E+13     0.0     2000.0
NH+O2=HNO+O                 4.000E+13     0.0    17880.0
NH+O2=NO+OH                 4.500E+08     0.79    1190.0
NH+H2O=HNO+H2                 2.000E+13     0.0    13850.0
NH+N2O=N2+HNO                 2.000E+12     0.0     6000.0
NNH+O=NH+NO                  2.000E+14     0.0     4000.0
NH+NO=N2+OH                 6.100E+13    -0.50     120.0
N2H4+O=N2H2+H2O               8.500E+13     0.0     1200.0
N2H4+O=N2H3+OH              2.500E+12     0.0     1200.0
N2H4+OH=N2H3+H2O             3.000E+10     0.68     1290.0
N2H4+OH=NH3+H2NO             3.670E+13     0.0        0.0
N2H4+HO2=N2H3+H2O2            4.000E+13     0.0     2000.0
N2H3+O=N2H2+OH              2.000E+13     0.0     1000.0
N2H3+O=NNH+H2O              3.160E+11     0.5        0.0
N2H3+O=NH2+HNO              1.000E+13     0.0        0.0
N2H3+OH=N2H2+H2O             3.000E+10     0.68     1290.0
N2H3+OH=NH3+HNO             1.000E+12     0.0    15000.0
N2H3+O2=N2H2+HO2             3.000E+12     0.0        0.0
N2H3+HO2=N2H2+H2O2            1.000E+13     0.0     2000.0
N2H3+HO2=N2H4+O2             8.000E+12     0.0        0.0
N2H3+NO=HNO+N2H2             1.000E+12     0.0        0.0
N2H2+O=NH2+NO              1.000E+13     0.0        0.0
N2H2+O=NNH+OH              2.000E+13     0.0     1000.0
N2H2+OH=NNH+H2O             5.920E+01     3.4    -1360.0
N2H2+HO2=NNH+H2O2            1.000E+13     0.0     2000.0
N2H2+NO=N2O+NH2             3.000E+10     0.0        0.0
NNH+O=N2+OH                1.700E+16    -1.23     500.0
NNH+OH=N2+H2O              2.400E+22    -2.88     2444.0
NNH+O2=N2+HO2              1.200E+12    -0.34     150.0
NNH+O2=N2O+OH              2.900E+11    -0.34     150.0
NNH+HO2=N2+H2O2             1.000E+13     0.0     2000.0
NNH+NO=N2+HNO              5.000E+13     0.0        0.0
!KD-> NH2OH+OH=HNOH+H2O            2.500E+13     0.0     4250.0
H2NO+M=H2+NO+M              7.830E+27    -4.29   60300.0
H2O/10.0/
H2NO+M=HNO+H+M              2.800E+24    -2.83   64915.0
H2O/10.0/
!KD-> H2NO+M=HNOH+M              1.100E+29    -3.99   43980.0
!KD->   H2O/10.0/
H2NO+H=HNO+H2              3.000E+07     2.0     2000.0
H2NO+H=NH2+OH              5.000E+13     0.0        0.0
H2NO+O=HNO+OH              3.000E+07     2.0     2000.0
H2NO+OH=HNO+H2O             2.000E+07     2.0     1000.0
H2NO+HO2=HNO+H2O2            2.900E+04     2.69    -1600.0
H2NO+NH2=HNO+NH3             3.000E+12     0.0     1000.0
H2NO+O2=HNO+HO2             3.000E+12     0.0    25000.0
H2NO+NO=HNO+HNO             2.000E+07     2.0    13000.0
```

```
!KD-> H2NO+NO2=HONO+HNO            6.000E+11     0.0     2000.0
!KD-> HNOH+M=HNO+H+M               2.000E+24    -2.84   58935.0
!KD->    H2O/10.0/
!KD-> HNOH+H=HNO+H2                4.800E+08     1.5      380.0
!KD-> HNOH+H=NH2+OH                4.000E+13     0.0        0.0
!KD-> HNOH+O=HNO+OH                7.000E+13     0.0        0.0
!KD->     DUPLICATE
!KD-> HNOH+O=HNO+OH                3.300E+08     1.5     -360.0
!KD->     DUPLICATE
!KD-> HNOH+OH=HNO+H2O              2.400E+06     2.0    -1190.0
!KD-> HNOH+HO2=HNO+H2O2            2.900E+04     2.69   -1600.0
!KD-> HNOH+NH2=HNO+NH3             1.800E+06     1.94   -1150.0
!KD-> HNOH+NO2=HONO+HNO            6.000E+11     0.0     2000.0
!KD-> HNOH+O2=HNO+HO2              3.000E+12     0.0    25000.0
!KD-> HNOH+HNO=NH2OH+NO            1.000E+12     0.0     3000.0
!END
CO+HO2=CO2+OH                1.500E+14     0.0    23650.0
CO+OH=CO2+H                  1.170E+07     1.354   -725.0
CO+O+M=CO2+M                 6.160E+14     0.0     3000.0
!KD->  H2/2.5/ H2O/6.2/ CO/1.875/ CO2/3.75/ AR/0.88/
H2/2.5/ H2O/6.2/ CO/1.875/ CO2/3.75/
CH4/3.2/ CH3OH/7.5/
CO+O2=CO2+O                  2.500E+12     0.0    47800.0
HCO+M=H+CO+M                 1.560E+14     0.0    15760.0
!KD->  H2/2.5/ H2O/6.2/ CO/1.875/ CO2/3.75/ AR/1.0/
H2/2.5/ H2O/6.2/ CO/1.875/ CO2/3.75/
CH4/3.2/ CH3OH/7.5/
HCO+OH=CO+H2O                1.000E+14     0.0        0.0
HCO+O=CO+OH                  3.000E+13     0.0        0.0
HCO+O=CO2+H                  3.000E+13     0.0        0.0
HCO+H=CO+H2                  9.000E+13     0.0        0.0
HCO+O2=CO+HO2                2.700E+13     0.0     1190.0
HCO+CH3=CO+CH4               1.200E+14     0.0        0.0
HCO+HO2=CO2+OH+H             3.000E+13     0.0        0.0
HCO+HCO=CH2O+CO              3.000E+13     0.0        0.0
HCO+HCO=H2+CO+CO             2.200E+13     0.0        0.0
CH4(+M)=CH3+H(+M)            2.400E+16     0.0   104913.0
LOW /4.5E+17 0.0 90800/
TROE /1.0 10.0 1350.0 7830.0/
CH4/0.0/ H2/2.0/ CO/2.0/ CO2/3.0/ H2O/5.0/
CH4(+CH4)=CH3+H(+CH4)        2.400E+16     0.0   104913.0
LOW /8.4E+18 0.0 90800/
TROE /0.31 2210.0 90/
CH4+HO2=CH3+H2O2             9.000E+12     0.0    24641.0
CH4+OH=CH3+H2O               1.548E+07     1.83    2774.0
CH4+O=CH3+OH                 7.200E+08     1.56    8485.0
CH4+H=CH3+H2                 1.300E+04     3.0     8050.0
CH4+CH2=CH3+CH3              4.300E+12     0.0    10038.0
CH4+O2=CH3+HO2               4.000E+13     0.0    56900.0
CH3+M=CH2+H+M                2.720E+36    -5.31  117100.0
!KD->  H2/2.5/ H2O/6.2/ CO/1.875/ CO2/3.75/ AR/1.0/
```

```
H2/2.5/ H2O/6.2/ CO/1.875/ CO2/3.75/
CH4/3.2/ CH3OH/7.5/
CH3+M=CH+H2+M               1.000E+16     0.0     85240.0
!KD->  H2/2.5/ H2O/6.2/ CO/1.875/ CO2/3.75/ AR/0.88/
H2/2.5/ H2O/6.2/ CO/1.875/ CO2/3.75/
CH4/3.2/ CH3OH/7.5/
CH3+HO2=CH3O+OH             1.800E+13     0.0         0.0
CH3+OH=CH2OH+H              2.640E+19    -1.8      8068.0
CH3+OH=CH3O+H               5.740E+12    -0.23    13931.0
CH3+OH=CH2+H2O              8.900E+18    -1.8      8067.0
CH3+OH=CH2O+H2              3.190E+12    -0.53    10810.0
CH3+O=H+CH2O                8.430E+13     0.0         0.0
CH3+O2=CH2O+OH              3.400E+11     0.0      8940.0
CH3+O2=CH3O+O               1.320E+14     0.0     31400.0
CH3+CH3=C2H5+H              5.000E+12     0.099   10600.0
CH3+CH3(+M)=C2H6(+M)        9.210E+16    -1.174     636.0
LOW /1.13E+36 -5.246 1705/
TROE /0.405 1120.0 69.6/
H2/2.0/ CO/2.0/ CO2/3.0/ H2O/5.0/
CH3+CH3O=CH4+CH2O           2.409E+13     0.0         0.0
CH3+CH2OH=CH4+CH2O          8.500E+13     0.0         0.0
CH3+H=SCH2+H2               6.000E+13     0.0     15100.0
CH3+O2(+M)=CH3O2(+M)        7.800E+08     1.2         0.0
LOW/5.8E+25 -3.30 0.0/
TROE /0.495 2325.5 10/
CH3+CH3=C2H4+H2             1.000E+14     0.0     32000.0
CH3+OH=SCH2+H2O             7.200E+13     0.0      2780.0
CH2+OH=CH2O+H               2.500E+13     0.0         0.0
CH2+O=CO+H2                 4.800E+13     0.0         0.0
CH2+O=CO+H+H                7.200E+13     0.0         0.0
CH2+O=CH+OH                 3.000E+14     0.0     11920.0
CH2+O=HCO+H                 3.000E+13     0.0         0.0
CH2+H=CH+H2                 3.120E+13     0.0     -1340.0
CH2+O2=HCO+OH               4.300E+10     0.0      -500.0
CH2+O2=CO2+H2               6.900E+11     0.0       500.0
CH2+O2=CO2+H+H              1.600E+12     0.0      1000.0
CH2+O2=CO+H2O               1.900E+10     0.0     -1000.0
CH2+O2=CO+OH+H              8.600E+10     0.0      -500.0
CH2+O2=CH2O+O               5.000E+13     0.0      9000.0
CH2+CO2=CH2O+CO             1.100E+11     0.0      1000.0
CH2+CH2=C2H2+H2             1.580E+15     0.0     11950.0
CH2+CH2=C2H2+H+H            2.000E+14     0.0     11000.0
CH2+CH2=CH3+CH              2.400E+14     0.0      9940.0
CH2+CH2=C2H3+H              2.000E+13     0.0         0.0
CH2+CH3=C2H4+H              4.200E+13     0.0         0.0
CH2+CH=C2H2+H               4.000E+13     0.0         0.0
!KD-> CH2+C=CH+CH                1.620E+12     0.67    46800.0
!KD-> CH2+M=C+H2+M               1.600E+14     0.0     64000.0
CH2+M=CH+H+M                5.600E+15     0.0     89600.0
SCH2+M=CH2+M                6.000E+12     0.0         0.0
!KD->  H2/2.5/ H2O/5.0/ CO/1.875/ CO2/3.75/ AR/0.6/ CH4/1.2/
```

```
H2/2.5/ H2O/5.0/ CO/1.875/ CO2/3.75/     CH4/1.2/
C2H2/8.0/ C2H4/4.0/ C2H6/3.6/ H/33.3/
SCH2+O2=CO+OH+H          3.000E+13    0.0      0.0
SCH2+H=CH+H2             3.000E+13    0.0      0.0
SCH2+O=CO+H+H            1.500E+13    0.0      0.0
SCH2+O=CO+H2             1.500E+13    0.0      0.0
SCH2+OH=CH2O+H           3.000E+13    0.0      0.0
SCH2+HO2=CH2O+OH         3.000E+13    0.0      0.0
SCH2+H2O2=CH3O+OH        3.000E+13    0.0      0.0
SCH2+H2O=>CH3OH          1.800E+13    0.0      0.0
SCH2+CH2O=CH3+HCO        1.200E+12    0.0      0.0
SCH2+HCO=CH3+CO          1.800E+13    0.0      0.0
SCH2+CH3=C2H4+H          1.800E+13    0.0      0.0
SCH2+CH4=CH3+CH3         4.000E+13    0.0      0.0
SCH2+C2H6=CH3+C2H5       1.200E+14    0.0      0.0
SCH2+CO2=CH2O+CO         3.000E+12    0.0      0.0
SCH2+CH2CO=C2H4+CO       1.600E+14    0.0      0.0
CH+OH=HCO+H              3.000E+13    0.0      0.0
CH+O=CO+H                4.000E+13    0.0      0.0
!KD-> CH+O=C+OH          1.520E+13    0.0      4730.0
!KD-> H2O+C=CH+OH        7.800E+11    0.67     39300.0
CH+O2=HCO+O              4.900E+13    0.0      0.0
CH+O2=CO+OH              4.900E+13    0.0      0.0
CH+CO2=HCO+CO            3.220E-02    4.44     -3530.0
CH+CH4=C2H4+H            3.900E+14    -0.4     0.0
CH+CH3=C2H3+H            3.000E+13    0.0      0.0
CH2+OH=CH+H2O            1.130E+07    2.0      3000.0
!KD-> CH+H=C+H2          7.900E+13    0.0      160.0
CH+H2O=CH2O+H            1.170E+15    -0.75    0.0
CH+H2O=CH2OH             5.700E+12    0.0      -760.0
CH+CH2O=CH2CO+H          1.000E+14    0.0      -515.0
CH3O+M=CH2O+H+M          5.400E+13    0.0      13500.0
!KD->  H2/2.5/ H2O/6.2/ CO/1.875/ CO2/3.75/ AR/0.88/
H2/2.5/ H2O/6.2/ CO/1.875/ CO2/3.75/
CH4/3.2/ CH3OH/7.5/
CH3O+HO2=CH2O+H2O2       3.000E+11    0.0      0.0
CH3O+OH=CH2O+H2O         1.800E+13    0.0      0.0
CH3O+O=CH2O+OH           1.800E+12    0.0      0.0
CH3O+H=CH2O+H2           1.800E+13    0.0      0.0
CH3O+O2=CH2O+HO2         2.200E+10    0.0      1750.0
CH3O+CH2O=CH3OH+HCO      1.000E+11    0.0      2980.0
CH3O+CO=CH3+CO2          6.810E-18    9.2      -2850.0
CH3O+HCO=CH3OH+CO        9.000E+13    0.0      0.0
CH3O+C2H5=CH2O+C2H6      2.410E+13    0.0      0.0
CH3O+C2H3=CH2O+C2H4      2.410E+13    0.0      0.0
CH3O+C2H4=CH2O+C2H5      1.200E+11    0.0      6750.0
CH3O+H=CH2OH+H           3.400E+06    1.6      0.0
CH3O+H=SCH2+H2O          1.000E+12    0.0      0.0
CH2O+M=HCO+H+M           5.000E+35    -5.54    96680.0
!KD->  H2/2.5/ H2O/6.2/ CO/1.875/ CO2/3.75/ AR/1.0/
H2/2.5/ H2O/6.2/ CO/1.875/ CO2/3.75/
```

```
CH4/3.2/ CH3OH/7.5/
CH2O+M=CO+H2+M              1.100E+36     -5.54    96680.0
!KD->  H2/2.5/ H2O/6.2/ CO/1.875/ CO2/3.75/ AR/1.0/
H2/2.5/ H2O/6.2/ CO/1.875/ CO2/3.75/
CH4/3.2/ CH3OH/7.5/
CH2O+HO2=HCO+H2O2           4.110E+04     2.5     10210.0
CH2O+OH=HCO+H2O             3.433E+09     1.18     -447.0
CH2O+O=HCO+OH               4.100E+11     0.57    2760.0
CH2O+H=HCO+H2               1.260E+08     1.62    2166.0
CH2O+O2=HCO+HO2             6.000E+13     0.0     40650.0
CH2O+CH3=HCO+CH4            7.800E-08     6.1      1970.0
C2H6(+M)=C2H5+H(+M)         8.850E+20     -1.228  102210.0
LOW /6.90E+42 -6.431 107175.0/
SRI /47.61 16182.0 3371.0/
!KD->  H2/2.0/ H2O/6.0/ CH4/2.0/ CO/1.5/ CO2/2.0/ C2H6/3.0/ AR/0.7/
H2/2.0/ H2O/6.0/ CH4/2.0/ CO/1.5/ CO2/2.0/ C2H6/3.0/
C2H6+HO2=C2H5+H2O2          1.330E+13     0.0     20535.0
C2H6+OH=C2H5+H2O            7.200E+06     2.0      870.0
C2H6+O=C2H5+OH              1.000E+09     1.5     5800.0
C2H6+H=C2H5+H2              1.400E+09     1.5     7400.0
C2H6+H=CH3+CH4              5.400E+04     0.0    11630.0
C2H6+O2=C2H5+HO2            6.000E+13     0.0     52000.0
C2H6+CH3=C2H5+CH4           1.470E-07     6.0     6060.0
C2H6+CH2=CH3+C2H5           6.500E+12     0.0     7911.0
C2H6+C2H3=C2H4+C2H5         8.566E-02     4.14    2543.0
C2H6+HCO=CH2O+C2H5          4.700E+04     2.72    18235.0
C2H5(+M)=C2H4+H(+M)         1.110E+10     1.037   36767.0
LOW /4.0E+33 -4.99 40000.0/
TROE /0.832 10 1203.0/
!KD->  H2/2.0/ CO/2.0/ CO2/3.0/ H2O/5.0/ CH4/2.0/ C2H6/0.0/ AR/0.7/
H2/2.0/ CO/2.0/ CO2/3.0/ H2O/5.0/ CH4/2.0/ C2H6/0.0/
C2H5(+C2H6)=C2H4+H(+C2H6)     8.200E+13     0.0     39880.0
LOW /1.0E+18 0.0 33380.0/
TROE /0.75 97.0 1379.0/
C2H5+HO2=C2H4+H2O2          1.800E+12     0.0       0.0
C2H5+OH=C2H4+H2O            2.409E+13     0.0       0.0
C2H5+OH=>CH3+CH2O+H         2.409E+13     0.0       0.0
C2H5+O=CH2O+CH3             4.240E+13     0.0       0.0
!KD-> C2H5+O=CH3HCO+H             5.300E+13     0.0       0.0
C2H5+O=C2H4+OH              3.460E+13     0.0       0.0
C2H5+H=C2H4+H2              1.700E+12     0.0       0.0
C2H5+O2=C2H4+HO2            2.560E+19     -2.77    1980.0
C2H5+CH3=C2H4+CH4           1.100E+12     0.0       0.0
C2H5+C2H5=C2H4+C2H6         1.400E+12     0.0       0.0
!KD-> C2H5+HO2=C2H5O+OH           3.000E+13     0.0       0.0
C2H4+M=C2H2+H2+M            3.500E+16     0.0     71530.0
!KD->    H2/2.5/ H2O/6.2/ CO/1.875/ CO2/3.75/ AR/1.0/
H2/2.5/ H2O/6.2/ CO/1.875/ CO2/3.75/
CH4/3.2/ CH3OH/7.5/
C2H4+M=C2H3+H+M             2.600E+17     0.0     96570.0
!KD->    H2/2.5/ H2O/6.2/ CO/1.875/ CO2/3.75/ AR/1.0/
```

```
H2/2.5/ H2O/6.2/ CO/1.875/ CO2/3.75/
CH4/3.2/ CH3OH/7.5/
C2H4+OH=C2H3+H2O          5.530E+05    2.31    2900.0
C2H4+O=CH3+HCO            8.100E+06    1.88     180.0
C2H4+H=C2H3+H2            4.490E+07    2.12   13366.0
C2H4+O2=C2H3+HO2          4.000E+13    0.0    61500.0
C2H4+C2H4=C2H5+C2H3       1.860E+14    0.0    64200.0
C2H4+CH3=C2H3+CH4         4.200E+12    0.0    11100.0
C2H4+O=CH2HCO+H           4.700E+06    1.88     180.0
C2H4+O=CH2O+CH2           3.000E+04    1.88     180.0
C2H4+O=CH2CO+H2           6.700E+05    1.88     180.0
C2H4+O=C2H3+OH            1.510E+07    1.91    3790.0
C2H4+OH=CH2O+CH3          2.000E+12    0.0      960.0
!KD-> C2H4+OH(+M)=PC2H5O(+M)      5.420E+12    0.0      0.0
!KD->     LOW /1.19E+27 -3.1 0.0/
C2H4+HO2=C2H3+H2O2        1.120E+13    0.0    30400.0
C2H4+CH3O=C2H3+CH3OH      1.000E+11    0.0    10000.0
C2H3(+M)=C2H2+H(+M)       2.100E+14    0.0    39740.0
LOW /4.15E+41 -7.5 45500.0/
TROE /0.65 100000 10/
!KD->  H2/2.0/ CO/2.0/ CO2/3.0/ H2O/5.0/ CH4/2.0/ C2H6/3.0/ AR/0.7/
H2/2.0/ CO/2.0/ CO2/3.0/ H2O/5.0/ CH4/2.0/ C2H6/3.0/
C2H3+HO2=>CH3+CO+OH       3.000E+13    0.0      0.0
C2H3+OH=C2H2+H2O          3.000E+13    0.0      0.0
C2H3+H=C2H2+H2            1.200E+13    0.0      0.0
C2H3+O=CH3+CO             1.000E+13    0.0      0.0
C2H3+O2=CH2O+HCO          1.700E+29   -5.312   6500.0
C2H3+CH=CH2+C2H2          5.000E+13    0.0      0.0
C2H3+CH3=C2H2+CH4         2.050E+13    0.0      0.0
C2H3+C2H=C2H2+C2H2        3.000E+13    0.0      0.0
C2H3+HCO=C2H4+CO          9.034E+13    0.0      0.0
C2H3+CH2O=C2H4+HCO        5.420E+03    2.81    5862.0
C2H3+C2H3=C2H2+C2H4       1.450E+13    0.0      0.0
C2H3+O=C2H2+OH            1.000E+13    0.0      0.0
C2H3+O=CH2+HCO            1.000E+13    0.0      0.0
C2H3+O=CH2CO+H            1.000E+13    0.0      0.0
!KD-> C2H3+OH=CH3HCO          3.000E+13    0.0      0.0
C2H3+O2=C2H2+HO2          5.190E+15   -1.26    3310.0
DUPLICATE
C2H3+O2=C2H2+HO2          2.120E-06    6.0     9484.0
DUPLICATE
C2H3+O2=CH2HCO+O          3.500E+14   -0.61    5260.0
C2H3+CH2=C2H2+CH3         3.000E+13    0.0      0.0
C2H2=C2H+H                2.373E+32   -5.28  130688.0
C2H2+O2=HCCO+OH           2.000E+08    1.5    30100.0
C2H2+O2=C2H+HO2           1.200E+13    0.0    74520.0
C2H2+OH=C2H+H2O           3.385E+07    2.0    14000.0
C2H2+OH=CH2CO+H           1.100E+13    0.0     7170.0
C2H2+O=CH2+CO             1.200E+06    2.1     1570.0
C2H2+O=HCCO+H             5.000E+06    2.1     1570.0
C2H2+CH3=C2H+CH4          1.800E+11    0.0    17290.0
```

```
C2H2+O=C2H+OH               3.000E+14     0.0    25000.0
C2H2+OH=CH3+CO              4.830E-04     4.0    -2000.0
C2H2+HO2=CH2CO+OH           6.100E+09     0.0     7950.0
C2H2+O2=HCO+HCO             4.000E+12     0.0    28000.0
C2H+OH=HCCO+H               2.000E+13     0.0        0.0
!KD-> C2H+OH=C2+H2O               4.000E+07     2.0     8000.0
C2H+O=CO+CH                 1.450E+13     0.0      460.0
C2H+O2=HCO+CO               9.000E+12     0.0        0.0
C2H+H2=C2H2+H               7.880E+05     2.39     346.0
C2H+O2=CO+CO+H              9.000E+12     0.0        0.0
C2H+O2=HCCO+O               6.000E+11     0.0        0.0
CH2CO(+M)=CH2+CO(+M)        3.000E+14     0.0    71000.0
LOW /2.300E+15   0.0  57600.0/
!KD->    H2/2.5/ H2O/6.2/ CO/1.875/ CO2/3.75/ AR/1.0/
H2/2.5/ H2O/6.2/ CO/1.875/ CO2/3.75/
CH4/3.2/ CH3OH/7.5/
CH2CO+O2=CH2O+CO2           2.000E+13     0.0    61500.0
CH2CO+HO2=>CH2O+CO+OH       6.000E+11     0.0    12738.0
CH2CO+O=HCCO+OH             1.000E+13     0.0     8000.0
CH2CO+OH=CH2OH+CO           1.000E+13     0.0        0.0
CH2CO+H=CH3+CO              3.280E+10     0.851   2840.0
CH2CO+CH3=C2H5+CO           2.400E+12     0.0     8000.0
CH2CO+CH2=C2H4+CO           2.900E+12     0.0     3800.0
CH2CO+CH2=HCCO+CH3          3.600E+13     0.0    11000.0
CH2CO+CH3=HCCO+CH4          7.500E+12     0.0    13000.0
CH2CO+OH=CH2O+HCO           2.800E+13     0.0        0.0
CH2CO+H=HCCO+H2             1.800E+14     0.0     8600.0
CH2CO+O=HCO+HCO             7.500E+11     0.0     1350.0
CH2CO+O=HCO+CO+H            7.500E+11     0.0     1350.0
CH2CO+O=CH2O+CO             7.500E+11     0.0     1350.0
CH2CO+OH=HCCO+H2O           7.500E+12     0.0     2000.0
HCCO+M=CH+CO+M              6.000E+15     0.0    58821.0
!KD->    H2/2.5/ H2O/6.2/ CO/1.875/ CO2/3.75/ AR/0.88/
H2/2.5/ H2O/6.2/ CO/1.875/ CO2/3.75/
CH4/3.2/ CH3OH/7.5/
HCCO+OH=HCO+CO+H            1.000E+13     0.0        0.0
!KD-> HCCO+OH=C2O+H2O             3.000E+13     0.0        0.0
HCCO+O=CO+CO+H              1.000E+14     0.0        0.0
HCCO+O=CH+CO2               2.950E+13     0.0     1110.0
HCCO+H=CH2+CO               1.500E+14     0.0        0.0
HCCO+O2=CO2+CO+H            5.400E+11     0.0      850.0
HCCO+CH2=C2H+CH2O           1.000E+13     0.0     2000.0
HCCO+CH2=C2H3+CO            3.000E+13     0.0        0.0
HCCO+CH3=C2H4+CO            2.000E+12     0.0        0.0
HCCO+CH=CO+C2H2             5.000E+13     0.0        0.0
HCCO+HCCO=CO+C2H2+CO        1.000E+13     0.0        0.0
HCCO+OH=HCO+HCO             1.000E+13     0.0        0.0
HCCO+O2=CO+CO+OH            5.400E+11     0.0      850.0
HCCO+O2=CO2+HCO             5.400E+11     0.0      850.0
CH3OH(+M)=CH3+OH(+M)        1.700E+16     0.0    90885.0
LOW /6.60E+16 0.0 65730.0/
```

```
TROE /0.82 200.0 1438.0/
CH3OH+HO2=CH2OH+H2O2          9.640E+10     0.0     12580.0
CH3OH+OH=CH2OH+H2O            1.440E+06     2.0      -840.0
CH3OH+OH=CH3O+H2O             1.000E+13     0.0      1700.0
CH3OH+O=CH2OH+OH              1.630E+13     0.0      5030.0
CH3OH+H=CH2OH+H2              1.640E+07     2.0      4520.0
CH3OH+CH3=CH2OH+CH4           3.190E+01     3.17     7172.0
CH3OH+CH3=CH3O+CH4            1.450E+01     3.1      6935.0
CH3OH+C2H5=C2H6+CH3O          1.440E+01     3.1      8942.0
CH3OH+H=CH3+H2O               2.000E+14     0.0      5300.0
CH3OH+O=CH3O+OH               1.000E+13     0.0      4680.0
CH3OH+CH3=C2H6+OH             2.000E+12     0.0     15000.0
CH3OH+CH3O=CH2OH+CH3OH        3.000E+11     0.0      4070.0
CH3OH(+M)=CH2OH+H(+M)         1.380E+16     0.0     95950.0
LOW /5.35E+16 0.0 70800.0/
TROE /0.82 200.0 1438.0/
CH3OH+H=H2+CH3O               4.000E+13     0.0      6095.0
CH3OH+O2=CH2OH+HO2            2.050E+13     0.0     44900.0
CH3OH+C2H5=C2H6+CH2OH         3.190E+01     3.2      9161.0
CH2OH+M=CH2O+H+M              1.140E+43    -8.0     43000.0
H2O/16.0/ CH4/3.0/ CO2/3.75/  CO/1.875/  H2/2.5/   CH3OH/6.0/
CH2OH+H=CH2O+H2               1.000E+13     0.0        0.0
CH2OH+O2=CH2O+HO2             1.500E+15    -1.0        0.0
DUPLICATE
CH2OH+O2=CH2O+HO2             7.200E+13     0.0      3570.0
DUPLICATE
H+CH2OH=SCH2+H2O              1.000E+12     0.0        0.0
CH2OH+O=CH2O+OH               9.000E+13     0.0        0.0
CH2OH+OH=CH2O+H2O             1.000E+13     0.0        0.0
CH2OH+HO2=CH2O+H2O2           1.210E+13     0.0        0.0
CH2OH+CH2OH=CH3OH+CH2O        4.820E+12     0.0        0.0
CH2OH+CH2OH=CH2O+CH2O+H2      1.000E+15    -0.7        0.0
CH2OH+HCO=CH3OH+CO            1.210E+14     0.0        0.0
CH2OH+CH2O=CH3OH+HCO          5.490E+03     2.8      5900.0
CH2OH+CH3O=CH3OH+CH2O         2.400E+13     0.0        0.0
CH3O+CH3O=CH3OH+CH2O          2.320E+13     0.0        0.0
!KD-> CH3HCO=CH3+HCO                7.100E+15     0.0     81790.0
!KD-> CH3HCO+HO2=CH3CO+H2O2         3.000E+12     0.0     12000.0
!KD-> CH3HCO+OH=CH3CO+H2O           2.300E+10     0.73    -1100.0
!KD-> CH3HCO+O=CH3CO+OH             5.800E+12     0.0      1800.0
!KD-> CH3HCO+H=CH3CO+H2             4.100E+09     1.16     2400.0
!KD-> CH3HCO+O2=CH3CO+HO2           3.000E+13     0.0     39200.0
!KD-> CH3HCO+CH3=CH3CO+CH4          7.600E+00     3.4      3740.0
!KD-> CH3HCO+H=CH2HCO+H2            7.000E+08     1.5      7400.0
!KD-> CH3HCO+O=CH2HCO+OH            5.000E+08     1.5      5800.0
!KD-> CH3HCO+OH=CH2HCO+H2O          2.000E+14     0.0      6000.0
!KD-> CH3HCO+HO2=CH2HCO+H2O2        3.000E+13     0.0     15000.0
!KD-> CH3HCO+CH2=CH3CO+CH3          1.660E+12     0.0      3510.0
!KD-> CH3HCO+CH3=CH2HCO+CH4         1.580E+00     4.0      7720.0
!KD-> CH3HCO+CH3O=CH3CO+CH3OH       5.000E+12     0.0        0.0
!KD-> CH3HCO+C2H5=CH3CO+C2H6        1.260E+12     0.0      8500.0
```

```
!KD-> CH3HCO+C2H3=CH3CO+C2H4        8.130E+10     0.0     3680.0
CH2HCO=CH3CO                 1.600E+11     0.0    21600.0
!KD-> CH3HCO+CH2HCO=CH3CO+CH3HCO    3.000E+12     0.0    11200.0
CH3CO(+M)=CH3+CO(+M)          2.800E+13     0.0    17150.0
LOW /6.0E+15 0.0 14070.0/
TROE /0.5 100000 10/
!KD->    H2/2.5/ H2O/6.2/ CO/1.875/ CO2/3.75/ AR/0.88/
H2/2.5/ H2O/6.2/ CO/1.875/ CO2/3.75/
CH4/3.2/ CH3OH/7.5/
CH3CO+H=CH2CO+H2            1.150E+13     0.0       0.0
CH3CO+H=CH3+HCO             2.150E+13     0.0       0.0
CH3CO+O=CH2CO+OH            4.000E+13     0.0       0.0
CH3CO+O=CH3+CO2             1.500E+14     0.0       0.0
CH3CO+CH3=C2H6+CO           3.300E+13     0.0       0.0
CH3CO+CH3=CH4+CH2CO         6.100E+12     0.0       0.0
CH2HCO+H=CH2CO+H2           2.000E+13     0.0       0.0
CH2HCO+O2=CH2O+OH+CO        1.800E+10     0.0       0.0
CH2HCO+O2=CH2CO+HO2         1.500E+11     0.0       0.0
CH2HCO=CH2CO+H              1.580E+13     0.0    35200.0
!KD-> C2H5O=CH3+CH2O              1.000E+15     0.0    21600.0
!KD-> C2H5O+O2=CH3HCO+HO2         3.600E+10     0.0     1090.0
!KD-> C2H5O=CH3HCO+H              2.000E+14     0.0    23300.0
!KD-> C2H5O+OH=CH3HCO+H2O         1.000E+14     0.0       0.0
!KD-> C2H5O+H=CH3HCO+H2           1.000E+14     0.0       0.0
!KD-> C2H5O+O=CH3HCO+OH           1.210E+14     0.0       0.0
!KD-> C2H5O+HO2=CH3HCO+H2O2       1.000E+14     0.0       0.0
!KD-> C2H5O+C2H5O=C2H5OH+CH3HCO    5.000E+13     0.0       0.0
!KD-> C2H5O+PC2H5O=C2H5OH+CH3HCO   5.000E+13     0.0       0.0
!KD-> C2H5O+SC2H5O=C2H5OH+CH3HCO   5.000E+13     0.0       0.0
!KD-> SC2H5O+M=CH3HCO+H+M         5.000E+13     0.0    21860.0
!KD-> SC2H5O+H=CH3HCO+H2          2.000E+13     0.0       0.0
!KD-> SC2H5O+OH=CH3HCO+H2O        1.500E+13     0.0       0.0
!KD-> SC2H5O+O=CH3HCO+OH          9.040E+13     0.0       0.0
!KD-> SC2H5O+O2=CH3HCO+HO2        8.400E+15    -1.20      0.0
!KD->    DUPLICATE
!KD-> SC2H5O+O2=CH3HCO+HO2        4.800E+14     0.0     5000.0
!KD->    DUPLICATE
!KD-> SC2H5O+HO2=CH3HCO+H2O2       1.000E+13     0.0       0.0
!KD-> SC2H5O+SC2H5O=C2H5OH+CH3HCO   3.500E+13     0.0       0.0
!KD-> SC2H5O+PC2H5O=C2H5OH+CH3HCO   5.000E+13     0.0       0.0
!KD-> PC2H5O=SC2H5O               1.000E+11     0.0    27000.0
!KD-> PC2H5O+PC2H5O=C2H5OH+CH3HCO   3.400E+13     0.0       0.0
!KD-> C2H5OH=CH2OH+CH3            3.100E+15     0.0    80600.0
!KD-> C2H5OH+OH=SC2H5O+H2O        3.000E+13     0.0     5960.0
!KD-> C2H5OH+OH=C2H5O+H2O         1.138E+06     2.0      914.0
!KD-> C2H5OH+OH=PC2H5O+H2O        2.563E+06     2.06     860.0
!KD-> C2H5OH+O=SC2H5O+OH          6.000E+05     2.46    1850.0
!KD-> C2H5OH+O=C2H5O+OH           4.820E+13     0.0     6856.0
!KD-> C2H5OH+O=PC2H5O+OH          5.000E+12     0.0     4411.0
!KD-> C2H5OH+H=C2H5+H2O           5.900E+11     0.0     3450.0
!KD-> C2H5OH+H=SC2H5O+H2          4.400E+12     0.0     4570.0
```

```
!KD-> C2H5OH+HO2=SC2H5O+H2O2        2.000E+13     0.0    17000.0
!KD-> C2H5OH+CH3=SC2H5O+CH4         4.000E+11     0.0     9700.0
!KD-> C2H5OH+CH3=PC2H5O+CH4         3.000E+00     4.0    10480.0
!KD-> C2H5OH+CH3=C2H5O+CH4          8.000E+10     0.0     9400.0
!KD-> C2H5OH+CH3O=SC2H5O+CH3OH      2.000E+11     0.0     7000.0
!KD-> C2H5OH+CH2O=C2H5O+CH3O        1.500E+12     0.0    79500.0
!KD-> C2H5OH+C2H5O=C2H5OH+SC2H5O    2.000E+11     0.0     7000.0
!KD-> C2H5OH=C2H5+OH                5.000E+16     0.0    91212.0
!KD-> C2H5OH=C2H4+H2O               1.000E+14     0.0    76706.0
!KD-> C2H5OH+O2=PC2H5O+HO2          4.000E+13     0.0    50900.0
!KD-> C2H5OH+O2=SC2H5O+HO2          4.000E+13     0.0    51200.0
!KD-> C2H5OH+O2=C2H5O+HO2           2.000E+13     0.0    56000.0
!KD-> C2H5OH+H=PC2H5O+H2            2.000E+12     0.0     9500.0
!KD-> C2H5OH+H=C2H5O+H2             1.760E+12     0.0     4570.0
!KD-> C2H5OH+HO2=H2O2+C2H5O         1.000E+11     0.0    15500.0
!KD-> C2H5OH+HO2=H2O2+PC2H5O        1.000E+11     0.0    12500.0
!KD-> C2H5OH+C2H5=PC2H5O+C2H6       1.500E+12     0.0    11700.0
!KD-> C2H5OH+C2H5=SC2H5O+C2H6       4.000E+13     0.0    10000.0
!KD-> C2H5OH+CH2OH=SC2H5O+CH3OH     4.000E+11     0.0     9700.0
!KD-> C+OH=CO+H                     5.000E+13     0.0        0.0
!KD-> C+O2=CO+O                     1.200E+14     0.0     4000.0
!KD-> C+CH3=C2H2+H                  5.000E+13     0.0        0.0
!KD-> C+CH2=C2H+H                   5.000E+13     0.0        0.0
!KD-> CH2O+CH3O2=HCO+CH3O2H         2.000E+12     0.0    11660.0
CH3O2+H=CH3O+OH                     9.600E+13     0.0        0.0
CH3O2+OH=CH3OH+O2                   6.000E+13     0.0        0.0
CH3O2+CH3=CH3O+CH3O                 2.400E+13     0.0        0.0
CH3O2+CH3O2=>CH2O+CH3OH+O2          2.700E+10     0.0     -780.0
CH3O2+CH3O2=>CH3O+CH3O+O2           2.800E+10     0.0     -780.0
!KD-> CH3O2+H2O2=CH3O2H+HO2         2.400E+12     0.0    10000.0
!KD-> CH3O2H=CH3O+OH                6.000E+14     0.0    42300.0
!KD-> CH3O2+HO2=CH3O2H+O2           2.290E+11     0.0    -1550.0
!KD-> CH3O2H+OH=CH3O2+H2O           1.150E+12     0.0     -380.0
!KD-> CH4+CH3O2=CH3+CH3O2H          1.810E+11     0.0    18600.0
!KD-> C2H6+CH3O2=C2H5+CH3O2H        2.950E+11     0.0    14940.0
!KD-> CH3OH+CH3O2=CH2OH+CH3O2H      1.810E+12     0.0    13800.0
!KD-> CH3O2H+O=OH+CH3O2             2.000E+13     0.0     4750.0
!KD-> CH3CO+O2=CH3CO3               1.000E+10     0.0    -2700.0
!KD-> CH3HCO+CH3CO3=CH3CO+CH3CO3H   1.200E+11     0.0     4900.0
!KD-> CH3HCO+C2H5O2=CH3CO+C2H5O2H   1.150E+11     0.0    10000.0
!KD-> C2H5+O2(+M)=C2H5O2(+M)        2.200E+10     0.772   -570.0
!KD->      LOW /7.10E+42 -8.24 4270.0 /
!KD-> C2H5O2=C2H4+HO2               5.620E+11     0.0    28900.0
!KD-> C2H5O2+HO2=C2H5O2H+O2         3.400E+11     0.0    -1300.0
!KD-> C2H5O2H=C2H5O+OH              4.000E+15     0.0    43000.0
!KD-> C2H5O2H+O=OH+C2H5O2           2.000E+13     0.0     4750.0
!KD-> C2H5O2H+OH=C2H5O2+H2O         2.000E+12     0.0     -370.0
!KD-> CH4+C2H5O2=CH3+C2H5O2H        1.140E+13     0.0    20460.0
!KD-> CH4+CH3CO3=CH3+CH3CO3H        1.140E+13     0.0    20460.0
!KD-> C2H4+C2H5O2=C2H3+C2H5O2H      1.000E+12     0.0    25000.0
!KD-> C2H4+CH3CO3=C2H3+CH3CO3H      3.000E+12     0.0    29000.0
```

```
!KD-> CH3CO3+HO2=CH3CO3H+O2         1.000E+12     0.0        0.0
!KD-> CH3CO3H=>CH3CO2+OH            1.150E+13     0.0    32550.0
!KD-> CH3CO3H=>CH3+CO2+OH           2.000E+14     0.0    40150.0
!KD-> CH3CO3+CH3O2=>CH3CO2+CH3O+O2  1.080E+15     0.0     3600.0
!KD-> CH3CO3+CH3O2=>CH3CO2H+CH2O+O2 2.470E+09     0.0    -4200.0
!KD-> CH3CO3+HO2=>CH3CO2+OH+O2      2.590E+11     0.0    -2080.0
!KD-> CH3CO3+CH3CO3=>CH3CO2+CH3CO2+O2  1.690E+12   0.0    -1060.0
!KD-> CH3CO2+M=>CH3+CO2+M           8.700E+15     0.0    14400.0
!KD-> CH3CO2H=CH4+CO2               7.080E+13     0.0    74600.0
!KD-> CH3CO2H=CH2CO+H2O             4.470E+14     0.0    79800.0
!KD-> CH3CO2H+OH=CH3CO2+H2O         2.400E+11     0.0     -400.0
!KD-> CH3OH+C2H5O2=CH2OH+C2H5O2H    6.300E+12     0.0    19360.0
!KD-> CH3OH+CH3CO3=CH2OH+CH3CO3H    6.300E+12     0.0    19360.0
!KD-> CH2O+C2H5O2=HCO+C2H5O2H       1.300E+11     0.0     9000.0
!KD-> CH2O+CH3CO3=HCO+CH3CO3H       1.000E+12     0.0    10560.0
!KD-> C2H4+CH3O2=C2H3+CH3O2H        1.000E+13     0.0    25000.0
!KD-> CH3HCO+CH3O2=CH3CO+CH3O2H     1.150E+11     0.0    10000.0
!KD-> C2H5OH+CH3O2=SC2H5O+CH3O2H    1.000E+13     0.0    10000.0
!KD-> C2H5+CH3O2=C2H5O+CH3O         2.410E+13     0.0        0.0
!KD-> C2H4+HO2=C2H4O+OH             2.200E+12     0.0    17200.0
!KD-> C2H4+CH3O=C2H4O+CH3           1.000E+11     0.0    14500.0
!KD-> C2H4+CH3O2=C2H4O+CH3O         7.000E+11     0.0    14500.0
!KD-> C2H4O=>CH3HCOW                1.600E+13     0.0    54300.0
!KD-> CH3HCOW+M=>CH3HCO+M           1.000E+14     0.0        0.0
!KD-> CH3HCOW=>CH3+HCO              5.000E+08     0.0        0.0
!KD-> C2H4O+H=H2+C2H3O              8.000E+13     0.0     9740.0
!KD-> C2H4O+H=H2O+C2H3              5.000E+09     0.0     5030.0
!KD-> C2H4O+H=C2H4+OH               9.510E+10     0.0     5030.0
!KD-> C2H4O+CH2HCO=CH3HCO+C2H3O     1.000E+11     0.0    14000.0
!KD-> C2H4O+CH3=CH4+C2H3O           1.070E+12     0.0    11900.0
!KD-> C2H4O+O=OH+C2H3O              1.910E+12     0.0     5300.0
!KD-> C2H4O+OH=H2O+C2H3O            1.780E+13     0.0     3600.0
!KD-> C2H3O=>CH2CHOW                1.000E+11     0.0    10000.0
!KD-> C2H3O=>CH3+CO                 8.000E+11     0.0    10000.0
!KD-> C2H3O+H+M=>C2H4O+M            4.000E+15     0.0        0.0
!KD-> CH2CHOW+M=>CH2HCO+M           1.000E+14     0.0        0.0
!KD-> CH2CHOW=>CH3+CO               1.000E+08     0.0        0.0
!KD-> CH2CHOW=>OH+C2H2              1.000E+11     0.0    17000.0
!KD-> CH2CHOW=>CH2CO+H              1.000E+08     0.0        0.0
!KD-> C2H4O+O2=HO2+C2H3O            1.000E+14     0.0    52000.0
!KD-> C2H4O+HO2=H2O2+C2H3O          5.000E+13     0.0    18000.0
!KD-> CH3HCOW+O2=>HO2+CH3CO         1.000E+14     0.0        0.0
!KD-> CH2CHOW+O2=>HO2+CH2CO         1.000E+14     0.0        0.0
CH2+C2H2=H+C3H3                     1.200E+13     0.0     6620.0
!KD-> CH2+C2H4=C3H6                 3.160E+12     0.0     5280.0
!KD-> SCH2+C2H4=>C3H6               1.000E+14     0.0        0.0
!KD-> CH2+C3H8=CH3+IC3H7            1.500E+00     3.46    7470.0
!KD-> CH2+C3H8=CH3+NC3H7            9.000E-01     3.65    7150.0
SCH2+C2H2=C3H3+H                    1.800E+14     0.0        0.0
!KD-> C2H3+CH2=C3H4+H               3.000E+13     0.0        0.0
!KD-> C2H3+C2H2=C4H4+H              1.930E+12     0.0     6000.0
```

```
!KD-> C2H3+C2H3=C4H6               7.230E+13     0.0       0.0
!KD-> C2H2+CH3=SC3H5               1.610E+40    -8.58   20331.0
!KD-> C2H2+CH3=C3H5                2.610E+46    -9.82   36951.0
!KD-> C2H2+CH3=C3H4+H              6.740E+19    -2.08   31591.0
!KD-> CH2CO+C2H3=C3H5+CO           1.000E+12     0.0     3000.0
HCCO+C2H2=C3H3+CO            1.000E+11     0.0     3000.0
!KD-> C3H8(+M)=C2H5+CH3(+M)        1.100E+17     0.0    84400.0
!KD->     LOW /7.83E+18 0.0 65000.0/
!KD-> C3H8+O2=NC3H7+HO2            4.000E+13     0.0    50870.0
!KD-> C3H8+O2=IC3H7+HO2            4.000E+13     0.0    47690.0
!KD-> C3H8+HO2=NC3H7+H2O2          4.760E+04     2.55   16490.0
!KD-> C3H8+HO2=IC3H7+H2O2          9.640E+03     2.6    13910.0
!KD-> C3H8+OH=NC3H7+H2O            3.160E+07     1.80     934.0
!KD-> C3H8+OH=IC3H7+H2O            7.060E+06     1.90    -159.0
!KD-> C3H8+O=NC3H7+OH              3.715E+06     2.4     5505.0
!KD-> C3H8+O=IC3H7+OH              5.495E+05     2.5     3140.0
!KD-> C3H8+H=NC3H7+H2              1.336E+06     2.54    6756.0
!KD-> C3H8+H=IC3H7+H2              1.300E+06     2.4     4470.0
!KD-> C3H8+CH3=NC3H7+CH4           9.000E-01     3.65    7150.0
!KD-> C3H8+CH3=IC3H7+CH4           1.500E+00     3.46    5480.0
!KD-> C3H8+C2H5=NC3H7+C2H6         9.000E-01     3.65    9140.0
!KD-> C3H8+C2H5=IC3H7+C2H6         1.200E+00     3.46    7470.0
!KD-> C3H8+C2H3=NC3H7+C2H4         6.000E+02     3.3    10502.0
!KD-> C3H8+C2H3=IC3H7+C2H4         1.000E+03     3.1     8829.0
!KD-> C3H8+IC3H7=NC3H7+C3H8        8.440E-03     4.2     8720.0
!KD-> C3H8+C3H5=NC3H7+C3H6         2.350E+02     3.3    19800.0
!KD-> C3H8+C3H5=IC3H7+C3H6         7.840E+01     3.3    18200.0
!KD-> C3H8+CH3O=NC3H7+CH3OH        4.340E+11     0.0     6460.0
!KD-> C3H8+CH3O=IC3H7+CH3OH        1.450E+11     0.0     4570.0
!KD-> NC3H7=C2H4+CH3               1.260E+13     0.0    30404.0
!KD-> NC3H7+O2=C3H6+HO2            1.000E+12     0.0     5000.0
!KD-> IC3H7=C2H4+CH3               1.000E+12     0.0    34500.0
!KD-> IC3H7+O2=C3H6+HO2            2.754E+10     0.0    -2151.0
!KD-> C3H6=C3H5+H                  4.570E+14     0.0    88900.0
!KD-> C3H6=SC3H5+H                 7.590E+14     0.0   101300.0
!KD-> C3H6=TC3H5+H                 1.450E+15     0.0    98060.0
!KD-> C3H6=C2H3+CH3                1.100E+21    -1.2    97720.0
!KD-> C3H6+HO2=C3H6O+OH            1.050E+12     0.0    14210.0
!KD-> C3H6+HO2=C3H5+H2O2           9.640E+03     2.6    13910.0
!KD-> C3H6+HO2=SC3H5+H2O2          7.500E+09     0.0    12570.0
!KD-> C3H6+HO2=TC3H5+H2O2          3.000E+09     0.0     9930.0
!KD-> C3H6+OH=C3H5+H2O             3.120E+06     2.0     -300.0
!KD-> C3H6+OH=SC3H5+H2O            2.140E+06     2.0     2780.0
!KD-> C3H6+OH=TC3H5+H2O            1.110E+06     2.0     1450.0
!KD-> C3H6+O=C2H5+HCO              6.833E+06     1.57    -628.0
!KD-> C3H6+O=CH3+CH3CO             9.111E+06     1.57    -628.0
!KD-> C3H6+O=C2H4+CH2O             4.555E+06     1.57    -628.0
!KD-> NC3H7=C3H6+H                 1.000E+14     0.0    37286.0
!KD-> C3H6+H=IC3H7                 5.704E+09     1.16     874.0
!KD-> C3H6+H=C3H5+H2               6.457E+12     0.0     4445.0
!KD-> C3H6+H=SC3H5+H2              7.810E+05     2.5    12280.0
```

```
!KD-> C3H6+O2=SC3H5+HO2            1.950E+12     0.0     39000.0
!KD-> C3H6+O2=TC3H5+HO2            1.950E+12     0.0     39000.0
!KD-> C3H6+O2=C3H5+HO2             1.950E+12     0.0     39000.0
!KD-> C3H6+CH3=C3H5+CH4            2.210E+00     3.5      5680.0
!KD-> C3H6+CH3=SC3H5+CH4           1.350E+00     3.5     12850.0
!KD-> C3H6+CH3=TC3H5+CH4           8.400E-01     3.5     11660.0
!KD-> C3H6+C2H5=C3H5+C2H6          2.230E+00     3.5      6640.0
!KD-> C3H6O=C2H5+HCO               2.450E+13     0.0     58500.0
!KD-> C3H6O=C2H5CHO                1.820E+14     0.0     58500.0
!KD-> C3H6O=CH3+CH3CO              4.540E+13     0.0     59900.0
!KD-> C3H6O=CH3+CH2HCO             2.450E+13     0.0     58820.0
!KD-> C3H6O=CH3+C2H3O              8.000E+15     0.0     92010.0
!KD-> C2H5CHO=C2H5+HCO             2.450E+16     0.0     73000.0
!KD-> C2H5CHO+O=C2H5CO+OH          5.680E+12     0.0      1540.0
!KD-> C2H5CHO+OH=C2H5CO+H2O        1.210E+13     0.0         0.0
!KD-> C2H5CHO+HO2=C2H5CO+H2O2      1.520E+09     0.0         0.0
!KD-> C2H5CHO+C2H5=C2H5CO+C2H6     5.000E+10     0.0      6290.0
!KD-> C2H5CO=C2H5+CO               5.890E+12     0.0     14400.0
!KD-> C3H5+O2=>CH2O+CH2HCO         5.000E+12     0.0     19190.0
!KD-> C3H5+H=C3H4+H2               1.800E+13     0.0         0.0
!KD-> C3H5+O=>C2H4+CO+H            1.807E+14     0.0         0.0
!KD-> C3H5+CH3=C3H4+CH4            3.000E+12    -0.32     -130.0
!KD-> C3H5+C2H5=C3H4+C2H6          9.640E+11     0.0      -130.0
!KD-> C3H5+C2H3=C3H4+C2H4          2.400E+12     0.0         0.0
!KD-> C3H5+C2H3=C3H6+C2H2          4.800E+12     0.0         0.0
!KD-> SC3H5+O2=CH3HCO+HCO          4.340E+12     0.0         0.0
!KD-> SC3H5+HO2=>CH2CO+CH3+OH      4.500E+12     0.0         0.0
!KD-> SC3H5+H=C3H4+H2              3.333E+12     0.0         0.0
!KD-> SC3H5+O=>CH2CO+CH3           1.807E+14     0.0         0.0
!KD-> SC3H5+CH3=C3H4+CH4           1.000E+11     0.0         0.0
!KD-> SC3H5+C2H5=C3H4+C2H6         1.000E+11     0.0         0.0
!KD-> SC3H5+C2H3=C3H4+C2H4         1.000E+11     0.0         0.0
!KD-> TC3H5+O2=CH3CO+CH2O          4.335E+11     0.0         0.0
!KD-> TC3H5+HO2=>CH2CO+CH3+OH      4.500E+12     0.0         0.0
!KD-> TC3H5+H=C3H4+H2              3.333E+12     0.0         0.0
!KD-> TC3H5+O=>HCCO+CH3+H          1.807E+14     0.0         0.0
!KD-> TC3H5+CH3=C3H4+CH4           1.000E+11     0.0         0.0
!KD-> TC3H5+C2H5=C3H4+C2H6         1.000E+11     0.0         0.0
!KD-> TC3H5+C2H3=C3H4+C2H4         1.000E+11     0.0         0.0
!KD-> C3H4+M=C3H3+H+M              2.000E+18     0.0     80000.0
!KD->   H2O/16.0/   CO2/3.75/   CO/1.875/   H2/2.5/   CH4/3.0/   C3H6/16.0/   C2H4/16.0/
C3H8/16.0/
!KD-> C3H4(+M)=PC3H4(+M)           1.070E+14     0.0     64300.0
!KD->     LOW /3.48E+17 0.0 48390.0/
!KD-> C3H4+O2=C3H3+HO2             4.000E+13     0.0     61500.0
!KD-> C3H4+HO2=>CH2CO+CH2+OH       8.000E+12     0.0     19000.0
!KD-> C3H4+OH=CH2CO+CH3            3.120E+12     0.0      -397.0
!KD-> C3H4+OH=C3H3+H2O             2.000E+07     2.0      1000.0
!KD-> C3H4+O=C2H3+HCO              1.100E-02     4.613   -4243.0
!KD-> C3H4+H=C3H5                  1.200E+11     0.69     3000.0
!KD-> C3H4+H=TC3H5                 8.500E+12     0.0      2000.0
```

```
!KD-> C3H4+H=C3H3+H2              2.000E+07     2.0     5000.0
!KD-> C3H4+CH3=C3H3+CH4           2.000E+11     0.0     7700.0
PC3H4+M=C3H3+H+M             4.700E+18     0.0    80000.0
!KD->  H2O/16.0/  CO2/3.75/  CO/1.875/  H2/2.5/  CH4/3.0/  C3H6/16.0/  C2H4/16.0/
C3H8/16.0/
H2O/16.0/ CO2/3.75/ CO/1.875/ H2/2.5/ CH4/3.0/          C2H4/16.0/
PC3H4+O2=>HCCO+OH+CH2        2.000E+08     1.5    30100.0
PC3H4+O2=C3H3+HO2            5.000E+12     0.0    51000.0
PC3H4+HO2=>C2H4+CO+OH        3.000E+12     0.0    19000.0
PC3H4+OH=C3H3+H2O            2.000E+07     2.0     1000.0
PC3H4+OH=CH2CO+CH3           5.000E-04     4.5    -1000.0
PC3H4+O=CH2CO+CH2            6.400E+12     0.0     2010.0
PC3H4+O=C2H3+HCO             3.200E+12     0.0     2010.0
PC3H4+O=HCCO+CH3             6.300E+12     0.0     2010.0
PC3H4+O=>HCCO+CH2+H          3.200E+11     0.0     2010.0
!KD-> PC3H4+H=TC3H5               6.500E+12     0.0     2000.0
PC3H4+H=C3H3+H2              2.000E+07     2.0     5000.0
PC3H4+H=C2H2+CH3             1.300E+05     2.5     1000.0
PC3H4+CH3=C3H3+CH4           1.500E+00     3.5     5600.0
PC3H4+C2H3=C3H3+C2H4         1.000E+12     0.0     7700.0
!KD-> PC3H4+C3H5=C3H3+C3H6        1.000E+12     0.0     7700.0
!KD-> C3H3+H=C3H2+H2              5.000E+13     0.0     3000.0
C3H3+O=>C2H+HCO+H            7.000E+13     0.0        0.0
C3H3+O=>C2H2+CO+H            7.000E+13     0.0        0.0
!KD-> C3H3+OH=C3H2+H2O            1.000E+13     0.0        0.0
C3H3+O2=CH2CO+HCO            3.010E+10     0.0     2870.0
!KD-> C3H3+CH=IC4H3+H             7.000E+13     0.0        0.0
!KD-> C3H3+CH=NC4H3+H             7.000E+13     0.0        0.0
!KD-> C3H3+CH2=C4H4+H             4.000E+13     0.0        0.0
!KD-> C3H3+C3H3=C6H5+H            2.000E+12     0.0        0.0
!KD-> CH+C2H2=C3H2+H              1.000E+14     0.0        0.0
!KD-> C3H2+O2=HCCO+CO+H           1.000E+14     0.0     3000.0
!KD-> C3H2+OH=C2H2+HCO            5.000E+13     0.0        0.0
!KD-> C3H2+CH2=IC4H3+H            3.000E+13     0.0        0.0
!KD-> C4H8=IC4H7+H                4.078E+18    -1.0    97350.0
!KD-> C4H8=C2C4H8                 4.000E+11     0.0    60000.0
!KD-> C4H8=T2C4H8                 4.000E+11     0.0    60000.0
!KD-> C4H8=C3H5+CH3               1.000E+16     0.0    73000.0
!KD-> C4H8=C2H3+C2H5              1.000E+19    -1.0    96770.0
!KD-> C4H8+O2=IC4H7+HO2           4.000E+12     0.0    33200.0
!KD-> C4H8+HO2=IC4H7+H2O2         1.000E+11     0.0    17060.0
!KD-> C4H8+OH=NC3H7+CH2O          6.500E+12     0.0        0.0
!KD-> C4H8+OH=CH3HCO+C2H5         1.000E+11     0.0        0.0
!KD-> C4H8+OH=C2H6+CH3CO          1.000E+10     0.0        0.0
!KD-> C4H8+OH=IC4H7+H2O           2.250E+13     0.0     2217.0
!KD-> C4H8+O=C3H6+CH2O            2.505E+12     0.0        0.0
!KD-> C4H8+O=CH3HCO+C2H4          1.250E+12     0.0      850.0
!KD-> C4H8+O=C2H5+CH3CO           1.625E+13     0.0      850.0
!KD-> C4H8+O=IC4H7+OH             9.600E+12     0.0     1970.0
!KD-> C4H8+O=NC3H7+HCO            1.800E+05     2.5    -1029.0
!KD-> C4H8+H=IC4H7+H2             5.000E+13     0.0     3900.0
```

```
!KD-> C4H8+CH3=IC4H7+CH4            1.000E+11     0.0     7300.0
!KD-> C4H8+C2H5=IC4H7+C2H6          1.000E+11     0.0     8000.0
!KD-> C4H8+C3H5=IC4H7+C3H6          7.900E+10     0.0    12400.0
!KD-> C4H8+SC3H5=IC4H7+C3H6         8.000E+10     0.0    12400.0
!KD-> C4H8+TC3H5=IC4H7+C3H6         8.000E+10     0.0    12400.0
!KD-> C2C4H8=T2C4H8                 4.000E+13     0.0    62000.0
!KD-> C2C4H8=C4H6+H2                1.000E+13     0.0    65500.0
!KD-> C2C4H8=IC4H7+H                4.074E+18    -1.0    97350.0
!KD-> C2C4H8=SC3H5+CH3              2.000E+16     0.0    95000.0
!KD-> C2C4H8+OH=IC4H7+H2O           1.250E+14     0.0     3060.0
!KD-> C2C4H8+OH=CH3HCO+C2H5         1.400E+13     0.0        0.0
!KD-> C2C4H8+O=IC3H7+HCO            6.030E+12     0.0        0.0
!KD-> C2C4H8+O=CH3HCO+C2H4          1.000E+12     0.0        0.0
!KD-> C2C4H8+H=IC4H7+H2             1.000E+13     0.0     3500.0
!KD-> C2C4H8+CH3=IC4H7+CH4          1.000E+11     0.0     8200.0
!KD-> T2C4H8=IC4H7+H                4.074E+18    -1.0    97350.0
!KD-> T2C4H8=SC3H5+CH3              2.000E+16     0.0    96000.0
!KD-> T2C4H8+OH=IC4H7+H2O           1.000E+14     0.0     3060.0
!KD-> T2C4H8+OH=CH3HCO+C2H5         1.500E+13     0.0        0.0
!KD-> T2C4H8+O=IC3H7+HCO            6.030E+12     0.0        0.0
!KD-> T2C4H8+O=CH3HCO+C2H4          1.000E+12     0.0        0.0
!KD-> T2C4H8+H=IC4H7+H2             5.000E+12     0.0     3500.0
!KD-> T2C4H8+CH3=IC4H7+CH4          1.000E+11     0.0     8200.0
!KD-> IC4H7=C4H6+H                  1.200E+14     0.0    49300.0
!KD-> IC4H7=C2H4+C2H3               1.000E+14     0.0    49000.0
!KD-> IC4H7+H=C4H6+H2               3.160E+12     0.0        0.0
!KD-> IC4H7+O2=C4H6+HO2             1.000E+11     0.0        0.0
!KD-> IC4H7+CH3=C4H6+CH4            1.000E+13     0.0        0.0
!KD-> IC4H7+C2H3=C4H6+C2H4          4.000E+12     0.0        0.0
!KD-> IC4H7+C2H5=C4H6+C2H6          4.000E+12     0.0        0.0
!KD-> IC4H7+C2H5=C4H8+C2H4          5.000E+11     0.0        0.0
!KD-> IC4H7+C2H5=T2C4H8+C2H4        5.000E+11     0.0        0.0
!KD-> IC4H7+C2H5=C2C4H8+C2H4        5.000E+11     0.0        0.0
!KD-> IC4H7+C3H5=C4H6+C3H6          4.000E+13     0.0        0.0
!KD-> IC4H7+IC4H7=C4H6+C4H8         3.160E+12     0.0        0.0
!KD-> C2H3+C2H4=C4H6+H              3.000E+12     0.0     1000.0
!KD-> C4H6+H=NC4H5+H2               3.000E+07     2.0    13000.0
!KD-> C4H6+H=IC4H5+H2               3.000E+07     2.0     6000.0
!KD-> C4H6+OH=NC4H5+H2O             2.000E+07     2.0     5000.0
!KD-> C4H6+OH=IC4H5+H2O             2.000E+07     2.0     2000.0
!KD-> C4H6+O=C2H4+CH2CO             1.000E+12     0.0        0.0
!KD-> C4H6+O=PC3H4+CH2O             1.000E+12     0.0        0.0
!KD-> C2H2+NC4H5=C6H6+H             2.800E+03     2.9     1400.0
!KD-> NC4H5+OH=C4H4+H2O             2.000E+07     2.0     1000.0
!KD-> NC4H5+H=C4H4+H2               3.000E+07     2.0     1000.0
!KD-> NC4H5+H=IC4H5+H               1.000E+14     0.0        0.0
!KD-> IC4H5=C4H4+H                  2.000E+15     0.0    45000.0
!KD-> NC4H5=C4H4+H                  1.600E+14     0.0    41400.0
!KD-> C4H4+OH=IC4H3+H2O             1.000E+07     2.0     2000.0
!KD-> C4H4+OH=NC4H3+H2O             7.500E+06     2.0     5000.0
!KD-> C4H4+H=NC4H3+H2               2.000E+07     2.0    15000.0
```

```
!KD-> NC4H3+H=IC4H3+H              1.000E+14     0.0        0.0
!KD-> IC4H3+CH2=C3H4+C2H           2.000E+13     0.0        0.0
!KD-> IC4H3+O2=CH2CO+HCCO          1.000E+12     0.0        0.0
!KD-> IC4H3+OH=C4H2+H2O            3.000E+13     0.0        0.0
!KD-> IC4H3+O=CH2CO+C2H            2.000E+13     0.0        0.0
!KD-> IC4H3+H=C4H2+H2              5.000E+13     0.0        0.0
!KD-> NC4H3+C2H2=C6H5              2.800E+03     2.9     1400.0
!KD-> NC4H3+M=C4H2+H+M             1.000E+16     0.0    59700.0
!KD->   H2O/16.0/   CO2/3.75/   CO/1.875/   H2/2.5/   CH4/3.0/   C3H6/16.0/   C2H4/16.0/
C3H8/16.0/
!KD-> IC4H3+M=C4H2+H+M             4.460E+15     0.0    46516.0
!KD->   H2O/16.0/   CO2/3.75/   CO/1.875/   H2/2.5/   CH4/3.0/   C3H6/16.0/   C2H4/16.0/
C3H8/16.0/
!KD-> IC4H3+O=H2C4O+H              2.000E+13     0.0        0.0
!KD-> H2C4O+H=C2H2+HCCO            5.000E+13     0.0     3000.0
!KD-> H2C4O+OH=CH2CO+HCCO          1.000E+07     2.0     2000.0
!KD-> C4H2+OH=H2C4O+H              6.660E+12     0.0     -410.0
!KD-> C2H2+C2H2=IC4H3+H            2.200E+12     0.0    64060.0
!KD-> C2H2+C2H2=NC4H3+H            1.000E+12     0.0    66000.0
!KD-> C2H2+C2H2=C4H4               5.500E+12     0.0    37000.0
!KD-> C4H2(+M)=C4H+H(+M)           2.200E+14     0.0   116740.0
!KD->       LOW /3.50E+17  0.0  80065.0/
!KD->       H2O /16.0/ H2 /2.5/ CO /1.875/ CO2 /3.75/ CH4 /3.0/
!KD->       C3H6 /16.0/ C2H4 /16.0/ C3H8 /16.0/
!KD-> C4H2+O=C3H2+CO               2.700E+13     0.0     1720.0
!KD-> C2H2+C2H=C4H2+H              1.820E+14     0.0      467.0
!KD-> C2H2+C2H=NC4H3               1.000E+13     0.0        0.0
!KD-> C4H+O2=C2H+CO+CO             1.000E+14     0.0        0.0
!KD-> C2O+H=CH+CO                  1.320E+13     0.0        0.0
!KD-> C2O+O=CO+CO                  5.200E+13     0.0        0.0
!KD-> C2O+OH=CO+CO+H               2.000E+13     0.0        0.0
!KD-> C2O+O2=CO+CO+O               2.000E+13     0.0        0.0
!KD-> C2O+O2=CO+CO2                2.000E+13     0.0        0.0
!KD-> C2+H2=C2H+H                  6.600E+13     0.0     7950.0
!KD-> C2+O=C+CO                    3.600E+14     0.0        0.0
!KD-> C2+O2=CO+CO                  9.000E+12     0.0      980.0
!KD-> C2+OH=C2O+H                  5.000E+13     0.0        0.0
!KD-> C6H5+OH=C6H5O+H              5.000E+13     0.0        0.0
!KD-> C6H5+O2=C6H5O+O              2.600E+13     0.0     6120.0
!KD-> C6H5+HO2=C6H5O+OH            5.000E+13     0.0     1000.0
!KD-> C6H6+H=C6H5+H2               3.000E+12     0.0     8100.0
!KD-> C6H6+OH=C6H5+H2O             1.680E+08     1.42    1450.0
!KD-> C6H6+O=C6H5O+H               2.780E+13     0.0     4910.0
!KD-> C6H6+O2=C6H5O+OH             4.000E+13     0.0    34000.0
!KD-> H+C6H5=C6H6                  7.800E+13     0.0        0.0
C3H3+O=>C2H3+CO              3.800E+13     0.0        0.0
C3H3+O=CH2O+C2H              2.000E+13     0.0        0.0
C3H3+O2=>HCCO+CH2O           6.000E+12     0.0        0.0
C3H3+CH3=C2H5+C2H            1.000E+13     0.0    37500.0
!KD-> C3H3+CH3=C4H6                5.000E+12     0.0        0.0
!KD-> C3H6+C2H3=C3H5+C2H4          2.210E+00     3.5     4680.0
```

```
!KD-> C3H6+C2H3=SC3H5+C2H4         1.350E+00     3.5     10860.0
!KD-> C3H6+C2H3=TC3H5+C2H4         8.400E-01     3.5     9670.0
!KD-> C3H6+CH3O=C3H5+CH3OH         9.000E+01     2.95    12000.0
!KD-> CH2+C2H2=C3H4                1.200E+13     0.0     6620.0
!KD-> C3H4+C3H4=C3H5+C3H3          5.000E+14     0.0     64700.0
!KD-> C3H4+OH=CH2O+C2H3            1.700E+12     0.0     -300.0
!KD-> C3H4+OH=HCO+C2H4             1.700E+12     0.0     -300.0
!KD-> C3H4+O=CH2O+C2H2             1.000E+12     0.0        0.0
!KD-> C3H4+O=>CO+C2H4              7.800E+12     0.0     1600.0
!KD-> C3H4+C3H5=C3H3+C3H6          2.000E+12     0.0     7700.0
!KD-> C3H4+C2H=C3H3+C2H2           1.000E+13     0.0        0.0
PC3H4=C2H+CH3                4.200E+16     0.0   100000.0
PC3H4+C2H=C3H3+C2H2          1.000E+13     0.0        0.0
!KD-> C3H2+O2=HCO+HCCO             1.000E+13     0.0        0.0
!KD-> C2H2+C2H3=NC4H5              2.510E+05     1.9     2100.0
!KD-> C2H3+C2H3=IC4H5+H            4.000E+13     0.0        0.0
!KD-> IC4H5+H=C4H4+H2              3.000E+07     2.0     1000.0
!KD-> C4H2+H=C4H+H2                1.000E+14     0.0     35000.0
!KD-> C4H6+OH=C3H5+CH2O            7.230E+12     0.0     -994.0
!KD-> C4H8+IC4H7=IC4H7+C2C4H8      3.980E+10     0.0     12400.0
!KD-> C4H8+IC4H7=IC4H7+T2C4H8      3.980E+10     0.0     12400.0
!KD-> C3H3+C3H3=C6H6               3.000E+11     0.0        0.0
!KD-> C3H3+C3H4=C6H6+H             1.400E+12     0.0     10000.0
!KD-> C3H5+C2H5=C3H6+C2H4          2.600E+12     0.0     -130.0
!KD-> C3H6+OH=C2H5+CH2O            8.000E+12     0.0        0.0
!KD-> C3H6+OH=CH3+CH3HCO           3.400E+11     0.0        0.0
!KD-> C3H5+O2=C3H4+HO2             1.200E+12     0.0     13550.0
!KD-> CH2O+C3H5=HCO+C3H6           8.000E+10     0.0     12400.0
!KD-> CH3HCO+C3H5=CH3CO+C3H6       3.800E+11     0.0     7200.0
!KD-> C3H8+CH3O2=NC3H7+CH3O2H      6.030E+12     0.0     19380.0
!KD-> C3H8+CH3O2=IC3H7+CH3O2H      1.990E+12     0.0     17050.0
!KD-> C3H8+C2H5O2=NC3H7+C2H5O2H    6.030E+12     0.0     19380.0
!KD-> C3H8+C2H5O2=IC3H7+C2H5O2H    1.990E+12     0.0     17050.0
!KD-> C3H8+IC3H7O2=NC3H7+IC3H7O2H  6.030E+12     0.0     19380.0
!KD-> C3H8+IC3H7O2=IC3H7+IC3H7O2H  1.990E+12     0.0     17050.0
!KD-> C3H8+NC3H7O2=NC3H7+NC3H7O2H  6.030E+12     0.0     19380.0
!KD-> C3H8+NC3H7O2=IC3H7+NC3H7O2H  1.990E+12     0.0     17050.0
!KD-> NC3H7+O2=NC3H7O2             4.820E+12     0.0        0.0
!KD-> IC3H7+O2=IC3H7O2             6.620E+12     0.0        0.0
!KD-> NC3H7+HO2=NC3H7O+OH          3.200E+13     0.0        0.0
!KD-> IC3H7+HO2=IC3H7O+OH          3.200E+13     0.0        0.0
!KD-> NC3H7+CH3O2=NC3H7O+CH3O      3.800E+12     0.0     -1200.0
!KD-> IC3H7+CH3O2=IC3H7O+CH3O      3.800E+12     0.0     -1200.0
!KD-> NC3H7+NC3H7O2=NC3H7O+NC3H7O  3.800E+12     0.0     -1200.0
!KD-> IC3H7+NC3H7O2=IC3H7O+NC3H7O  3.800E+12     0.0     -1200.0
!KD-> NC3H7+IC3H7O2=NC3H7O+IC3H7O  3.800E+12     0.0     -1200.0
!KD-> IC3H7+IC3H7O2=IC3H7O+IC3H7O  3.800E+12     0.0     -1200.0
!KD-> NC3H7O2+HO2=NC3H7O2H+O2      4.600E+10     0.0     -2600.0
!KD-> IC3H7O2+HO2=IC3H7O2H+O2      4.600E+10     0.0     -2600.0
!KD-> CH3+NC3H7O2=CH3O+NC3H7O      3.800E+12     0.0     -1200.0
!KD-> CH3+IC3H7O2=CH3O+IC3H7O      3.800E+12     0.0     -1200.0
```

```
!KD-> NC3H7O2H=NC3H7O+OH            4.000E+15     0.0    43000.0
!KD-> IC3H7O2H=IC3H7O+OH            4.000E+15     0.0    43000.0
!KD-> NC3H7O=C2H5+CH2O              5.000E+13     0.0    15700.0
!KD-> IC3H7O=CH3+CH3HCO             4.000E+14     0.0    17200.0
!KD-> C3H6+OH(+M)=C3H6OH(+M)        1.810E+13     0.0        0.0
!KD->     LOW /1.33E+30  -3.5  0.0/
!KD-> C3H6OH=>C2H5+CH2O             1.400E+09     0.0    17200.0
!KD-> C3H6OH=>CH3+CH3HCO            1.000E+09     0.0    17200.0
!KD-> C3H6OH+O2=O2C3H6OH            1.000E+12     0.0    -1100.0
!KD-> O2C3H6OH=>CH3HCO+CH2O+OH      1.000E+16     0.0    25000.0
!KD-> C3H6+CH3O2=C3H5+CH3O2H        2.000E+12     0.0    17000.0
!KD-> C3H6+CH3O2=C3H6O+CH3O         4.000E+11     0.0    11720.0
!KD-> C3H6+C2H5O2=C3H5+C2H5O2H      3.200E+11     0.0    14900.0
!KD-> C3H6+C3H5O2=C3H5+C3H5O2H      3.200E+11     0.0    14900.0
!KD-> C3H6+C3H5O2=C3H6O+C3H5O       1.050E+11     0.0    14200.0
!KD-> C3H6+CH3CO3=C3H5+CH3CO3H      3.200E+11     0.0    14900.0
!KD-> C3H6+NC3H7O2=C3H5+NC3H7O2H    3.200E+11     0.0    14900.0
!KD-> C3H6+IC3H7O2=C3H5+IC3H7O2H    3.200E+11     0.0    14900.0
!KD-> C3H6+NC3H7O2=C3H6O+NC3H7O     1.700E+07     0.0        0.0
!KD-> C3H5+O2=C3H5O2                1.200E+10     0.0    -2300.0
!KD-> C3H5+HO2=C3H5O+OH             9.000E+12     0.0        0.0
!KD-> C3H5+CH3O2=C3H5O+CH3O         3.800E+11     0.0    -1200.0
!KD-> C3H5O2+CH3=C3H5O+CH3O         3.800E+11     0.0    -1200.0
!KD-> C3H5O2+C3H5=C3H5O+C3H5O       3.800E+11     0.0    -1200.0
!KD-> C3H5O2+HO2=C3H5O2H+O2         4.600E+10     0.0    -2600.0
!KD-> C3H5O2+HO2=>C3H5O+OH+O2       1.000E+12     0.0        0.0
!KD-> C3H5O2+CH3O2=>C3H5O+CH3O+O2   1.700E+11     0.0    -1000.0
!KD-> C3H5O2+C3H5O2=>C3H5O+C3H5O+O2  3.700E+12     0.0     2200.0
!KD-> C3H5O=CH2O+C2H3               1.000E+14     0.0    21600.0
!KD-> C3H5O2H=C3H5O+OH              4.000E+15     0.0    43000.0
!KD-> CH2O+C3H5O2=HCO+C3H5O2H       1.300E+11     0.0    10500.0
!KD-> CH2O+NC3H7O2=HCO+NC3H7O2H     1.300E+11     0.0     9000.0
!KD-> CH2O+IC3H7O2=HCO+IC3H7O2H     1.300E+11     0.0     9000.0
!KD-> C2H4+NC3H7O2=C2H3+NC3H7O2H    7.100E+11     0.0    25000.0
!KD-> C2H4+IC3H7O2=C2H3+IC3H7O2H    7.100E+11     0.0    25000.0
!KD-> CH4+C3H5O2=CH3+C3H5O2H        1.140E+13     0.0    20460.0
!KD-> CH4+NC3H7O2=CH3+NC3H7O2H      1.140E+13     0.0    20460.0
!KD-> CH4+IC3H7O2=CH3+IC3H7O2H      1.140E+13     0.0    20460.0
!KD-> CH3OH+NC3H7O2=CH2OH+NC3H7O2H   6.300E+12     0.0    19360.0
!KD-> CH3OH+IC3H7O2=CH2OH+IC3H7O2H   6.300E+12     0.0    19360.0
!KD-> CH3HCO+C3H5O2=CH3CO+C3H5O2H    1.150E+11     0.0    10000.0
!KD-> CH3HCO+NC3H7O2=CH3CO+NC3H7O2H  1.150E+11     0.0    10000.0
!KD-> CH3HCO+IC3H7O2=CH3CO+IC3H7O2H  1.150E+11     0.0    10000.0
!KD-> C+N2+M=CNN+M                  1.120E+15     0.0        0.0
!KD-> C2H+NO=HCN+CO                 6.000E+13     0.0      570.0
!KD-> C2H+HCN=CN+C2H2               3.200E+12     0.0     1530.0
!KD-> CH2+NO=HCN+OH                 5.000E+11     0.0     2870.0
!KD-> HCN+M=H+CN+M                  3.570E+26    -2.6   124900.0
!KD-> C2N2+M=CN+CN+M                3.200E+16     0.0    94400.0
!KD-> CH+N2(+M)=HCNN(+M)            3.100E+12     0.15       0.0
!KD->      LOW / 1.30E+25 -3.16 740.0 /
```

```
!KD->      TROE /0.667 235.0 2117.0 4536.0 /
!KD->      H2O/10.0/ O2/2.0/ AR/0.75/ H2/2.0/
!KD-> HCNN+H=H2+CNN                5.000E+13     0.0        0.0
!KD-> HCNN+H=>CH2+N2               2.000E+13     0.0     3000.0
!KD-> HCNN+O=OH+CNN                2.000E+13     0.0    20000.0
!KD-> HCNN+O=CO+H+N2               5.000E+13     0.0    15000.0
!KD-> HCNN+O=HCN+NO                5.000E+13     0.0    15000.0
!KD-> HCNN+OH=H2O+CNN              1.000E+13     0.0     8000.0
!KD-> HCNN+OH=H+HCO+N2             1.000E+13     0.0    16000.0
!KD-> HCNN+O2=HO2+CNN              1.000E+12     0.0     4000.0
!KD-> HCNN+O2=>H+CO2+N2            4.000E+12     0.0        0.0
!KD-> HCNN+O2=HCO+N2O              4.000E+12     0.0        0.0
!KD-> CNN+O=CO+N2                  1.000E+13     0.0        0.0
!KD-> CNN+O=CN+NO                  1.000E+14     0.0    20000.0
!KD-> CNN+OH=H+CO+N2               1.000E+13     0.0     1000.0
!KD-> CNN+H=NH+CN                  5.000E+14     0.0    40000.0
!KD-> CNN+OH=HCN+NO                1.000E+12     0.0     1000.0
!KD-> CNN+H=HCN+N                  5.000E+13     0.0    25000.0
!KD-> CNN+O2=NO+NCO                1.000E+13     0.0     5000.0
HNO+CH3=NO+CH4                8.200E+05     1.87     954.0
!KD-> HONO+CH3=NO2+CH4             8.100E+05     1.87    5504.0
H2NO+CH3=CH3O+NH2             2.000E+13     0.0        0.0
H2NO+CH3=HNO+CH4              1.600E+06     1.87    2960.0
!KD-> HNOH+CH3=HNO+CH4             1.600E+06     1.87    2096.0
!KD-> NH2OH+CH3=HNOH+CH4           1.600E+06     1.87    6350.0
!KD-> NH2OH+CH3=H2NO+CH4           8.200E+05     1.87    5500.0
N2H2+CH3=NNH+CH4              1.600E+06     1.87    2970.0
N2H3+CH3=N2H2+CH4             8.200E+05     1.87    1818.0
N2H4+CH3=N2H3+CH4             3.300E+06     1.87    5325.0
CH4+NH=CH3+NH2                9.000E+13     0.0    20080.0
CH4+NH2=CH3+NH3               1.200E+13     0.0    15150.0
CH3+NH2=CH2+NH3               1.600E+06     1.87    7570.0
C2H6+NH=C2H5+NH2              7.000E+13     0.0    16700.0
C2H6+NH2=C2H5+NH3             9.700E+12     0.0    11470.0
!KD-> C3H8+NH2=NC3H7+NH3           1.700E+13     0.0    10660.0
!KD-> C3H8+NH2=IC3H7+NH3           4.500E+11     0.0     6150.0
!KD-> CH3+NO(+M)=CH3NO(+M)         1.000E+13     0.0        0.0
!KD->     LOW /1.90E+18 0.0 0.0/
!KD->     SRI /0.03 -790.0 1.0/
!KD-> CH3NO+H=H2CNO+H2             4.400E+08     1.5      377.0
!KD-> CH3NO+H=CH3+HNO              1.800E+13     0.0     2800.0
!KD-> CH3NO+O=H2CNO+OH             3.300E+08     1.5     3615.0
!KD-> CH3NO+O=CH3+NO2              1.700E+06     2.08       0.0
!KD-> CH3NO+OH=H2CNO+H2O           3.600E+06     2.0    -1192.0
!KD-> CH3NO+OH=CH3+HONO            2.500E+12     0.0     1000.0
!KD-> CH3NO+CH3=H2CNO+CH4          7.900E+05     1.87    5415.0
!KD-> CH3NO+NH2=H2CNO+NH3          2.800E+06     1.94    1073.0
!KD-> H2CNO=HNCO+H                 2.300E+42    -9.11   53840.0
!KD-> H2CNO+O2=CH2O+NO2            2.900E+12    -0.31   17700.0
!KD-> H2CNO+H=CH3+NO               4.000E+13     0.0        0.0
!KD-> H2CNO+H=HCNO+H2              4.800E+08     1.5     -894.0
```

```
!KD-> H2CNO+O=HCNO+OH          3.300E+08    1.5     -894.0
!KD-> H2CNO+O=CH2O+NO          7.000E+13    0.0       0.0
!KD-> H2CNO+OH=CH2OH+NO        4.000E+13    0.0       0.0
!KD-> H2CNO+OH=HCNO+H2O        2.400E+06    2.0    -1192.0
!KD-> H2CNO+CH3=C2H5+NO        3.000E+13    0.0       0.0
!KD-> H2CNO+CH3=HCNO+CH4       1.600E+06    1.87   -1113.0
!KD-> H2CNO+NH2=HCNO+NH3       1.800E+06    1.94   -1152.0
CH3+NO2=CH3O+NO          1.400E+13    0.0       0.0
CH+NO2=HCO+NO            1.200E+14    0.0       0.0
CH2+NO2=CH2O+NO          4.200E+13    0.0       0.0
!KD-> CN+NO=N2+CO              1.000E+11    0.0       0.0
!KD-> HNCO+M=H+NCO+M           5.000E+15    0.0   120000.0
!KD-> HNCO+N=NH+NCO            4.000E+13    0.0    36000.0
CH3O+HNO=CH3OH+NO        3.160E+13    0.0       0.0
!KD-> NCO+HO2=HNCO+O2          2.000E+13    0.0       0.0
N2O+CO=CO2+N2            2.510E+14    0.0    46000.0
N2O+CH2=CH2O+N2          1.000E+12    0.0       0.0
N2O+CH3=CH3O+N2          9.000E+09    0.0       0.0
N2O+HCO=CO2+H+N2         1.700E+14    0.0    20000.0
N2O+HCCO=CO+HCO+N2       1.700E+14    0.0    25500.0
N2O+C2H2=HCCO+H+N2       6.590E+16    0.0    61200.0
N2O+C2H3=CH2HCO+N2       1.000E+11    0.0       0.0
!KD-> HOCN+O=NCO+OH            1.500E+04    2.64    4000.0
!KD-> HOCN+H=NCO+H2            2.000E+07    2.0     2000.0
!KD-> HOCN+H=NH2+CO            1.200E+08    0.61    2080.0
!KD-> HOCN+OH=NCO+H2O          6.380E+05    2.0     2560.0
!KD-> HOCN+CH3=NCO+CH4         8.200E+05    1.87    6620.0
!KD-> HOCN+NH2=NCO+NH3         9.200E+05    1.94    3645.0
!KD-> CN+NO2=CO+N2O            4.930E+14   -0.752    344.0
!KD-> CN+NO2=CO2+N2            3.700E+14   -0.752    344.0
!KD-> CN+CO2=NCO+CO            3.670E+06    2.16   26900.0
!KD-> CN+NH3=HCN+NH2           9.200E+12    0.0     -357.0
!KD-> HNCO+CN=HCN+NCO          1.500E+13    0.0       0.0
!KD-> HONO+NCO=HNCO+NO2        3.600E+12    0.0       0.0
!KD-> NCO+CH2O=HNCO+HCO        6.000E+12    0.0       0.0
!CH+N2=HCN+N             3.680E+07    1.42   20723.0
!KD-> NH2+C=CH+NH              5.800E+11    0.67   20900.0
!KD-> C+N2=CN+N                5.200E+13    0.0    44700.0
!KD-> CH2+N2=HCN+NH            4.800E+12    0.0    35850.0
!KD-> C2+N2=CN+CN              1.500E+13    0.0    41700.0
!KD-> H2CN+N=N2+CH2            6.000E+13    0.0      400.0
!KD-> H2CN+H=HCN+H2            2.400E+08    1.5     -894.0
!KD-> H2CN+O=HCN+OH            1.700E+08    1.5     -894.0
!KD-> H2CN+O=HNCO+H            6.000E+13    0.0       0.0
!KD-> H2CN+O=HCNO+H            2.000E+13    0.0       0.0
!KD-> H2CN+M=HCN+H+M           3.000E+14    0.0    22000.0
!KD-> H2CN+HO2=HCN+H2O2        1.400E+04    2.69   -1610.0
!KD-> H2CN+O2=CH2O+NO          3.000E+12    0.0     6000.0
!KD-> H2CN+CH3=HCN+CH4         8.100E+05    1.87   -1113.0
!KD-> H2CN+OH=HCN+H2O          1.200E+06    2.0    -1192.0
!KD-> H2CN+NH2=HCN+NH3         9.200E+05    1.94   -1152.0
```

```
!KD-> C+NO=CN+O                2.000E+13     0.0        0.0
!KD-> CH+NO=HCN+O              8.690E+13     0.0        0.0
!KD-> CH+NO=CN+OH              1.680E+12     0.0        0.0
CH+NO=CO+NH              9.840E+12     0.0        0.0
!KD-> CH+NO=NCO+H              1.670E+13     0.0        0.0
!KD-> CH2+NO=HNCO+H            2.500E+12     0.0     5970.0
!KD-> CH2+NO=HCNO+H            3.800E+13    -0.36     576.0
CH2+NO=NH2+CO            2.300E+16    -1.43    1331.0
!KD-> CH2+NO=H2CN+O            8.100E+07     1.42    4110.0
!KD-> CH3+NO=HCN+H2O           2.400E+12     0.0    15700.0
!KD-> CH3+NO=H2CN+OH           5.200E+12     0.0    24240.0
!KD-> HCCO+NO=HCNO+CO          4.640E+13     0.0      700.0
!KD-> HCCO+NO=HCN+CO2          1.390E+13     0.0      700.0
!KD-> SCH2+NO=HCN+OH           1.000E+14     0.0        0.0
!KD-> HCNO=HCN+O               4.200E+31    -6.12   61210.0
!KD-> HCNO+H=HCN+OH            1.000E+14     0.0    12000.0
!KD-> HCNO+H=HNCO+H            2.100E+15    -0.69    2850.0
!KD-> HCNO+H=HOCN+H            1.400E+11    -0.19    2484.0
!KD-> HCNO+H=NH2+CO            1.700E+14    -0.75    2890.0
!KD-> HCNO+O=HCO+NO            7.000E+13     0.0        0.0
!KD-> CH2+N=HCN+H              5.000E+13     0.0        0.0
CH2+N=NH+CH              6.000E+11     0.67   40500.0
!KD-> CH+N=CN+H                1.670E+14    -0.09       0.0
!KD-> CH+N=C+NH                4.500E+11     0.65    2400.0
N+CO2=NO+CO              1.900E+11     0.0     3400.0
!KD-> N+HCCO=HCN+CO            5.000E+13     0.0        0.0
!KD-> CH3+N=H2CN+H             7.100E+13     0.0        0.0
!KD-> CH3+N=HCNH+H             1.200E+11     0.52     367.6
!KD-> HCNH=HCN+H               6.100E+28    -5.69   24270.0
!KD-> HCNH+H=H2CN+H            2.000E+13     0.0        0.0
!KD-> HCNH+H=HCN+H2            2.400E+08     1.5     -894.0
!KD-> HCNH+O=HNCO+H            7.000E+13     0.0        0.0
!KD-> HCNH+O=HCN+OH            1.700E+08     1.5     -894.0
!KD-> HCNH+OH=HCN+H2O          1.200E+06     2.0    -1192.0
!KD-> HCNH+CH3=HCN+CH4         8.200E+05     1.87   -1113.0
!KD-> C2H3+N=HCN+CH2           2.000E+13     0.0        0.0
!KD-> CN+H2O=HCN+OH            4.000E+12     0.0     7400.0
!KD-> CN+H2O=HOCN+H            4.000E+12     0.0     7400.0
!KD-> OH+HCN=HOCN+H            3.200E+04     2.45   12120.0
!KD-> OH+HCN=HNCO+H            5.600E-06     4.71    -490.0
!KD-> OH+HCN=NH2+CO            6.440E+10     0.0    11700.0
!KD-> HOCN+H=HNCO+H            1.000E+13     0.0        0.0
!KD-> HCN+O=NCO+H              1.380E+04     2.64    4980.0
!KD-> HCN+O=NH+CO              3.450E+03     2.64    4980.0
!KD-> HCN+O=CN+OH              2.700E+09     1.58   26600.0
!KD-> CN+H2=HCN+H              2.000E+04     2.87    1600.0
!KD-> CN+O=CO+N                1.900E+12     0.46     720.0
!KD-> CN+O2=NCO+O              7.200E+12     0.0     -400.0
!KD-> CN+OH=NCO+H              4.000E+13     0.0        0.0
!KD-> CN+HCN=C2N2+H            1.510E+07     1.71    1530.0
!KD-> CN+NO2=NCO+NO            5.320E+15    -0.752    344.0
```

```
!KD-> CN+N2O=NCO+N2               6.000E+12     0.0     15360.0
!KD-> C2N2+O=NCO+CN               4.570E+12     0.0      8880.0
!KD-> C2N2+OH=HNCO+CN             1.860E+11     0.0      2900.0
!KD-> C2N2+OH=HOCN+CN             2.000E+12     0.0     19000.0
!KD-> HNCO+H=H2+NCO               1.760E+05     2.41    12300.0
!KD-> HNCO+H=NH2+CO               3.600E+04     2.49     2340.0
!KD-> HNCO+M=NH+CO+M              1.100E+16     0.0     86000.0
!KD->   N2/1.5/ O2/1.5/ H2O/18.6/
!KD-> HNCO+O=NCO+OH               2.200E+06     2.11    11430.0
!KD-> HNCO+O=NH+CO2               9.800E+07     1.41     8530.0
!KD-> HNCO+O=HNO+CO               1.500E+08     1.57    44012.0
!KD-> HNCO+OH=NCO+H2O             3.450E+07     1.5      3600.0
!KD-> HNCO+OH=NH2+CO2             6.300E+10    -0.06    11645.0
!KD-> HNCO+HO2=NCO+H2O2           3.000E+11     0.0     29000.0
!KD-> HNCO+O2=HNO+CO2             1.000E+12     0.0     35000.0
!KD-> HNCO+NH2=NCO+NH3            5.000E+12     0.0      6200.0
!KD-> HNCO+NH=NCO+NH2             1.040E+15     0.0     39390.0
!KD-> NCO+H=NH+CO                 5.360E+13     0.0         0.0
!KD-> NCO+O=NO+CO                 4.200E+13     0.0         0.0
!KD-> NCO+O=N+CO2                 8.000E+12     0.0      2500.0
!KD-> NCO+N=N2+CO                 2.000E+13     0.0         0.0
!KD-> NCO+OH=NO+HCO               5.000E+12     0.0     15000.0
!KD-> NCO+M=N+CO+M                2.200E+14     0.0     54050.0
!KD-> NCO+NO=N2O+CO               4.600E+18    -2.01      934.0
!KD-> NCO+NO=N2+CO2               5.800E+18    -2.01      934.0
!KD-> NCO+O2=NO+CO2               2.000E+12     0.0     20000.0
!KD-> NCO+HCO=HNCO+CO             3.600E+13     0.0         0.0
!KD-> NCO+NO2=CO+NO+NO            2.830E+13    -0.646    -326.0
!KD-> NCO+NO2=CO2+N2O             3.570E+14    -0.646    -326.0
!KD-> NCO+HNO=HNCO+NO             1.800E+13     0.0         0.0
!KD-> NCO+NCO=CO+CO+N2            3.000E+12     0.0         0.0
NO+HCO=CO+HNO               7.240E+13    -0.4        0.0
NO2+CO=CO2+NO               9.000E+13     0.0     33800.0
NO2+HCO=H+CO2+NO            8.400E+15    -0.75     1930.0
!KD-> CH3O+NO2=HONO+CH2O          3.000E+12     0.0         0.0
CH3O+NO=CH2O+HNO            1.300E+14    -0.7        0.0
!KD-> NO2+CH2O=HONO+HCO           1.000E+10     0.0     15100.0
NO+CH2O=HNO+HCO             1.000E+13     0.0     40820.0
!KD-> NO2+HCO=HONO+CO             1.000E+13     0.0         0.0
NO2+HCO=OH+NO+CO            1.000E+14     0.0        0.0
!KD-> NCO+N=NO+CN                 2.700E+18    -0.995   17200.0
!KD-> CN+CH4=HCN+CH3              9.000E+04     2.64     -300.0
!KD-> C+NO=CO+N                   2.800E+13     0.0         0.0
NH+CO2=HNO+CO               1.000E+13     0.0     14350.0
!KD-> NCO+CH4=HNCO+CH3            1.000E+13     0.0      8130.0
!KD-> C+N2O=CN+NO                 4.800E+12     0.0         0.0
!KD-> CH+NH2=HCN+H+H              3.000E+13     0.0         0.0
!KD-> CH+NH=HCN+H                 5.000E+13     0.0         0.0
!KD-> CH2+NH=HCN+H+H              3.000E+13     0.0         0.0
!KD-> CH3+N=HCN+H+H               2.000E+11     0.0         0.0
!KD-> CH3+N=HCN+H2                7.100E+12     0.0         0.0
```

```
CH4+N=NH+CH3                    1.000E+13      0.0     24000.0
!KD-> C3H3+N=HCN+C2H2               1.000E+13      0.0         0.0
!KD-> CH+N2O=HCN+NO                 1.340E+13      0.0      -510.0
CH+N2O=CO+H+N2                  5.200E+12      0.0      -510.0
!KD-> C2O+N2=>NCO+CN                7.000E+11      0.0     17000.0
END
```

Mech.5

```
ELEM H C O N AR
END
SPECIES
!KD->  C2H6 C2H5 CH2 CH2OH CH
!KD->  C2H2 C2H4 C2H3 CH3HCO C2H
!KD->  CH2CO HCCO C2H4O C2 C2O
!KD->  CH3CO C CH3CO3 CH3CO3H CH3O2
!KD->  CH3O2H C2H5O2H C2H5O2 CH3CO2 CH3CO2H
!KD->  C2H5OH C2H5O SC2H5O PC2H5O CH2HCO
!KD->  CN H2CN HCN HCNO HOCN
!KD->  HNCO NCO N2O N2O3 C2N2
!KD->  HONO NO3 HNO3 CNN HCNN
!KD->  N2O4 NH2OH HNOH HNNO HCNH
!KD->  NCN HNCN H2CNO CH3NO CH2CHOW
!KD->  C2H3O CH3HCOW C3H6OH O2C3H6OH C3H5O2
!KD->  C3H5O2H C3H5O NC3H7O2 NC3H7O2H IC3H7O2
!KD->  IC3H7O2H IC3H7O NC3H7O C3H6 C3H8
!KD->  IC3H7 NC3H7 C3H2 C3H3 SC3H5
!KD->  PC3H4 TC3H5 C3H6O C2H5CHO C2H5CO
!KD->  C3H5 C3H4 IC4H7 C4H2 C4H
!KD->  C4H6 H2C4O C4H4 IC4H5 NC4H5
!KD->  C4H8 T2C4H8 C2C4H8 IC4H3 NC4H3
!KD->  C6H6 C6H5O C6H5 AR
H H2 O O2 OH
HO2 H2O H2O2 CO CO2
HCO CH3 CH4 CH2O CH3O
CH3OH SCH2 N NH NO
NH2 HNO NO2 NNH NH3
N2H2 N2H3 N2H4 H2NO N2
END
```

REACTIONS, A_i ((cm^3/mol)$^{(r-1)}$/s), β_i, E_i (cal/mol)

```
! CH + N2 = HCN + N       3.68E+05 1.42 20723
!KD-> CH+N2=NCN+H                  3.00E+12       0.0     22157.
!KD-> CN+N2O=NCN+NO                6.000E+13       0.0     15360.0
!KD->      DUPLICATE
!KD-> CN+N2O=NCN+NO                1.800E+10       0.0      1450.0
!KD->      DUPLICATE
!KD-> CN + NCO = NCN + CO          1.800E+13       0           0
!KD-> C2O + N2 = NCN + CO          7.00E+11       0       17000
```

```
!KD-> CH + N2 = HNCN              1.65E+21     -3.62    14196
!KD-> HNCN + M = H + NCN + M        1.79E+28     -3.44    64502
!KD-> HNCN + O = NO + HCN          1.22E+14      0.05      73.5
!KD-> HNCN + O = NH + NCO          5.60E+13      0.05      73.5
!KD-> HNCN + O = CN + HNO          9.36E+12      0.05      73.5
!KD-> HNCN + OH = NCN + H2O         8.28E+03      2.78     3135
!KD-> HNCN + O2 = HO2 + NCN         1.26E+08      1.28    24240
!KD-> NCN = N + CN               2.95E+30     -5.29   117090
!KD-> NCN = C + N2               2.66E+28     -5.32    83110
!KD-> NCN = CNN                 3.69E+29     -5.84    78410
!KD-> NCN + H = HCN +N            1.89E+14      0       8425
!KD-> NCN + O = CN + NO           2.54E+13      0.15      -34
!KD-> NCN + O = CO + N2           2.42E+02      2.32    -1135
!KD-> NCN + O = N + NCO           2.20E+09      0.42     -157
!KD-> NCN + N= N2 + CN            1.00E+13      0         0
!KD-> NCN + C = CN +CN            1.00E+13      0         0
!KD-> NCN + OH = HCN + NO          3.32E+10     -0.97     7290.
!KD->    DUPLICATE
!KD-> NCN + OH = HCN + NO          4.69E+10      0.44     4000.
!KD-> DUPLICATE
!KD-> NCN + O2 = NO + NCO          3.80E+09      0.51    24590
!KD-> NCN + CH = HCN +CN           3.21E+13      0       -860
!KD-> NCN + CN = C2N2 +N           1.25E+14      0       8020
!KD-> NCN + CH2 = H2CN + CN         7.99E+13      0       4630
H+H+M=H2+M                  7.000E+17    -1.0        0.0
H2/0.0/ N2/0.0/ H/0.0/ H2O/14.3/ CO/3.0/ CO2/3.0/
H+H+H2=H2+H2                1.000E+17    -0.6        0.0
H+H+N2=H2+N2                5.400E+18    -1.3        0.0
H+H+H=H2+H                 3.200E+15     0.0        0.0
O+O+M=O2+M                  1.000E+17    -1.0        0.0
O/71.0/ O2/20.0/ NO/5.0/ N2/5.0/ N/5.0/ H2O/5.0/
O+H+M=OH+M                  6.200E+16    -0.6        0.0
H2O/5.0/
H2+O2=OH+OH                 2.500E+12     0.0    39000.0
O+H2=OH+H                  5.060E+04     2.67    6290.0
H+O2=OH+O                  9.750E+13     0.0    14850.0
H+O2(+M)=HO2(+M)            1.480E+12     0.6        0.0
LOW /3.50E+16 -0.41 -1116.0/
TROE /0.5 100000 10/
!KD->  AR/0.0/ H2O/10.6/ H2/1.5/ CO2/2.4/
H2O/10.6/ H2/1.5/ CO2/2.4/
!KD-> H+O2(+AR)=HO2(+AR)          1.480E+12     0.6        0.0
!KD->    LOW /7.00E+17 -0.8  0.0/
!KD->    TROE /0.45 10 100000/
H+OH+M=H2O+M                2.200E+22    -2.0        0.0
!KD->  H2O/6.4/ AR/0.38/ CO2/1.9/
H2O/6.4/        CO2/1.9/
H2+OH=H2O+H                 1.000E+08     1.6     3300.0
OH+OH=H2O+O                 1.500E+09     1.14     100.0
HO2+OH=H2O+O2                2.890E+13     0.0     -500.0
HO2+O=OH+O2                 1.630E+13     0.0     -445.0
```

```
H+HO2=H2+O2                  4.280E+13     0.0     1411.0
H+HO2=OH+OH                   1.700E+14     0.0      875.0
H+HO2=H2O+O                   3.000E+13     0.0     1720.0
HO2+HO2=H2O2+O2               4.200E+14     0.0    12000.0
DUPLICATE
HO2+HO2=H2O2+O2               1.300E+11     0.0    -1640.0
DUPLICATE
OH+OH(+M)=H2O2(+M)            7.200E+13    -0.37       0.0
LOW /2.2E+19 -0.76 0.0/
TROE /0.5 100000 10/
H2O/0.0/
OH+OH(+H2O)=H2O2(+H2O)        7.200E+13    -0.37       0.0
LOW /1.45E+18 0.0 0.0/
H2O2+OH=HO2+H2O               1.000E+12     0.0        0.0
DUPLICATE
H2O2+OH=HO2+H2O               5.800E+14     0.0     9560.0
DUPLICATE
H2O2+H=HO2+H2                 1.700E+12     0.0     3755.0
H2O2+H=H2O+OH                 1.000E+13     0.0     3575.0
H2O2+O=HO2+OH                 2.800E+13     0.0     6400.0
N2+O=NO+N                    1.800E+14     0.0    76100.0
N+O2=NO+O                    9.000E+09     1.0     6500.0
NO+M=N+O+M                    9.640E+14     0.0   148300.0
N2 /1.5/ NO /3.0/ CO2/2.5/
NO+NO=N2+O2                  3.000E+11     0.0    65000.0
!KD-> N2O(+M)=N2+O(+M)             1.260E+12     0.0    62620.0
!KD->    LOW / 4.000E+14 0.0 56640.0/
!KD->    O2/1.4/ N2/1.7/ H2O/12.0/ NO/3.0/ N2O/3.5/
!KD-> N2O+O=N2+O2                 1.000E+14     0.0    28200.0
!KD-> N2O+O=NO+NO                  6.920E+13     0.0    26630.0
!KD-> N2O+N=N2+NO                 1.000E+13     0.0    20000.0
!KD-> N2O+NO=N2+NO2                2.750E+14     0.0    50000.0
NO+O(+M)=NO2(+M)              1.300E+15    -0.75       0.0
LOW /4.72E+24 -2.87 1551.0/
TROE /0.962 10.0 7962.0 /
!KD->    AR /0.6/ NO2 /6.2/ NO /1.8/ O2 /0.8/ N2O /4.4/ CO2/0/
NO2 /6.2/ NO /1.8/ O2 /0.8/ CO2/0/
H2O /10.0/
NO+O(+CO2)=NO2(+CO2)          1.300E+15    -0.75       0.0
LOW /4.0E+22 -2.16 1051.0/
TROE /0.962 10.0 7962.0 /
NO2+O=NO+O2                  3.910E+12     0.0     -238.0
!KD-> NO2+N=N2O+O                 8.400E+11     0.0        0.0
NO2+N=NO+NO                   1.000E+12     0.0        0.0
!KD-> NO2+NO=N2O+O2                1.000E+12     0.0    60000.0
NO2+NO2=NO+NO+O2              3.950E+12     0.0    27590.0
!KD-> NO2+NO2=NO3+NO               1.130E+04     2.58   22720.0
!KD-> NO2+O(+M)=NO3(+M)            1.330E+13     0.0        0.0
!KD->    LOW / 1.49E+28 -4.08 2467.0 /
!KD->    TROE /0.86 10.0 2800.0 /
!KD->    H2O/10.0/ O2/0.8/ H2/2.0/ CO2 /0/
```

```
!KD-> NO2+O(+CO2)=NO3(+CO2)         1.330E+13     0.0        0.0
!KD->     LOW / 1.34E+28 -3.94 2277.0 /
!KD->     TROE /0.86 10.0 2800.0 /
!KD-> NO3=NO+O2                    2.500E+06     0.0     12120.0
!KD-> NO3+NO2=NO+NO2+O2            1.200E+11     0.0     3200.0
!KD-> NO3+O=NO2+O2                 1.020E+13     0.0        0.0
!KD-> NO3+NO3=NO2+NO2+O2           5.120E+11     0.0     4870.0
!KD-> N2O4(+M)=NO2+NO2(+M)         4.050E+18     -1.1    12840.0
!KD->      LOW /1.96E+28  -3.8  12840./
!KD->      AR/0.8/ N2O4/2.0/ NO2/2.0/
!KD-> N2O4+O=N2O3+O2               1.210E+12     0.0        0.0
!KD-> NO2+NO(+M)=N2O3(+M)          1.600E+09     1.4        0.0
!KD->      LOW /1.0E+33  -7.7  0.0/
!KD->      N2/1.36/
!KD-> N2O3+O=NO2+NO2               2.710E+11     0.0        0.0
N2+M=N+N+M                 1.000E+28    -3.33   225000.0
N/5/ O/2.2/
NH+M=N+H+M                 2.650E+14     0.0    75500.0
NH+H=N+H2                 3.200E+13     0.0      325.0
NH+N=N2+H                 9.000E+11     0.5        0.0
NH+NH=NNH+H                5.100E+13     0.0        0.0
NH+NH=NH2+N                5.950E+02     2.89    -2030.0
NH+NH=N2+H2                1.000E+08     1.0        0.0
NH2+M=NH+H+M                3.160E+23     -2.0    91400.0
NH+H2=NH2+H                1.000E+14     0.0    20070.0
NH2+N=N2+H+H               6.900E+13     0.0        0.0
NH2+NH=N2H2+H               1.500E+15     -0.5        0.0
NH2+NH=NH3+N               1.000E+13     0.0      2000.0
NH3+NH=NH2+NH2              3.160E+14     0.0    26770.0
NH2+NH2=N2H2+H2             1.000E+13     0.0     1500.0
N2H3+H=NH2+NH2              5.000E+13     0.0     2000.0
NH3+M=NH2+H+M               2.200E+16     0.0    93470.0
NH3+M=NH+H2+M               6.300E+14     0.0    93390.0
NH3+H=NH2+H2               5.420E+05     2.4      9920.0
NH3+NH2=N2H3+H2             1.000E+11     0.5    21600.0
NNH=N2+H                  3.000E+08     0.0        0.0
!    DUPLICATE
NNH+M=N2+H+M                1.000E+13     0.5     3060.0
!    DUPLICATE
NNH+H=N2+H2                1.000E+14     0.0        0.0
NNH+N=NH+N2                3.000E+13     0.0     2000.0
NNH+NH=N2+NH2               2.000E+11     0.5     2000.0
NNH+NH2=N2+NH3              1.000E+13     0.0        0.0
NNH+NNH=N2H2+N2             1.000E+13     0.0     4000.0
N2H2+M=NNH+H+M              5.000E+16     0.0    50000.0
H2O/15.0/ O2/2.0/ N2/2.0/ H2/2.0/
N2H2+M=NH+NH+M              3.160E+16     0.0    99400.0
H2O/15.0/ O2/2.0/ N2/2.0/ H2/2.0/
N2H2+H=NNH+H2              8.500E+04     2.63    -230.0
N2H2+N=NNH+NH              1.000E+06     2.0        0.0
N2H2+NH=NNH+NH2             1.000E+13     0.0     6000.0
```

```
N2H2+NH2=NH3+NNH          8.800E-02   4.05   -1610.0
N2H3+NH=N2H2+NH2          2.000E+13   0.0       0.0
N2H3+NNH=N2H2+N2H2        1.000E+13   0.0    4000.0
N2H3+M=NH2+NH+M           5.000E+16   0.0   60000.0
N2H3+M=N2H2+H+M           1.000E+16   0.0   37000.0
N2H3+H=N2H2+H2            1.000E+13   0.0       0.0
N2H3+H=NH+NH3             1.000E+11   0.0       0.0
N2H3+N=N2H2+NH            1.000E+06   2.0       0.0
N2H3+NH2=NH3+N2H2         1.000E+11   0.5       0.0
N2H3+N2H2=N2H4+NNH        1.000E+13   0.0    6000.0
N2H3+N2H3=NH3+NH3+N2      3.000E+12   0.0       0.0
N2H3+N2H3=N2H4+N2H2       1.200E+13   0.0       0.0
N2H4(+M)=NH2+NH2(+M)      5.000E+14   0.0   60000.0
LOW/1.50E+15 0.0 39000.0 /
N2/2.4/ NH3/3.0/ N2H4/4.0/
N2H4+M=N2H3+H+M           1.000E+15   0.0   63600.0
N2/2.4/ NH3/3.0/ N2H4/4.0/
N2H4+H=N2H3+H2            7.000E+12   0.0    2500.0
N2H4+H=NH2+NH3            2.400E+09   0.0    3100.0
N2H4+N=N2H3+NH            1.000E+10   1.0    2000.0
N2H4+NH=NH2+N2H3          1.000E+09   1.5    2000.0
N2H4+NH2=N2H3+NH3         1.800E+06   1.71   -1380.0
N+OH=NO+H                 2.800E+13   0.0       0.0
!KD-> N2O+H=N2+OH              2.200E+14   0.0   16750.0
!KD-> N2O+H=NH+NO              6.700E+22   -2.16   37155.0
!KD-> N2O+H=NNH+O              5.500E+18   -1.06   47290.0
!KD-> N2O+H=HNNO               8.000E+24   -4.39   10530.0
!KD-> N2O+OH=N2+HO2            1.000E+14   0.0   30000.0
!KD-> HNO+NO=N2O+OH            8.500E+12   0.0   29580.0
!KD-> HNO+NO+NO=HNNO+NO2       1.600E+11   0.0    2090.0
!KD-> NH+NO+M=HNNO+M           1.630E+23   -2.6    1820.0
!KD-> HNNO+H=N2O+H2            2.000E+13   0.0       0.0
!KD-> HNNO+H=NH2+NO            1.000E+12   0.0       0.0
!KD-> HNNO+O=N2O+OH            2.000E+13   0.0       0.0
!KD-> HNNO+OH=H2O+N2O          2.000E+13   0.0       0.0
!KD-> HNNO+OH=HNOH+NO          1.000E+12   0.0       0.0
!KD-> HNNO+NO=N2+HONO          2.600E+11   0.0    1610.0
!KD-> HNNO+NO=NNH+NO2          3.200E+12   0.0     540.0
!KD-> HNNO+NO=N2O+HNO          1.000E+12   0.0       0.0
!KD-> HNNO+NO2=N2O+HONO        1.000E+12   0.0       0.0
!KD-> HNNO+NO2=NNH+NO3         1.000E+13   0.0   17000.0
NO2+H=NO+OH               1.320E+14   0.0     362.0
NO2+OH=HO2+NO             1.810E+13   0.0    6676.0
!KD-> NO2+HO2=HONO+O2          4.640E+11   0.0    -479.0
!KD-> NO2+H2=HONO+H            7.330E+11   0.0   28800.0
!KD-> NO2+NH=N2O+OH            8.650E+10   0.0   -2270.0
NO2+NH=NO+HNO             1.245E+11   0.0   -2270.0
!KD-> NO3+H=NO2+OH             6.620E+13   0.0       0.0
!KD-> NO3+OH=NO2+HO2           1.210E+13   0.0       0.0
!KD-> NO3+HO2=HNO3+O2          5.550E+11   0.0       0.0
!KD-> NO3+HO2=NO2+OH+O2        1.510E+12   0.0       0.0
```

```
!KD-> N2O4+H2O=HONO+HNO3          2.520E+14    0.0    11590.0
!KD-> N2O3+H2O=HONO+HONO          3.790E+13    0.0     8880.0
H+NO(+M)=HNO(+M)            1.520E+15    -0.41      0.0
LOW /4.00E+20 -1.75 0.0 /
!KD->    H2O/10.0/ O2/1.5/ AR/0.75/ H2/2.0/ CO2/3.0/
H2O/10.0/ O2/1.5/        H2/2.0/ CO2/3.0/
HNO+H=NO+H2                 4.460E+11    0.72    655.0
HNO+OH=NO+H2O               1.300E+07    1.88    -956.0
HNO+O=OH+NO                 5.000E+11    0.5    2000.0
HNO+O=NO2+H                 5.000E+10    0.0    2000.0
HNO+O2=NO+HO2               2.200E+10    0.0    9140.0
HNO+N=NO+NH                 1.000E+11    0.5    2000.0
!KD-> HNO+N=H+N2O                 5.000E+10    0.5    3000.0
HNO+NH=NH2+NO               5.000E+11    0.5      0.0
HNO+NH2=NH3+NO              2.000E+13    0.0    1000.0
!KD-> HNO+HNO=N2O+H2O             3.630E-03    3.98    1190.0
!KD-> HNO+HNO=HNOH+NO             2.000E+08    0.0    4170.0
!KD-> HNO+NO2=HONO+NO             6.020E+11    0.0    2000.0
!KD-> NO+OH(+M)=HONO(+M)          2.000E+12    -0.05    -721.0
!KD->    LOW / 5.08E+23 -2.51 -67.6 /
!KD->    TROE /0.62 10.0 100000.0 /
!KD->    H2O/10.0/ O2/2.0/ AR/0.75/ H2/2.0/ CO2/0.0/
!KD-> NO+OH(+CO2)=HONO(+CO2)       2.000E+12    -0.05    -721.0
!KD->    LOW / 1.70E+23 -2.3 -246.0 /
!KD->    TROE /0.62 10.0 100000.0 /
!KD-> NO2+H+M=HONO+M              1.400E+18    -1.5     900.0
!KD-> HONO+H=HNO+OH               5.640E+10    0.86    4970.0
!KD-> HONO+H=NO+H2O               8.120E+06    1.89    3840.0
!KD-> HONO+O=OH+NO2               1.200E+13    0.0    5960.0
!KD-> HONO+OH=H2O+NO2             1.690E+12    0.0    -517.0
!KD-> HONO+NH=NH2+NO2             1.000E+13    0.0      0.0
!KD-> HONO+HONO=H2O+NO2+NO         1.000E+13    0.0    8540.0
!KD-> HONO+NH2=NO2+NH3            5.000E+12    0.0      0.0
!KD-> NO2+OH(+M)=HNO3(+M)          2.410E+13    0.0      0.0
!KD->    LOW / 6.42E+32 -5.49 2350.0 /
!KD->    TROE /1.0 10.0 1168.0 /
!KD->    H2O/10.0/ O2/2.0/ AR/0.75/ H2/2.0/ CO2/0.0/
!KD-> NO2+OH(+CO2)=HNO3(+CO2)      2.410E+13    0.0      0.0
!KD->    LOW / 5.80E+32 -5.4 2186.0 /
!KD->    TROE /1.0 10.0 1168.0 /
!KD-> NO+HO2+M=HNO3+M             1.500E+24    -3.5    2200.0
!KD-> HNO3+H=H2+NO3               5.560E+08    1.53   16400.0
!KD-> HNO3+H=H2O+NO2              6.080E+01    3.29    6290.0
!KD-> HNO3+H=OH+HONO              3.820E+05    2.3    6980.0
!KD-> HNO3+OH=NO3+H2O             1.030E+10    0.0    -1240.0
NH3+O=NH2+OH                1.100E+06    2.1    5210.0
NH3+OH=NH2+H2O              5.000E+07    1.6     950.0
NH3+HO2=NH2+H2O2            3.000E+11    0.0    22000.0
NH2+HO2=NH3+O2              1.650E+04    1.55    2027.0
NH2+O=H2+NO                 5.000E+12    0.0      0.0
NH2+O=HNO+H                 4.500E+13    0.0      0.0
```

```
NH2+O=NH+OH                  7.000E+12     0.0       0.0
NH2+OH=NH+H2O                 9.000E+07     1.5     -460.0
!KD-> NH2+OH=NH2OH              1.790E+13     0.2       0.0
NH2+HO2=HNO+H2O              5.680E+15    -1.12     707.0
NH2+HO2=H2NO+OH              2.910E+17    -1.32    1248.0
NH2+O2=HNO+OH               1.000E+13     0.0    26290.0
NH2+O2=H2NO+O               6.000E+13     0.0    29880.0
NH2+NO=NNH+OH               2.290E+10     0.425   -814.0
NH2+NO=N2+H2O               2.770E+20    -2.65    1258.0
!KD-> NH2+NO=H2+N2O              1.000E+13     0.0    33700.0
!KD-> NH2+NO2=N2O+H2O             1.620E+16    -1.44     270.0
NH2+NO2=H2NO+NO              6.480E+16    -1.44     270.0
NH+O=NO+H                   7.000E+13     0.0       0.0
NH+O=N+OH                   7.000E+12     0.0       0.0
NH+OH=HNO+H                  2.000E+13     0.0       0.0
NH+OH=N+H2O                  2.000E+09     1.2       0.0
NH+OH=NO+H2                  2.000E+13     0.0       0.0
NH+HO2=HNO+OH                 1.000E+13     0.0     2000.0
NH+O2=HNO+O                  4.000E+13     0.0    17880.0
NH+O2=NO+OH                  4.500E+08     0.79    1190.0
NH+H2O=HNO+H2                 2.000E+13     0.0    13850.0
!KD-> NH+N2O=N2+HNO              2.000E+12     0.0     6000.0
NNH+O=NH+NO                  2.000E+14     0.0     4000.0
NH+NO=N2+OH                  6.100E+13    -0.50     120.0
N2H4+O=N2H2+H2O               8.500E+13     0.0     1200.0
N2H4+O=N2H3+OH               2.500E+12     0.0     1200.0
N2H4+OH=N2H3+H2O              3.000E+10     0.68    1290.0
N2H4+OH=NH3+H2NO              3.670E+13     0.0       0.0
N2H4+HO2=N2H3+H2O2             4.000E+13     0.0     2000.0
N2H3+O=N2H2+OH               2.000E+13     0.0     1000.0
N2H3+O=NNH+H2O               3.160E+11     0.5       0.0
N2H3+O=NH2+HNO               1.000E+13     0.0       0.0
N2H3+OH=N2H2+H2O              3.000E+10     0.68    1290.0
N2H3+OH=NH3+HNO              1.000E+12     0.0    15000.0
N2H3+O2=N2H2+HO2             3.000E+12     0.0       0.0
N2H3+HO2=N2H2+H2O2             1.000E+13     0.0     2000.0
N2H3+HO2=N2H4+O2             8.000E+12     0.0       0.0
N2H3+NO=HNO+N2H2              1.000E+12     0.0       0.0
N2H2+O=NH2+NO               1.000E+13     0.0       0.0
N2H2+O=NNH+OH               2.000E+13     0.0     1000.0
N2H2+OH=NNH+H2O              5.920E+01     3.4    -1360.0
N2H2+HO2=NNH+H2O2             1.000E+13     0.0     2000.0
!KD-> N2H2+NO=N2O+NH2             3.000E+10     0.0       0.0
NNH+O=N2+OH                 1.700E+16    -1.23     500.0
NNH+OH=N2+H2O                2.400E+22    -2.88    2444.0
NNH+O2=N2+HO2                1.200E+12    -0.34     150.0
!KD-> NNH+O2=N2O+OH              2.900E+11    -0.34     150.0
NNH+HO2=N2+H2O2               1.000E+13     0.0     2000.0
NNH+NO=N2+HNO                5.000E+13     0.0       0.0
!KD-> NH2OH+OH=HNOH+H2O            2.500E+13     0.0     4250.0
H2NO+M=H2+NO+M               7.830E+27    -4.29   60300.0
```

```
H2O/10.0/
H2NO+M=HNO+H+M                2.800E+24     -2.83    64915.0
H2O/10.0/
!KD-> H2NO+M=HNOH+M               1.100E+29     -3.99    43980.0
!KD->   H2O/10.0/
H2NO+H=HNO+H2               3.000E+07      2.0      2000.0
H2NO+H=NH2+OH               5.000E+13      0.0        0.0
H2NO+O=HNO+OH               3.000E+07      2.0      2000.0
H2NO+OH=HNO+H2O               2.000E+07      2.0      1000.0
H2NO+HO2=HNO+H2O2             2.900E+04      2.69    -1600.0
H2NO+NH2=HNO+NH3              3.000E+12      0.0      1000.0
H2NO+O2=HNO+HO2              3.000E+12      0.0     25000.0
H2NO+NO=HNO+HNO              2.000E+07      2.0     13000.0
!KD-> H2NO+NO2=HONO+HNO            6.000E+11      0.0      2000.0
!KD-> HNOH+M=HNO+H+M              2.000E+24     -2.84    58935.0
!KD->    H2O/10.0/
!KD-> HNOH+H=HNO+H2               4.800E+08      1.5       380.0
!KD-> HNOH+H=NH2+OH               4.000E+13      0.0        0.0
!KD-> HNOH+O=HNO+OH               7.000E+13      0.0        0.0
!KD->     DUPLICATE
!KD-> HNOH+O=HNO+OH               3.300E+08      1.5      -360.0
!KD->     DUPLICATE
!KD-> HNOH+OH=HNO+H2O              2.400E+06      2.0     -1190.0
!KD-> HNOH+HO2=HNO+H2O2            2.900E+04      2.69    -1600.0
!KD-> HNOH+NH2=HNO+NH3             1.800E+06      1.94    -1150.0
!KD-> HNOH+NO2=HONO+HNO            6.000E+11      0.0      2000.0
!KD-> HNOH+O2=HNO+HO2              3.000E+12      0.0     25000.0
!KD-> HNOH+HNO=NH2OH+NO            1.000E+12      0.0      3000.0
!END
CO+HO2=CO2+OH               1.500E+14      0.0     23650.0
CO+OH=CO2+H                1.170E+07      1.354    -725.0
CO+O+M=CO2+M               6.160E+14      0.0      3000.0
!KD->  H2/2.5/ H2O/6.2/ CO/1.875/ CO2/3.75/ AR/0.88/
H2/2.5/ H2O/6.2/ CO/1.875/ CO2/3.75/
CH4/3.2/ CH3OH/7.5/
CO+O2=CO2+O                2.500E+12      0.0     47800.0
HCO+M=H+CO+M               1.560E+14      0.0     15760.0
!KD->  H2/2.5/ H2O/6.2/ CO/1.875/ CO2/3.75/ AR/1.0/
H2/2.5/ H2O/6.2/ CO/1.875/ CO2/3.75/
CH4/3.2/ CH3OH/7.5/
HCO+OH=CO+H2O               1.000E+14      0.0        0.0
HCO+O=CO+OH                3.000E+13      0.0        0.0
HCO+O=CO2+H                3.000E+13      0.0        0.0
HCO+H=CO+H2                9.000E+13      0.0        0.0
HCO+O2=CO+HO2               2.700E+13      0.0      1190.0
HCO+CH3=CO+CH4              1.200E+14      0.0        0.0
HCO+HO2=CO2+OH+H             3.000E+13      0.0        0.0
HCO+HCO=CH2O+CO             3.000E+13      0.0        0.0
HCO+HCO=H2+CO+CO             2.200E+13      0.0        0.0
CH4(+M)=CH3+H(+M)           2.400E+16      0.0    104913.0
LOW /4.5E+17 0.0 90800/
```

```
TROE /1.0 10.0 1350.0 7830.0/
CH4/0.0/ H2/2.0/ CO/2.0/ CO2/3.0/ H2O/5.0/
CH4(+CH4)=CH3+H(+CH4)         2.400E+16      0.0    104913.0
LOW /8.4E+18 0.0 90800/
TROE /0.31 2210.0 90/
CH4+HO2=CH3+H2O2              9.000E+12      0.0     24641.0
CH4+OH=CH3+H2O                1.548E+07      1.83     2774.0
CH4+O=CH3+OH                  7.200E+08      1.56     8485.0
CH4+H=CH3+H2                  1.300E+04      3.0      8050.0
!KD-> CH4+CH2=CH3+CH3              4.300E+12      0.0     10038.0
CH4+O2=CH3+HO2                4.000E+13      0.0     56900.0
!KD-> CH3+M=CH2+H+M                2.720E+36     -5.31   117100.0
!KD->  H2/2.5/ H2O/6.2/ CO/1.875/ CO2/3.75/ AR/1.0/
!KD->  CH4/3.2/ CH3OH/7.5/
!KD-> CH3+M=CH+H2+M                1.000E+16      0.0     85240.0
!KD->  H2/2.5/ H2O/6.2/ CO/1.875/ CO2/3.75/ AR/0.88/
!KD->  CH4/3.2/ CH3OH/7.5/
CH3+HO2=CH3O+OH               1.800E+13      0.0        0.0
!KD-> CH3+OH=CH2OH+H               2.640E+19     -1.8      8068.0
CH3+OH=CH3O+H                 5.740E+12     -0.23    13931.0
!KD-> CH3+OH=CH2+H2O               8.900E+18     -1.8      8067.0
CH3+OH=CH2O+H2                3.190E+12     -0.53    10810.0
CH3+O=H+CH2O                  8.430E+13      0.0        0.0
CH3+O2=CH2O+OH                3.400E+11      0.0      8940.0
CH3+O2=CH3O+O                 1.320E+14      0.0     31400.0
!KD-> CH3+CH3=C2H5+H               5.000E+12      0.099   10600.0
!KD-> CH3+CH3(+M)=C2H6(+M)         9.210E+16     -1.174     636.0
!KD->    LOW /1.13E+36 -5.246 1705/
!KD->    TROE /0.405 1120.0 69.6/
!KD->    H2/2.0/ CO/2.0/ CO2/3.0/ H2O/5.0/
CH3+CH3O=CH4+CH2O             2.409E+13      0.0        0.0
!KD-> CH3+CH2OH=CH4+CH2O           8.500E+13      0.0        0.0
CH3+H=SCH2+H2                 6.000E+13      0.0     15100.0
!KD-> CH3+O2(+M)=CH3O2(+M)         7.800E+08      1.2        0.0
!KD->    LOW/5.8E+25 -3.30 0.0/
!KD->    TROE /0.495 2325.5 10/
!KD-> CH3+CH3=C2H4+H2              1.000E+14      0.0     32000.0
CH3+OH=SCH2+H2O               7.200E+13      0.0      2780.0
!KD-> CH2+OH=CH2O+H                2.500E+13      0.0        0.0
!KD-> CH2+O=CO+H2                  4.800E+13      0.0        0.0
!KD-> CH2+O=CO+H+H                 7.200E+13      0.0        0.0
!KD-> CH2+O=CH+OH                  3.000E+14      0.0     11920.0
!KD-> CH2+O=HCO+H                  3.000E+13      0.0        0.0
!KD-> CH2+H=CH+H2                  3.120E+13      0.0     -1340.0
!KD-> CH2+O2=HCO+OH                4.300E+10      0.0      -500.0
!KD-> CH2+O2=CO2+H2                6.900E+11      0.0       500.0
!KD-> CH2+O2=CO2+H+H               1.600E+12      0.0      1000.0
!KD-> CH2+O2=CO+H2O                1.900E+10      0.0     -1000.0
!KD-> CH2+O2=CO+OH+H               8.600E+10      0.0      -500.0
!KD-> CH2+O2=CH2O+O                5.000E+13      0.0      9000.0
!KD-> CH2+CO2=CH2O+CO              1.100E+11      0.0      1000.0
```

```
!KD-> CH2+CH2=C2H2+H2            1.580E+15     0.0     11950.0
!KD-> CH2+CH2=C2H2+H+H           2.000E+14     0.0     11000.0
!KD-> CH2+CH2=CH3+CH             2.400E+14     0.0      9940.0
!KD-> CH2+CH2=C2H3+H             2.000E+13     0.0         0.0
!KD-> CH2+CH3=C2H4+H             4.200E+13     0.0         0.0
!KD-> CH2+CH=C2H2+H              4.000E+13     0.0         0.0
!KD-> CH2+C=CH+CH                1.620E+12     0.67    46800.0
!KD-> CH2+M=C+H2+M               1.600E+14     0.0     64000.0
!KD-> CH2+M=CH+H+M               5.600E+15     0.0     89600.0
!KD-> SCH2+M=CH2+M               6.000E+12     0.0         0.0
!KD->  H2/2.5/ H2O/5.0/ CO/1.875/ CO2/3.75/ AR/0.6/ CH4/1.2/
!KD->  C2H2/8.0/ C2H4/4.0/ C2H6/3.6/ H/33.3/
SCH2+O2=CO+OH+H              3.000E+13     0.0         0.0
!KD-> SCH2+H=CH+H2               3.000E+13     0.0         0.0
SCH2+O=CO+H+H                1.500E+13     0.0         0.0
SCH2+O=CO+H2                 1.500E+13     0.0         0.0
SCH2+OH=CH2O+H               3.000E+13     0.0         0.0
SCH2+HO2=CH2O+OH             3.000E+13     0.0         0.0
SCH2+H2O2=CH3O+OH            3.000E+13     0.0         0.0
SCH2+H2O=>CH3OH              1.800E+13     0.0         0.0
SCH2+CH2O=CH3+HCO            1.200E+12     0.0         0.0
SCH2+HCO=CH3+CO              1.800E+13     0.0         0.0
!KD-> SCH2+CH3=C2H4+H            1.800E+13     0.0         0.0
SCH2+CH4=CH3+CH3             4.000E+13     0.0         0.0
!KD-> SCH2+C2H6=CH3+C2H5         1.200E+14     0.0         0.0
SCH2+CO2=CH2O+CO             3.000E+12     0.0         0.0
!KD-> SCH2+CH2CO=C2H4+CO         1.600E+14     0.0         0.0
!KD-> CH+OH=HCO+H                3.000E+13     0.0         0.0
!KD-> CH+O=CO+H                  4.000E+13     0.0         0.0
!KD-> CH+O=C+OH                  1.520E+13     0.0      4730.0
!KD-> H2O+C=CH+OH                7.800E+11     0.67    39300.0
!KD-> CH+O2=HCO+O                4.900E+13     0.0         0.0
!KD-> CH+O2=CO+OH                4.900E+13     0.0         0.0
!KD-> CH+CO2=HCO+CO              3.220E-02     4.44    -3530.0
!KD-> CH+CH4=C2H4+H              3.900E+14    -0.4         0.0
!KD-> CH+CH3=C2H3+H              3.000E+13     0.0         0.0
!KD-> CH2+OH=CH+H2O              1.130E+07     2.0      3000.0
!KD-> CH+H=C+H2                  7.900E+13     0.0       160.0
!KD-> CH+H2O=CH2O+H              1.170E+15    -0.75        0.0
!KD-> CH+H2O=CH2OH               5.700E+12     0.0      -760.0
!KD-> CH+CH2O=CH2CO+H            1.000E+14     0.0      -515.0
CH3O+M=CH2O+H+M              5.400E+13     0.0     13500.0
!KD->  H2/2.5/ H2O/6.2/ CO/1.875/ CO2/3.75/ AR/0.88/
H2/2.5/ H2O/6.2/ CO/1.875/ CO2/3.75/
CH4/3.2/ CH3OH/7.5/
CH3O+HO2=CH2O+H2O2           3.000E+11     0.0         0.0
CH3O+OH=CH2O+H2O             1.800E+13     0.0         0.0
CH3O+O=CH2O+OH               1.800E+12     0.0         0.0
CH3O+H=CH2O+H2               1.800E+13     0.0         0.0
CH3O+O2=CH2O+HO2             2.200E+10     0.0      1750.0
CH3O+CH2O=CH3OH+HCO          1.000E+11     0.0      2980.0
```

```
CH3O+CO=CH3+CO2              6.810E-18     9.2     -2850.0
CH3O+HCO=CH3OH+CO            9.000E+13     0.0        0.0
!KD-> CH3O+C2H5=CH2O+C2H6          2.410E+13     0.0        0.0
!KD-> CH3O+C2H3=CH2O+C2H4          2.410E+13     0.0        0.0
!KD-> CH3O+C2H4=CH2O+C2H5          1.200E+11     0.0     6750.0
!KD-> CH3O+H=CH2OH+H               3.400E+06     1.6        0.0
CH3O+H=SCH2+H2O              1.000E+12     0.0        0.0
CH2O+M=HCO+H+M               5.000E+35    -5.54   96680.0
!KD->  H2/2.5/ H2O/6.2/ CO/1.875/ CO2/3.75/ AR/1.0/
H2/2.5/ H2O/6.2/ CO/1.875/ CO2/3.75/
CH4/3.2/ CH3OH/7.5/
CH2O+M=CO+H2+M               1.100E+36    -5.54   96680.0
!KD->  H2/2.5/ H2O/6.2/ CO/1.875/ CO2/3.75/ AR/1.0/
H2/2.5/ H2O/6.2/ CO/1.875/ CO2/3.75/
CH4/3.2/ CH3OH/7.5/
CH2O+HO2=HCO+H2O2            4.110E+04     2.5     10210.0
CH2O+OH=HCO+H2O              3.433E+09     1.18     -447.0
CH2O+O=HCO+OH                4.100E+11     0.57     2760.0
CH2O+H=HCO+H2                1.260E+08     1.62     2166.0
CH2O+O2=HCO+HO2              6.000E+13     0.0     40650.0
CH2O+CH3=HCO+CH4             7.800E-08     6.1      1970.0
!KD-> C2H6(+M)=C2H5+H(+M)          8.850E+20    -1.228  102210.0
!KD->    LOW /6.90E+42 -6.431 107175.0/
!KD->    SRI /47.61 16182.0 3371.0/
!KD->  H2/2.0/ H2O/6.0/ CH4/2.0/ CO/1.5/ CO2/2.0/ C2H6/3.0/ AR/0.7/
!KD-> C2H6+HO2=C2H5+H2O2           1.330E+13     0.0     20535.0
!KD-> C2H6+OH=C2H5+H2O             7.200E+06     2.0       870.0
!KD-> C2H6+O=C2H5+OH               1.000E+09     1.5      5800.0
!KD-> C2H6+H=C2H5+H2               1.400E+09     1.5      7400.0
!KD-> C2H6+H=CH3+CH4               5.400E+04     0.0     11630.0
!KD-> C2H6+O2=C2H5+HO2             6.000E+13     0.0     52000.0
!KD-> C2H6+CH3=C2H5+CH4            1.470E-07     6.0      6060.0
!KD-> C2H6+CH2=CH3+C2H5            6.500E+12     0.0      7911.0
!KD-> C2H6+C2H3=C2H4+C2H5          8.566E-02     4.14     2543.0
!KD-> C2H6+HCO=CH2O+C2H5           4.700E+04     2.72    18235.0
!KD-> C2H5(+M)=C2H4+H(+M)          1.110E+10     1.037   36767.0
!KD->    LOW /4.0E+33 -4.99 40000.0/
!KD->    TROE /0.832 10 1203.0/
!KD->  H2/2.0/ CO/2.0/ CO2/3.0/ H2O/5.0/ CH4/2.0/ C2H6/0.0/ AR/0.7/
!KD-> C2H5(+C2H6)=C2H4+H(+C2H6)     8.200E+13     0.0     39880.0
!KD->    LOW /1.0E+18 0.0 33380.0/
!KD->    TROE /0.75 97.0 1379.0/
!KD-> C2H5+HO2=C2H4+H2O2           1.800E+12     0.0        0.0
!KD-> C2H5+OH=C2H4+H2O             2.409E+13     0.0        0.0
!KD-> C2H5+OH=>CH3+CH2O+H          2.409E+13     0.0        0.0
!KD-> C2H5+O=CH2O+CH3              4.240E+13     0.0        0.0
!KD-> C2H5+O=CH3HCO+H              5.300E+13     0.0        0.0
!KD-> C2H5+O=C2H4+OH               3.460E+13     0.0        0.0
!KD-> C2H5+H=C2H4+H2               1.700E+12     0.0        0.0
!KD-> C2H5+O2=C2H4+HO2             2.560E+19    -2.77     1980.0
!KD-> C2H5+CH3=C2H4+CH4            1.100E+12     0.0        0.0
```

```
!KD-> C2H5+C2H5=C2H4+C2H6          1.400E+12     0.0       0.0
!KD-> C2H5+HO2=C2H5O+OH            3.000E+13     0.0       0.0
!KD-> C2H4+M=C2H2+H2+M             3.500E+16     0.0    71530.0
!KD->    H2/2.5/ H2O/6.2/ CO/1.875/ CO2/3.75/ AR/1.0/
!KD->    CH4/3.2/ CH3OH/7.5/
!KD-> C2H4+M=C2H3+H+M              2.600E+17     0.0    96570.0
!KD->    H2/2.5/ H2O/6.2/ CO/1.875/ CO2/3.75/ AR/1.0/
!KD->    CH4/3.2/ CH3OH/7.5/
!KD-> C2H4+OH=C2H3+H2O             5.530E+05     2.31    2900.0
!KD-> C2H4+O=CH3+HCO               8.100E+06     1.88     180.0
!KD-> C2H4+H=C2H3+H2               4.490E+07     2.12   13366.0
!KD-> C2H4+O2=C2H3+HO2             4.000E+13     0.0    61500.0
!KD-> C2H4+C2H4=C2H5+C2H3          1.860E+14     0.0    64200.0
!KD-> C2H4+CH3=C2H3+CH4            4.200E+12     0.0    11100.0
!KD-> C2H4+O=CH2HCO+H              4.700E+06     1.88     180.0
!KD-> C2H4+O=CH2O+CH2              3.000E+04     1.88     180.0
!KD-> C2H4+O=CH2CO+H2              6.700E+05     1.88     180.0
!KD-> C2H4+O=C2H3+OH               1.510E+07     1.91    3790.0
!KD-> C2H4+OH=CH2O+CH3             2.000E+12     0.0      960.0
!KD-> C2H4+OH(+M)=PC2H5O(+M)       5.420E+12     0.0       0.0
!KD->      LOW /1.19E+27 -3.1 0.0/
!KD-> C2H4+HO2=C2H3+H2O2           1.120E+13     0.0    30400.0
!KD-> C2H4+CH3O=C2H3+CH3OH         1.000E+11     0.0    10000.0
!KD-> C2H3(+M)=C2H2+H(+M)          2.100E+14     0.0    39740.0
!KD->    LOW /4.15E+41 -7.5 45500.0/
!KD->    TROE /0.65 100000 10/
!KD->  H2/2.0/ CO/2.0/ CO2/3.0/ H2O/5.0/ CH4/2.0/ C2H6/3.0/ AR/0.7/
!KD-> C2H3+HO2=>CH3+CO+OH          3.000E+13     0.0       0.0
!KD-> C2H3+OH=C2H2+H2O             3.000E+13     0.0       0.0
!KD-> C2H3+H=C2H2+H2               1.200E+13     0.0       0.0
!KD-> C2H3+O=CH3+CO                1.000E+13     0.0       0.0
!KD-> C2H3+O2=CH2O+HCO             1.700E+29    -5.312   6500.0
!KD-> C2H3+CH=CH2+C2H2             5.000E+13     0.0       0.0
!KD-> C2H3+CH3=C2H2+CH4            2.050E+13     0.0       0.0
!KD-> C2H3+C2H=C2H2+C2H2           3.000E+13     0.0       0.0
!KD-> C2H3+HCO=C2H4+CO             9.034E+13     0.0       0.0
!KD-> C2H3+CH2O=C2H4+HCO           5.420E+03     2.81    5862.0
!KD-> C2H3+C2H3=C2H2+C2H4          1.450E+13     0.0       0.0
!KD-> C2H3+O=C2H2+OH               1.000E+13     0.0       0.0
!KD-> C2H3+O=CH2+HCO               1.000E+13     0.0       0.0
!KD-> C2H3+O=CH2CO+H               1.000E+13     0.0       0.0
!KD-> C2H3+OH=CH3HCO               3.000E+13     0.0       0.0
!KD-> C2H3+O2=C2H2+HO2             5.190E+15    -1.26    3310.0
!KD->      DUPLICATE
!KD-> C2H3+O2=C2H2+HO2             2.120E-06     6.0     9484.0
!KD->      DUPLICATE
!KD-> C2H3+O2=CH2HCO+O             3.500E+14    -0.61    5260.0
!KD-> C2H3+CH2=C2H2+CH3            3.000E+13     0.0       0.0
!KD-> C2H2=C2H+H                   2.373E+32    -5.28  130688.0
!KD-> C2H2+O2=HCCO+OH              2.000E+08     1.5    30100.0
!KD-> C2H2+O2=C2H+HO2              1.200E+13     0.0    74520.0
```

```
!KD-> C2H2+OH=C2H+H2O              3.385E+07     2.0    14000.0
!KD-> C2H2+OH=CH2CO+H              1.100E+13     0.0     7170.0
!KD-> C2H2+O=CH2+CO              1.200E+06     2.1     1570.0
!KD-> C2H2+O=HCCO+H              5.000E+06     2.1     1570.0
!KD-> C2H2+CH3=C2H+CH4             1.800E+11     0.0    17290.0
!KD-> C2H2+O=C2H+OH              3.000E+14     0.0    25000.0
!KD-> C2H2+OH=CH3+CO              4.830E-04     4.0    -2000.0
!KD-> C2H2+HO2=CH2CO+OH            6.100E+09     0.0     7950.0
!KD-> C2H2+O2=HCO+HCO              4.000E+12     0.0    28000.0
!KD-> C2H+OH=HCCO+H              2.000E+13     0.0        0.0
!KD-> C2H+OH=C2+H2O              4.000E+07     2.0     8000.0
!KD-> C2H+O=CO+CH              1.450E+13     0.0      460.0
!KD-> C2H+O2=HCO+CO              9.000E+12     0.0        0.0
!KD-> C2H+H2=C2H2+H              7.880E+05     2.39     346.0
!KD-> C2H+O2=CO+CO+H              9.000E+12     0.0        0.0
!KD-> C2H+O2=HCCO+O              6.000E+11     0.0        0.0
!KD-> CH2CO(+M)=CH2+CO(+M)          3.000E+14     0.0    71000.0
!KD->     LOW /2.300E+15   0.0  57600.0/
!KD->     H2/2.5/ H2O/6.2/ CO/1.875/ CO2/3.75/ AR/1.0/
!KD->     CH4/3.2/ CH3OH/7.5/
!KD-> CH2CO+O2=CH2O+CO2            2.000E+13     0.0    61500.0
!KD-> CH2CO+HO2=>CH2O+CO+OH         6.000E+11     0.0    12738.0
!KD-> CH2CO+O=HCCO+OH              1.000E+13     0.0     8000.0
!KD-> CH2CO+OH=CH2OH+CO            1.000E+13     0.0        0.0
!KD-> CH2CO+H=CH3+CO              3.280E+10     0.851    2840.0
!KD-> CH2CO+CH3=C2H5+CO            2.400E+12     0.0     8000.0
!KD-> CH2CO+CH2=C2H4+CO            2.900E+12     0.0     3800.0
!KD-> CH2CO+CH2=HCCO+CH3           3.600E+13     0.0    11000.0
!KD-> CH2CO+CH3=HCCO+CH4           7.500E+12     0.0    13000.0
!KD-> CH2CO+OH=CH2O+HCO            2.800E+13     0.0        0.0
!KD-> CH2CO+H=HCCO+H2              1.800E+14     0.0     8600.0
!KD-> CH2CO+O=HCO+HCO              7.500E+11     0.0     1350.0
!KD-> CH2CO+O=HCO+CO+H             7.500E+11     0.0     1350.0
!KD-> CH2CO+O=CH2O+CO              7.500E+11     0.0     1350.0
!KD-> CH2CO+OH=HCCO+H2O            7.500E+12     0.0     2000.0
!KD-> HCCO+M=CH+CO+M              6.000E+15     0.0    58821.0
!KD->     H2/2.5/ H2O/6.2/ CO/1.875/ CO2/3.75/ AR/0.88/
!KD->     CH4/3.2/ CH3OH/7.5/
!KD-> HCCO+OH=HCO+CO+H             1.000E+13     0.0        0.0
!KD-> HCCO+OH=C2O+H2O              3.000E+13     0.0        0.0
!KD-> HCCO+O=CO+CO+H              1.000E+14     0.0        0.0
!KD-> HCCO+O=CH+CO2              2.950E+13     0.0     1110.0
!KD-> HCCO+H=CH2+CO              1.500E+14     0.0        0.0
!KD-> HCCO+O2=CO2+CO+H             5.400E+11     0.0      850.0
!KD-> HCCO+CH2=C2H+CH2O            1.000E+13     0.0     2000.0
!KD-> HCCO+CH2=C2H3+CO            3.000E+13     0.0        0.0
!KD-> HCCO+CH3=C2H4+CO            2.000E+12     0.0        0.0
!KD-> HCCO+CH=CO+C2H2             5.000E+13     0.0        0.0
!KD-> HCCO+HCCO=CO+C2H2+CO          1.000E+13     0.0        0.0
!KD-> HCCO+OH=HCO+HCO             1.000E+13     0.0        0.0
!KD-> HCCO+O2=CO+CO+OH             5.400E+11     0.0      850.0
```

```
!KD-> HCCO+O2=CO2+HCO              5.400E+11     0.0      850.0
CH3OH(+M)=CH3+OH(+M)          1.700E+16     0.0    90885.0
LOW /6.60E+16 0.0 65730.0/
TROE /0.82 200.0 1438.0/
!KD-> CH3OH+HO2=CH2OH+H2O2         9.640E+10     0.0    12580.0
!KD-> CH3OH+OH=CH2OH+H2O           1.440E+06     2.0     -840.0
CH3OH+OH=CH3O+H2O            1.000E+13     0.0     1700.0
!KD-> CH3OH+O=CH2OH+OH            1.630E+13     0.0     5030.0
!KD-> CH3OH+H=CH2OH+H2            1.640E+07     2.0     4520.0
!KD-> CH3OH+CH3=CH2OH+CH4          3.190E+01     3.17    7172.0
CH3OH+CH3=CH3O+CH4           1.450E+01     3.1     6935.0
!KD-> CH3OH+C2H5=C2H6+CH3O         1.440E+01     3.1     8942.0
CH3OH+H=CH3+H2O              2.000E+14     0.0     5300.0
CH3OH+O=CH3O+OH              1.000E+13     0.0     4680.0
!KD-> CH3OH+CH3=C2H6+OH            2.000E+12     0.0    15000.0
!KD-> CH3OH+CH3O=CH2OH+CH3OH       3.000E+11     0.0     4070.0
!KD-> CH3OH(+M)=CH2OH+H(+M)        1.380E+16     0.0    95950.0
!KD->    LOW /5.35E+16 0.0 70800.0/
!KD->    TROE /0.82 200.0 1438.0/
CH3OH+H=H2+CH3O              4.000E+13     0.0     6095.0
!KD-> CH3OH+O2=CH2OH+HO2           2.050E+13     0.0    44900.0
!KD-> CH3OH+C2H5=C2H6+CH2OH        3.190E+01     3.2     9161.0
!KD-> CH2OH+M=CH2O+H+M             1.140E+43    -8.0    43000.0
!KD->    H2O/16.0/ CH4/3.0/ CO2/3.75/  CO/1.875/  H2/2.5/  CH3OH/6.0/
!KD-> CH2OH+H=CH2O+H2              1.000E+13     0.0        0.0
!KD-> CH2OH+O2=CH2O+HO2            1.500E+15    -1.0        0.0
!KD->    DUPLICATE
!KD-> CH2OH+O2=CH2O+HO2            7.200E+13     0.0     3570.0
!KD->    DUPLICATE
!KD-> H+CH2OH=SCH2+H2O             1.000E+12     0.0        0.0
!KD-> CH2OH+O=CH2O+OH              9.000E+13     0.0        0.0
!KD-> CH2OH+OH=CH2O+H2O            1.000E+13     0.0        0.0
!KD-> CH2OH+HO2=CH2O+H2O2          1.210E+13     0.0        0.0
!KD-> CH2OH+CH2OH=CH3OH+CH2O       4.820E+12     0.0        0.0
!KD-> CH2OH+CH2OH=CH2O+CH2O+H2     1.000E+15    -0.7        0.0
!KD-> CH2OH+HCO=CH3OH+CO           1.210E+14     0.0        0.0
!KD-> CH2OH+CH2O=CH3OH+HCO         5.490E+03     2.8     5900.0
!KD-> CH2OH+CH3O=CH3OH+CH2O        2.400E+13     0.0        0.0
CH3O+CH3O=CH3OH+CH2O         2.320E+13     0.0        0.0
!KD-> CH3HCO=CH3+HCO              7.100E+15     0.0    81790.0
!KD-> CH3HCO+HO2=CH3CO+H2O2        3.000E+12     0.0    12000.0
!KD-> CH3HCO+OH=CH3CO+H2O          2.300E+10     0.73   -1100.0
!KD-> CH3HCO+O=CH3CO+OH            5.800E+12     0.0     1800.0
!KD-> CH3HCO+H=CH3CO+H2            4.100E+09     1.16    2400.0
!KD-> CH3HCO+O2=CH3CO+HO2          3.000E+13     0.0    39200.0
!KD-> CH3HCO+CH3=CH3CO+CH4         7.600E+00     3.4     3740.0
!KD-> CH3HCO+H=CH2HCO+H2           7.000E+08     1.5     7400.0
!KD-> CH3HCO+O=CH2HCO+OH           5.000E+08     1.5     5800.0
!KD-> CH3HCO+OH=CH2HCO+H2O         2.000E+14     0.0     6000.0
!KD-> CH3HCO+HO2=CH2HCO+H2O2       3.000E+13     0.0    15000.0
!KD-> CH3HCO+CH2=CH3CO+CH3         1.660E+12     0.0     3510.0
```

```
!KD-> CH3HCO+CH3=CH2HCO+CH4        1.580E+00    4.0    7720.0
!KD-> CH3HCO+CH3O=CH3CO+CH3OH      5.000E+12    0.0       0.0
!KD-> CH3HCO+C2H5=CH3CO+C2H6       1.260E+12    0.0    8500.0
!KD-> CH3HCO+C2H3=CH3CO+C2H4       8.130E+10    0.0    3680.0
!KD-> CH2HCO=CH3CO                 1.600E+11    0.0   21600.0
!KD-> CH3HCO+CH2HCO=CH3CO+CH3HCO   3.000E+12    0.0   11200.0
!KD-> CH3CO(+M)=CH3+CO(+M)         2.800E+13    0.0   17150.0
!KD->    LOW /6.0E+15 0.0 14070.0/
!KD->    TROE /0.5 100000 10/
!KD->    H2/2.5/ H2O/6.2/ CO/1.875/ CO2/3.75/ AR/0.88/
!KD->    CH4/3.2/ CH3OH/7.5/
!KD-> CH3CO+H=CH2CO+H2             1.150E+13    0.0       0.0
!KD-> CH3CO+H=CH3+HCO              2.150E+13    0.0       0.0
!KD-> CH3CO+O=CH2CO+OH             4.000E+13    0.0       0.0
!KD-> CH3CO+O=CH3+CO2              1.500E+14    0.0       0.0
!KD-> CH3CO+CH3=C2H6+CO            3.300E+13    0.0       0.0
!KD-> CH3CO+CH3=CH4+CH2CO          6.100E+12    0.0       0.0
!KD-> CH2HCO+H=CH2CO+H2            2.000E+13    0.0       0.0
!KD-> CH2HCO+O2=CH2O+OH+CO         1.800E+10    0.0       0.0
!KD-> CH2HCO+O2=CH2CO+HO2          1.500E+11    0.0       0.0
!KD-> CH2HCO=CH2CO+H               1.580E+13    0.0   35200.0
!KD-> C2H5O=CH3+CH2O               1.000E+15    0.0   21600.0
!KD-> C2H5O+O2=CH3HCO+HO2          3.600E+10    0.0    1090.0
!KD-> C2H5O=CH3HCO+H               2.000E+14    0.0   23300.0
!KD-> C2H5O+OH=CH3HCO+H2O          1.000E+14    0.0       0.0
!KD-> C2H5O+H=CH3HCO+H2            1.000E+14    0.0       0.0
!KD-> C2H5O+O=CH3HCO+OH            1.210E+14    0.0       0.0
!KD-> C2H5O+HO2=CH3HCO+H2O2        1.000E+14    0.0       0.0
!KD-> C2H5O+C2H5O=C2H5OH+CH3HCO    5.000E+13    0.0       0.0
!KD-> C2H5O+PC2H5O=C2H5OH+CH3HCO   5.000E+13    0.0       0.0
!KD-> C2H5O+SC2H5O=C2H5OH+CH3HCO   5.000E+13    0.0       0.0
!KD-> SC2H5O+M=CH3HCO+H+M          5.000E+13    0.0   21860.0
!KD-> SC2H5O+H=CH3HCO+H2           2.000E+13    0.0       0.0
!KD-> SC2H5O+OH=CH3HCO+H2O         1.500E+13    0.0       0.0
!KD-> SC2H5O+O=CH3HCO+OH           9.040E+13    0.0       0.0
!KD-> SC2H5O+O2=CH3HCO+HO2         8.400E+15   -1.20      0.0
!KD->    DUPLICATE
!KD-> SC2H5O+O2=CH3HCO+HO2         4.800E+14    0.0    5000.0
!KD->    DUPLICATE
!KD-> SC2H5O+HO2=CH3HCO+H2O2       1.000E+13    0.0       0.0
!KD-> SC2H5O+SC2H5O=C2H5OH+CH3HCO  3.500E+13    0.0       0.0
!KD-> SC2H5O+PC2H5O=C2H5OH+CH3HCO  5.000E+13    0.0       0.0
!KD-> PC2H5O=SC2H5O                1.000E+11    0.0   27000.0
!KD-> PC2H5O+PC2H5O=C2H5OH+CH3HCO  3.400E+13    0.0       0.0
!KD-> C2H5OH=CH2OH+CH3             3.100E+15    0.0   80600.0
!KD-> C2H5OH+OH=SC2H5O+H2O         3.000E+13    0.0    5960.0
!KD-> C2H5OH+OH=C2H5O+H2O          1.138E+06    2.0     914.0
!KD-> C2H5OH+OH=PC2H5O+H2O         2.563E+06    2.06    860.0
!KD-> C2H5OH+O=SC2H5O+OH           6.000E+05    2.46   1850.0
!KD-> C2H5OH+O=C2H5O+OH            4.820E+13    0.0    6856.0
!KD-> C2H5OH+O=PC2H5O+OH           5.000E+12    0.0    4411.0
```

```
!KD-> C2H5OH+H=C2H5+H2O            5.900E+11     0.0     3450.0
!KD-> C2H5OH+H=SC2H5O+H2           4.400E+12     0.0     4570.0
!KD-> C2H5OH+HO2=SC2H5O+H2O2       2.000E+13     0.0    17000.0
!KD-> C2H5OH+CH3=SC2H5O+CH4        4.000E+11     0.0     9700.0
!KD-> C2H5OH+CH3=PC2H5O+CH4        3.000E+00     4.0    10480.0
!KD-> C2H5OH+CH3=C2H5O+CH4         8.000E+10     0.0     9400.0
!KD-> C2H5OH+CH3O=SC2H5O+CH3OH     2.000E+11     0.0     7000.0
!KD-> C2H5OH+CH2O=C2H5O+CH3O       1.500E+12     0.0    79500.0
!KD-> C2H5OH+C2H5O=C2H5OH+SC2H5O   2.000E+11     0.0     7000.0
!KD-> C2H5OH=C2H5+OH               5.000E+16     0.0    91212.0
!KD-> C2H5OH=C2H4+H2O              1.000E+14     0.0    76706.0
!KD-> C2H5OH+O2=PC2H5O+HO2         4.000E+13     0.0    50900.0
!KD-> C2H5OH+O2=SC2H5O+HO2         4.000E+13     0.0    51200.0
!KD-> C2H5OH+O2=C2H5O+HO2          2.000E+13     0.0    56000.0
!KD-> C2H5OH+H=PC2H5O+H2           2.000E+12     0.0     9500.0
!KD-> C2H5OH+H=C2H5O+H2            1.760E+12     0.0     4570.0
!KD-> C2H5OH+HO2=H2O2+C2H5O        1.000E+11     0.0    15500.0
!KD-> C2H5OH+HO2=H2O2+PC2H5O       1.000E+11     0.0    12500.0
!KD-> C2H5OH+C2H5=PC2H5O+C2H6      1.500E+12     0.0    11700.0
!KD-> C2H5OH+C2H5=SC2H5O+C2H6      4.000E+13     0.0    10000.0
!KD-> C2H5OH+CH2OH=SC2H5O+CH3OH    4.000E+11     0.0     9700.0
!KD-> C+OH=CO+H                    5.000E+13     0.0        0.0
!KD-> C+O2=CO+O                    1.200E+14     0.0     4000.0
!KD-> C+CH3=C2H2+H                 5.000E+13     0.0        0.0
!KD-> C+CH2=C2H+H                  5.000E+13     0.0        0.0
!KD-> CH2O+CH3O2=HCO+CH3O2H        2.000E+12     0.0    11660.0
!KD-> CH3O2+H=CH3O+OH              9.600E+13     0.0        0.0
!KD-> CH3O2+OH=CH3OH+O2            6.000E+13     0.0        0.0
!KD-> CH3O2+CH3=CH3O+CH3O          2.400E+13     0.0        0.0
!KD-> CH3O2+CH3O2=>CH2O+CH3OH+O2   2.700E+10     0.0     -780.0
!KD-> CH3O2+CH3O2=>CH3O+CH3O+O2    2.800E+10     0.0     -780.0
!KD-> CH3O2+H2O2=CH3O2H+HO2        2.400E+12     0.0    10000.0
!KD-> CH3O2H=CH3O+OH               6.000E+14     0.0    42300.0
!KD-> CH3O2+HO2=CH3O2H+O2          2.290E+11     0.0    -1550.0
!KD-> CH3O2H+OH=CH3O2+H2O          1.150E+12     0.0     -380.0
!KD-> CH4+CH3O2=CH3+CH3O2H         1.810E+11     0.0    18600.0
!KD-> C2H6+CH3O2=C2H5+CH3O2H       2.950E+11     0.0    14940.0
!KD-> CH3OH+CH3O2=CH2OH+CH3O2H     1.810E+12     0.0    13800.0
!KD-> CH3O2H+O=OH+CH3O2            2.000E+13     0.0     4750.0
!KD-> CH3CO+O2=CH3CO3              1.000E+10     0.0    -2700.0
!KD-> CH3HCO+CH3CO3=CH3CO+CH3CO3H  1.200E+11     0.0     4900.0
!KD-> CH3HCO+C2H5O2=CH3CO+C2H5O2H  1.150E+11     0.0    10000.0
!KD-> C2H5+O2(+M)=C2H5O2(+M)       2.200E+10     0.772   -570.0
!KD->     LOW /7.10E+42 -8.24 4270.0 /
!KD-> C2H5O2=C2H4+HO2              5.620E+11     0.0    28900.0
!KD-> C2H5O2+HO2=C2H5O2H+O2        3.400E+11     0.0    -1300.0
!KD-> C2H5O2H=C2H5O+OH             4.000E+15     0.0    43000.0
!KD-> C2H5O2H+O=OH+C2H5O2          2.000E+13     0.0     4750.0
!KD-> C2H5O2H+OH=C2H5O2+H2O        2.000E+12     0.0     -370.0
!KD-> CH4+C2H5O2=CH3+C2H5O2H       1.140E+13     0.0    20460.0
!KD-> CH4+CH3CO3=CH3+CH3CO3H       1.140E+13     0.0    20460.0
```

```
!KD-> C2H4+C2H5O2=C2H3+C2H5O2H      1.000E+12     0.0    25000.0
!KD-> C2H4+CH3CO3=C2H3+CH3CO3H      3.000E+12     0.0    29000.0
!KD-> CH3CO3+HO2=CH3CO3H+O2         1.000E+12     0.0        0.0
!KD-> CH3CO3H=>CH3CO2+OH            1.150E+13     0.0    32550.0
!KD-> CH3CO3H=>CH3+CO2+OH           2.000E+14     0.0    40150.0
!KD-> CH3CO3+CH3O2=>CH3CO2+CH3O+O2  1.080E+15     0.0     3600.0
!KD-> CH3CO3+CH3O2=>CH3CO2H+CH2O+O2  2.470E+09     0.0    -4200.0
!KD-> CH3CO3+HO2=>CH3CO2+OH+O2      2.590E+11     0.0    -2080.0
!KD-> CH3CO3+CH3CO3=>CH3CO2+CH3CO2+O2  1.690E+12   0.0    -1060.0
!KD-> CH3CO2+M=>CH3+CO2+M           8.700E+15     0.0    14400.0
!KD-> CH3CO2H=CH4+CO2               7.080E+13     0.0    74600.0
!KD-> CH3CO2H=CH2CO+H2O             4.470E+14     0.0    79800.0
!KD-> CH3CO2H+OH=CH3CO2+H2O         2.400E+11     0.0     -400.0
!KD-> CH3OH+C2H5O2=CH2OH+C2H5O2H    6.300E+12     0.0    19360.0
!KD-> CH3OH+CH3CO3=CH2OH+CH3CO3H    6.300E+12     0.0    19360.0
!KD-> CH2O+C2H5O2=HCO+C2H5O2H       1.300E+11     0.0     9000.0
!KD-> CH2O+CH3CO3=HCO+CH3CO3H       1.000E+12     0.0    10560.0
!KD-> C2H4+CH3O2=C2H3+CH3O2H        1.000E+13     0.0    25000.0
!KD-> CH3HCO+CH3O2=CH3CO+CH3O2H     1.150E+11     0.0    10000.0
!KD-> C2H5OH+CH3O2=SC2H5O+CH3O2H    1.000E+13     0.0    10000.0
!KD-> C2H5+CH3O2=C2H5O+CH3O         2.410E+13     0.0        0.0
!KD-> C2H4+HO2=C2H4O+OH             2.200E+12     0.0    17200.0
!KD-> C2H4+CH3O=C2H4O+CH3           1.000E+11     0.0    14500.0
!KD-> C2H4+CH3O2=C2H4O+CH3O         7.000E+11     0.0    14500.0
!KD-> C2H4O=>CH3HCOW                1.600E+13     0.0    54300.0
!KD-> CH3HCOW+M=>CH3HCO+M           1.000E+14     0.0        0.0
!KD-> CH3HCOW=>CH3+HCO              5.000E+08     0.0        0.0
!KD-> C2H4O+H=H2+C2H3O              8.000E+13     0.0     9740.0
!KD-> C2H4O+H=H2O+C2H3              5.000E+09     0.0     5030.0
!KD-> C2H4O+H=C2H4+OH               9.510E+10     0.0     5030.0
!KD-> C2H4O+CH2HCO=CH3HCO+C2H3O     1.000E+11     0.0    14000.0
!KD-> C2H4O+CH3=CH4+C2H3O           1.070E+12     0.0    11900.0
!KD-> C2H4O+O=OH+C2H3O              1.910E+12     0.0     5300.0
!KD-> C2H4O+OH=H2O+C2H3O            1.780E+13     0.0     3600.0
!KD-> C2H3O=>CH2CHOW                1.000E+11     0.0    10000.0
!KD-> C2H3O=>CH3+CO                 8.000E+11     0.0    10000.0
!KD-> C2H3O+H+M=>C2H4O+M            4.000E+15     0.0        0.0
!KD-> CH2CHOW+M=>CH2HCO+M           1.000E+14     0.0        0.0
!KD-> CH2CHOW=>CH3+CO               1.000E+08     0.0        0.0
!KD-> CH2CHOW=>OH+C2H2              1.000E+11     0.0    17000.0
!KD-> CH2CHOW=>CH2CO+H              1.000E+08     0.0        0.0
!KD-> C2H4O+O2=HO2+C2H3O            1.000E+14     0.0    52000.0
!KD-> C2H4O+HO2=H2O2+C2H3O          5.000E+13     0.0    18000.0
!KD-> CH3HCOW+O2=>HO2+CH3CO         1.000E+14     0.0        0.0
!KD-> CH2CHOW+O2=>HO2+CH2CO         1.000E+14     0.0        0.0
!KD-> CH2+C2H2=H+C3H3               1.200E+13     0.0     6620.0
!KD-> CH2+C2H4=C3H6                 3.160E+12     0.0     5280.0
!KD-> SCH2+C2H4=>C3H6               1.000E+14     0.0        0.0
!KD-> CH2+C3H8=CH3+IC3H7            1.500E+00     3.46    7470.0
!KD-> CH2+C3H8=CH3+NC3H7            9.000E-01     3.65    7150.0
!KD-> SCH2+C2H2=C3H3+H              1.800E+14     0.0        0.0
```

```
!KD-> C2H3+CH2=C3H4+H            3.000E+13    0.0       0.0
!KD-> C2H3+C2H2=C4H4+H           1.930E+12    0.0    6000.0
!KD-> C2H3+C2H3=C4H6             7.230E+13    0.0       0.0
!KD-> C2H2+CH3=SC3H5             1.610E+40   -8.58  20331.0
!KD-> C2H2+CH3=C3H5              2.610E+46   -9.82  36951.0
!KD-> C2H2+CH3=C3H4+H            6.740E+19   -2.08  31591.0
!KD-> CH2CO+C2H3=C3H5+CO         1.000E+12    0.0    3000.0
!KD-> HCCO+C2H2=C3H3+CO          1.000E+11    0.0    3000.0
!KD-> C3H8(+M)=C2H5+CH3(+M)      1.100E+17    0.0   84400.0
!KD->    LOW /7.83E+18 0.0 65000.0/
!KD-> C3H8+O2=NC3H7+HO2          4.000E+13    0.0   50870.0
!KD-> C3H8+O2=IC3H7+HO2          4.000E+13    0.0   47690.0
!KD-> C3H8+HO2=NC3H7+H2O2        4.760E+04    2.55  16490.0
!KD-> C3H8+HO2=IC3H7+H2O2        9.640E+03    2.6   13910.0
!KD-> C3H8+OH=NC3H7+H2O          3.160E+07    1.80    934.0
!KD-> C3H8+OH=IC3H7+H2O          7.060E+06    1.90   -159.0
!KD-> C3H8+O=NC3H7+OH            3.715E+06    2.4    5505.0
!KD-> C3H8+O=IC3H7+OH            5.495E+05    2.5    3140.0
!KD-> C3H8+H=NC3H7+H2            1.336E+06    2.54   6756.0
!KD-> C3H8+H=IC3H7+H2            1.300E+06    2.4    4470.0
!KD-> C3H8+CH3=NC3H7+CH4         9.000E-01    3.65   7150.0
!KD-> C3H8+CH3=IC3H7+CH4         1.500E+00    3.46   5480.0
!KD-> C3H8+C2H5=NC3H7+C2H6       9.000E-01    3.65   9140.0
!KD-> C3H8+C2H5=IC3H7+C2H6       1.200E+00    3.46   7470.0
!KD-> C3H8+C2H3=NC3H7+C2H4       6.000E+02    3.3   10502.0
!KD-> C3H8+C2H3=IC3H7+C2H4       1.000E+03    3.1    8829.0
!KD-> C3H8+IC3H7=NC3H7+C3H8      8.440E-03    4.2    8720.0
!KD-> C3H8+C3H5=NC3H7+C3H6       2.350E+02    3.3   19800.0
!KD-> C3H8+C3H5=IC3H7+C3H6       7.840E+01    3.3   18200.0
!KD-> C3H8+CH3O=NC3H7+CH3OH      4.340E+11    0.0    6460.0
!KD-> C3H8+CH3O=IC3H7+CH3OH      1.450E+11    0.0    4570.0
!KD-> NC3H7=C2H4+CH3             1.260E+13    0.0   30404.0
!KD-> NC3H7+O2=C3H6+HO2          1.000E+12    0.0    5000.0
!KD-> IC3H7=C2H4+CH3             1.000E+12    0.0   34500.0
!KD-> IC3H7+O2=C3H6+HO2          2.754E+10    0.0   -2151.0
!KD-> C3H6=C3H5+H                4.570E+14    0.0   88900.0
!KD-> C3H6=SC3H5+H               7.590E+14    0.0  101300.0
!KD-> C3H6=TC3H5+H               1.450E+15    0.0   98060.0
!KD-> C3H6=C2H3+CH3              1.100E+21   -1.2   97720.0
!KD-> C3H6+HO2=C3H6O+OH          1.050E+12    0.0   14210.0
!KD-> C3H6+HO2=C3H5+H2O2         9.640E+03    2.6   13910.0
!KD-> C3H6+HO2=SC3H5+H2O2        7.500E+09    0.0   12570.0
!KD-> C3H6+HO2=TC3H5+H2O2        3.000E+09    0.0    9930.0
!KD-> C3H6+OH=C3H5+H2O           3.120E+06    2.0    -300.0
!KD-> C3H6+OH=SC3H5+H2O          2.140E+06    2.0    2780.0
!KD-> C3H6+OH=TC3H5+H2O          1.110E+06    2.0    1450.0
!KD-> C3H6+O=C2H5+HCO            6.833E+06    1.57   -628.0
!KD-> C3H6+O=CH3+CH3CO           9.111E+06    1.57   -628.0
!KD-> C3H6+O=C2H4+CH2O           4.555E+06    1.57   -628.0
!KD-> NC3H7=C3H6+H               1.000E+14    0.0   37286.0
!KD-> C3H6+H=IC3H7               5.704E+09    1.16    874.0
```

```
!KD-> C3H6+H=C3H5+H2               6.457E+12     0.0     4445.0
!KD-> C3H6+H=SC3H5+H2              7.810E+05     2.5    12280.0
!KD-> C3H6+O2=SC3H5+HO2            1.950E+12     0.0    39000.0
!KD-> C3H6+O2=TC3H5+HO2            1.950E+12     0.0    39000.0
!KD-> C3H6+O2=C3H5+HO2             1.950E+12     0.0    39000.0
!KD-> C3H6+CH3=C3H5+CH4            2.210E+00     3.5     5680.0
!KD-> C3H6+CH3=SC3H5+CH4           1.350E+00     3.5    12850.0
!KD-> C3H6+CH3=TC3H5+CH4           8.400E-01     3.5    11660.0
!KD-> C3H6+C2H5=C3H5+C2H6          2.230E+00     3.5     6640.0
!KD-> C3H6O=C2H5+HCO               2.450E+13     0.0    58500.0
!KD-> C3H6O=C2H5CHO                1.820E+14     0.0    58500.0
!KD-> C3H6O=CH3+CH3CO              4.540E+13     0.0    59900.0
!KD-> C3H6O=CH3+CH2HCO             2.450E+13     0.0    58820.0
!KD-> C3H6O=CH3+C2H3O              8.000E+15     0.0    92010.0
!KD-> C2H5CHO=C2H5+HCO             2.450E+16     0.0    73000.0
!KD-> C2H5CHO+O=C2H5CO+OH          5.680E+12     0.0     1540.0
!KD-> C2H5CHO+OH=C2H5CO+H2O        1.210E+13     0.0        0.0
!KD-> C2H5CHO+HO2=C2H5CO+H2O2      1.520E+09     0.0        0.0
!KD-> C2H5CHO+C2H5=C2H5CO+C2H6     5.000E+10     0.0     6290.0
!KD-> C2H5CO=C2H5+CO               5.890E+12     0.0    14400.0
!KD-> C3H5+O2=>CH2O+CH2HCO         5.000E+12     0.0    19190.0
!KD-> C3H5+H=C3H4+H2               1.800E+13     0.0        0.0
!KD-> C3H5+O=>C2H4+CO+H            1.807E+14     0.0        0.0
!KD-> C3H5+CH3=C3H4+CH4            3.000E+12    -0.32    -130.0
!KD-> C3H5+C2H5=C3H4+C2H6          9.640E+11     0.0     -130.0
!KD-> C3H5+C2H3=C3H4+C2H4          2.400E+12     0.0        0.0
!KD-> C3H5+C2H3=C3H6+C2H2          4.800E+12     0.0        0.0
!KD-> SC3H5+O2=CH3HCO+HCO          4.340E+12     0.0        0.0
!KD-> SC3H5+HO2=>CH2CO+CH3+OH      4.500E+12     0.0        0.0
!KD-> SC3H5+H=C3H4+H2              3.333E+12     0.0        0.0
!KD-> SC3H5+O=>CH2CO+CH3           1.807E+14     0.0        0.0
!KD-> SC3H5+CH3=C3H4+CH4           1.000E+11     0.0        0.0
!KD-> SC3H5+C2H5=C3H4+C2H6         1.000E+11     0.0        0.0
!KD-> SC3H5+C2H3=C3H4+C2H4         1.000E+11     0.0        0.0
!KD-> TC3H5+O2=CH3CO+CH2O          4.335E+11     0.0        0.0
!KD-> TC3H5+HO2=>CH2CO+CH3+OH      4.500E+12     0.0        0.0
!KD-> TC3H5+H=C3H4+H2              3.333E+12     0.0        0.0
!KD-> TC3H5+O=>HCCO+CH3+H          1.807E+14     0.0        0.0
!KD-> TC3H5+CH3=C3H4+CH4           1.000E+11     0.0        0.0
!KD-> TC3H5+C2H5=C3H4+C2H6         1.000E+11     0.0        0.0
!KD-> TC3H5+C2H3=C3H4+C2H4         1.000E+11     0.0        0.0
!KD-> C3H4+M=C3H3+H+M              2.000E+18     0.0    80000.0
!KD->   H2O/16.0/   CO2/3.75/   CO/1.875/   H2/2.5/   CH4/3.0/   C3H6/16.0/   C2H4/16.0/
C3H8/16.0/
!KD-> C3H4(+M)=PC3H4(+M)           1.070E+14     0.0    64300.0
!KD->    LOW /3.48E+17 0.0 48390.0/
!KD-> C3H4+O2=C3H3+HO2             4.000E+13     0.0    61500.0
!KD-> C3H4+HO2=>CH2CO+CH2+OH       8.000E+12     0.0    19000.0
!KD-> C3H4+OH=CH2CO+CH3            3.120E+12     0.0     -397.0
!KD-> C3H4+OH=C3H3+H2O             2.000E+07     2.0     1000.0
!KD-> C3H4+O=C2H3+HCO              1.100E-02     4.613  -4243.0
```

```
!KD-> C3H4+H=C3H5                 1.200E+11    0.69    3000.0
!KD-> C3H4+H=TC3H5                8.500E+12    0.0     2000.0
!KD-> C3H4+H=C3H3+H2              2.000E+07    2.0     5000.0
!KD-> C3H4+CH3=C3H3+CH4           2.000E+11    0.0     7700.0
!KD-> PC3H4+M=C3H3+H+M            4.700E+18    0.0    80000.0
!KD->  H2O/16.0/  CO2/3.75/  CO/1.875/  H2/2.5/  CH4/3.0/  C3H6/16.0/  C2H4/16.0/
C3H8/16.0/
!KD-> PC3H4+O2=>HCCO+OH+CH2       2.000E+08    1.5    30100.0
!KD-> PC3H4+O2=C3H3+HO2           5.000E+12    0.0    51000.0
!KD-> PC3H4+HO2=>C2H4+CO+OH       3.000E+12    0.0    19000.0
!KD-> PC3H4+OH=C3H3+H2O           2.000E+07    2.0     1000.0
!KD-> PC3H4+OH=CH2CO+CH3          5.000E-04    4.5    -1000.0
!KD-> PC3H4+O=CH2CO+CH2           6.400E+12    0.0     2010.0
!KD-> PC3H4+O=C2H3+HCO            3.200E+12    0.0     2010.0
!KD-> PC3H4+O=HCCO+CH3            6.300E+12    0.0     2010.0
!KD-> PC3H4+O=>HCCO+CH2+H         3.200E+11    0.0     2010.0
!KD-> PC3H4+H=TC3H5               6.500E+12    0.0     2000.0
!KD-> PC3H4+H=C3H3+H2             2.000E+07    2.0     5000.0
!KD-> PC3H4+H=C2H2+CH3            1.300E+05    2.5     1000.0
!KD-> PC3H4+CH3=C3H3+CH4          1.500E+00    3.5     5600.0
!KD-> PC3H4+C2H3=C3H3+C2H4        1.000E+12    0.0     7700.0
!KD-> PC3H4+C3H5=C3H3+C3H6        1.000E+12    0.0     7700.0
!KD-> C3H3+H=C3H2+H2              5.000E+13    0.0     3000.0
!KD-> C3H3+O=>C2H+HCO+H           7.000E+13    0.0        0.0
!KD-> C3H3+O=>C2H2+CO+H           7.000E+13    0.0        0.0
!KD-> C3H3+OH=C3H2+H2O            1.000E+13    0.0        0.0
!KD-> C3H3+O2=CH2CO+HCO           3.010E+10    0.0     2870.0
!KD-> C3H3+CH=IC4H3+H             7.000E+13    0.0        0.0
!KD-> C3H3+CH=NC4H3+H             7.000E+13    0.0        0.0
!KD-> C3H3+CH2=C4H4+H             4.000E+13    0.0        0.0
!KD-> C3H3+C3H3=C6H5+H            2.000E+12    0.0        0.0
!KD-> CH+C2H2=C3H2+H              1.000E+14    0.0        0.0
!KD-> C3H2+O2=HCCO+CO+H           1.000E+14    0.0     3000.0
!KD-> C3H2+OH=C2H2+HCO            5.000E+13    0.0        0.0
!KD-> C3H2+CH2=IC4H3+H            3.000E+13    0.0        0.0
!KD-> C4H8=IC4H7+H                4.078E+18   -1.0    97350.0
!KD-> C4H8=C2C4H8                 4.000E+11    0.0    60000.0
!KD-> C4H8=T2C4H8                 4.000E+11    0.0    60000.0
!KD-> C4H8=C3H5+CH3               1.000E+16    0.0    73000.0
!KD-> C4H8=C2H3+C2H5              1.000E+19   -1.0    96770.0
!KD-> C4H8+O2=IC4H7+HO2           4.000E+12    0.0    33200.0
!KD-> C4H8+HO2=IC4H7+H2O2         1.000E+11    0.0    17060.0
!KD-> C4H8+OH=NC3H7+CH2O          6.500E+12    0.0        0.0
!KD-> C4H8+OH=CH3HCO+C2H5         1.000E+11    0.0        0.0
!KD-> C4H8+OH=C2H6+CH3CO          1.000E+10    0.0        0.0
!KD-> C4H8+OH=IC4H7+H2O           2.250E+13    0.0     2217.0
!KD-> C4H8+O=C3H6+CH2O            2.505E+12    0.0        0.0
!KD-> C4H8+O=CH3HCO+C2H4          1.250E+12    0.0      850.0
!KD-> C4H8+O=C2H5+CH3CO           1.625E+13    0.0      850.0
!KD-> C4H8+O=IC4H7+OH             9.600E+12    0.0     1970.0
!KD-> C4H8+O=NC3H7+HCO            1.800E+05    2.5    -1029.0
```

```
!KD-> C4H8+H=IC4H7+H2              5.000E+13     0.0     3900.0
!KD-> C4H8+CH3=IC4H7+CH4           1.000E+11     0.0     7300.0
!KD-> C4H8+C2H5=IC4H7+C2H6         1.000E+11     0.0     8000.0
!KD-> C4H8+C3H5=IC4H7+C3H6         7.900E+10     0.0    12400.0
!KD-> C4H8+SC3H5=IC4H7+C3H6        8.000E+10     0.0    12400.0
!KD-> C4H8+TC3H5=IC4H7+C3H6        8.000E+10     0.0    12400.0
!KD-> C2C4H8=T2C4H8                4.000E+13     0.0    62000.0
!KD-> C2C4H8=C4H6+H2               1.000E+13     0.0    65500.0
!KD-> C2C4H8=IC4H7+H               4.074E+18    -1.0    97350.0
!KD-> C2C4H8=SC3H5+CH3             2.000E+16     0.0    95000.0
!KD-> C2C4H8+OH=IC4H7+H2O          1.250E+14     0.0     3060.0
!KD-> C2C4H8+OH=CH3HCO+C2H5        1.400E+13     0.0        0.0
!KD-> C2C4H8+O=IC3H7+HCO           6.030E+12     0.0        0.0
!KD-> C2C4H8+O=CH3HCO+C2H4         1.000E+12     0.0        0.0
!KD-> C2C4H8+H=IC4H7+H2            1.000E+13     0.0     3500.0
!KD-> C2C4H8+CH3=IC4H7+CH4         1.000E+11     0.0     8200.0
!KD-> T2C4H8=IC4H7+H               4.074E+18    -1.0    97350.0
!KD-> T2C4H8=SC3H5+CH3             2.000E+16     0.0    96000.0
!KD-> T2C4H8+OH=IC4H7+H2O          1.000E+14     0.0     3060.0
!KD-> T2C4H8+OH=CH3HCO+C2H5        1.500E+13     0.0        0.0
!KD-> T2C4H8+O=IC3H7+HCO           6.030E+12     0.0        0.0
!KD-> T2C4H8+O=CH3HCO+C2H4         1.000E+12     0.0        0.0
!KD-> T2C4H8+H=IC4H7+H2            5.000E+12     0.0     3500.0
!KD-> T2C4H8+CH3=IC4H7+CH4         1.000E+11     0.0     8200.0
!KD-> IC4H7=C4H6+H                 1.200E+14     0.0    49300.0
!KD-> IC4H7=C2H4+C2H3              1.000E+14     0.0    49000.0
!KD-> IC4H7+H=C4H6+H2              3.160E+12     0.0        0.0
!KD-> IC4H7+O2=C4H6+HO2            1.000E+11     0.0        0.0
!KD-> IC4H7+CH3=C4H6+CH4           1.000E+13     0.0        0.0
!KD-> IC4H7+C2H3=C4H6+C2H4         4.000E+12     0.0        0.0
!KD-> IC4H7+C2H5=C4H6+C2H6         4.000E+12     0.0        0.0
!KD-> IC4H7+C2H5=C4H8+C2H4         5.000E+11     0.0        0.0
!KD-> IC4H7+C2H5=T2C4H8+C2H4       5.000E+11     0.0        0.0
!KD-> IC4H7+C2H5=C2C4H8+C2H4       5.000E+11     0.0        0.0
!KD-> IC4H7+C3H5=C4H6+C3H6         4.000E+13     0.0        0.0
!KD-> IC4H7+IC4H7=C4H6+C4H8        3.160E+12     0.0        0.0
!KD-> C2H3+C2H4=C4H6+H             3.000E+12     0.0     1000.0
!KD-> C4H6+H=NC4H5+H2              3.000E+07     2.0    13000.0
!KD-> C4H6+H=IC4H5+H2              3.000E+07     2.0     6000.0
!KD-> C4H6+OH=NC4H5+H2O            2.000E+07     2.0     5000.0
!KD-> C4H6+OH=IC4H5+H2O            2.000E+07     2.0     2000.0
!KD-> C4H6+O=C2H4+CH2CO            1.000E+12     0.0        0.0
!KD-> C4H6+O=PC3H4+CH2O            1.000E+12     0.0        0.0
!KD-> C2H2+NC4H5=C6H6+H            2.800E+03     2.9     1400.0
!KD-> NC4H5+OH=C4H4+H2O            2.000E+07     2.0     1000.0
!KD-> NC4H5+H=C4H4+H2              3.000E+07     2.0     1000.0
!KD-> NC4H5+H=IC4H5+H              1.000E+14     0.0        0.0
!KD-> IC4H5=C4H4+H                 2.000E+15     0.0    45000.0
!KD-> NC4H5=C4H4+H                 1.600E+14     0.0    41400.0
!KD-> C4H4+OH=IC4H3+H2O            1.000E+07     2.0     2000.0
!KD-> C4H4+OH=NC4H3+H2O            7.500E+06     2.0     5000.0
```

```
!KD-> C4H4+H=NC4H3+H2              2.000E+07     2.0    15000.0
!KD-> NC4H3+H=IC4H3+H              1.000E+14     0.0        0.0
!KD-> IC4H3+CH2=C3H4+C2H           2.000E+13     0.0        0.0
!KD-> IC4H3+O2=CH2CO+HCCO          1.000E+12     0.0        0.0
!KD-> IC4H3+OH=C4H2+H2O            3.000E+13     0.0        0.0
!KD-> IC4H3+O=CH2CO+C2H            2.000E+13     0.0        0.0
!KD-> IC4H3+H=C4H2+H2              5.000E+13     0.0        0.0
!KD-> NC4H3+C2H2=C6H5              2.800E+03     2.9     1400.0
!KD-> NC4H3+M=C4H2+H+M             1.000E+16     0.0    59700.0
!KD->   H2O/16.0/   CO2/3.75/   CO/1.875/   H2/2.5/   CH4/3.0/   C3H6/16.0/   C2H4/16.0/
C3H8/16.0/
!KD-> IC4H3+M=C4H2+H+M             4.460E+15     0.0    46516.0
!KD->   H2O/16.0/   CO2/3.75/   CO/1.875/   H2/2.5/   CH4/3.0/   C3H6/16.0/   C2H4/16.0/
C3H8/16.0/
!KD-> IC4H3+O=H2C4O+H              2.000E+13     0.0        0.0
!KD-> H2C4O+H=C2H2+HCCO            5.000E+13     0.0     3000.0
!KD-> H2C4O+OH=CH2CO+HCCO          1.000E+07     2.0     2000.0
!KD-> C4H2+OH=H2C4O+H              6.660E+12     0.0     -410.0
!KD-> C2H2+C2H2=IC4H3+H            2.200E+12     0.0    64060.0
!KD-> C2H2+C2H2=NC4H3+H            1.000E+12     0.0    66000.0
!KD-> C2H2+C2H2=C4H4               5.500E+12     0.0    37000.0
!KD-> C4H2(+M)=C4H+H(+M)           2.200E+14     0.0   116740.0
!KD->      LOW /3.50E+17  0.0  80065.0/
!KD->      H2O /16.0/ H2 /2.5/ CO /1.875/ CO2 /3.75/ CH4 /3.0/
!KD->      C3H6 /16.0/ C2H4 /16.0/ C3H8 /16.0/
!KD-> C4H2+O=C3H2+CO               2.700E+13     0.0     1720.0
!KD-> C2H2+C2H=C4H2+H              1.820E+14     0.0      467.0
!KD-> C2H2+C2H=NC4H3               1.000E+13     0.0        0.0
!KD-> C4H+O2=C2H+CO+CO             1.000E+14     0.0        0.0
!KD-> C2O+H=CH+CO                  1.320E+13     0.0        0.0
!KD-> C2O+O=CO+CO                  5.200E+13     0.0        0.0
!KD-> C2O+OH=CO+CO+H               2.000E+13     0.0        0.0
!KD-> C2O+O2=CO+CO+O               2.000E+13     0.0        0.0
!KD-> C2O+O2=CO+CO2                2.000E+13     0.0        0.0
!KD-> C2+H2=C2H+H                  6.600E+13     0.0     7950.0
!KD-> C2+O=C+CO                    3.600E+14     0.0        0.0
!KD-> C2+O2=CO+CO                  9.000E+12     0.0      980.0
!KD-> C2+OH=C2O+H                  5.000E+13     0.0        0.0
!KD-> C6H5+OH=C6H5O+H              5.000E+13     0.0        0.0
!KD-> C6H5+O2=C6H5O+O              2.600E+13     0.0     6120.0
!KD-> C6H5+HO2=C6H5O+OH            5.000E+13     0.0     1000.0
!KD-> C6H6+H=C6H5+H2               3.000E+12     0.0     8100.0
!KD-> C6H6+OH=C6H5+H2O             1.680E+08     1.42    1450.0
!KD-> C6H6+O=C6H5O+H               2.780E+13     0.0     4910.0
!KD-> C6H6+O2=C6H5O+OH             4.000E+13     0.0    34000.0
!KD-> H+C6H5=C6H6                  7.800E+13     0.0        0.0
!KD-> C3H3+O=>C2H3+CO              3.800E+13     0.0        0.0
!KD-> C3H3+O=CH2O+C2H              2.000E+13     0.0        0.0
!KD-> C3H3+O2=>HCCO+CH2O           6.000E+12     0.0        0.0
!KD-> C3H3+CH3=C2H5+C2H            1.000E+13     0.0    37500.0
!KD-> C3H3+CH3=C4H6                5.000E+12     0.0        0.0
```

```
!KD-> C3H6+C2H3=C3H5+C2H4          2.210E+00     3.5     4680.0
!KD-> C3H6+C2H3=SC3H5+C2H4         1.350E+00     3.5    10860.0
!KD-> C3H6+C2H3=TC3H5+C2H4         8.400E-01     3.5     9670.0
!KD-> C3H6+CH3O=C3H5+CH3OH         9.000E+01     2.95   12000.0
!KD-> CH2+C2H2=C3H4               1.200E+13     0.0     6620.0
!KD-> C3H4+C3H4=C3H5+C3H3          5.000E+14     0.0    64700.0
!KD-> C3H4+OH=CH2O+C2H3            1.700E+12     0.0     -300.0
!KD-> C3H4+OH=HCO+C2H4             1.700E+12     0.0     -300.0
!KD-> C3H4+O=CH2O+C2H2             1.000E+12     0.0        0.0
!KD-> C3H4+O=>CO+C2H4              7.800E+12     0.0     1600.0
!KD-> C3H4+C3H5=C3H3+C3H6          2.000E+12     0.0     7700.0
!KD-> C3H4+C2H=C3H3+C2H2           1.000E+13     0.0        0.0
!KD-> PC3H4=C2H+CH3               4.200E+16     0.0   100000.0
!KD-> PC3H4+C2H=C3H3+C2H2          1.000E+13     0.0        0.0
!KD-> C3H2+O2=HCO+HCCO             1.000E+13     0.0        0.0
!KD-> C2H2+C2H3=NC4H5              2.510E+05     1.9     2100.0
!KD-> C2H3+C2H3=IC4H5+H            4.000E+13     0.0        0.0
!KD-> IC4H5+H=C4H4+H2              3.000E+07     2.0     1000.0
!KD-> C4H2+H=C4H+H2               1.000E+14     0.0    35000.0
!KD-> C4H6+OH=C3H5+CH2O            7.230E+12     0.0     -994.0
!KD-> C4H8+IC4H7=IC4H7+C2C4H8      3.980E+10     0.0    12400.0
!KD-> C4H8+IC4H7=IC4H7+T2C4H8      3.980E+10     0.0    12400.0
!KD-> C3H3+C3H3=C6H6               3.000E+11     0.0        0.0
!KD-> C3H3+C3H4=C6H6+H             1.400E+12     0.0    10000.0
!KD-> C3H5+C2H5=C3H6+C2H4          2.600E+12     0.0     -130.0
!KD-> C3H6+OH=C2H5+CH2O            8.000E+12     0.0        0.0
!KD-> C3H6+OH=CH3+CH3HCO           3.400E+11     0.0        0.0
!KD-> C3H5+O2=C3H4+HO2             1.200E+12     0.0    13550.0
!KD-> CH2O+C3H5=HCO+C3H6           8.000E+10     0.0    12400.0
!KD-> CH3HCO+C3H5=CH3CO+C3H6       3.800E+11     0.0     7200.0
!KD-> C3H8+CH3O2=NC3H7+CH3O2H      6.030E+12     0.0    19380.0
!KD-> C3H8+CH3O2=IC3H7+CH3O2H      1.990E+12     0.0    17050.0
!KD-> C3H8+C2H5O2=NC3H7+C2H5O2H    6.030E+12     0.0    19380.0
!KD-> C3H8+C2H5O2=IC3H7+C2H5O2H    1.990E+12     0.0    17050.0
!KD-> C3H8+IC3H7O2=NC3H7+IC3H7O2H   6.030E+12     0.0    19380.0
!KD-> C3H8+IC3H7O2=IC3H7+IC3H7O2H   1.990E+12     0.0    17050.0
!KD-> C3H8+NC3H7O2=NC3H7+NC3H7O2H   6.030E+12     0.0    19380.0
!KD-> C3H8+NC3H7O2=IC3H7+NC3H7O2H   1.990E+12     0.0    17050.0
!KD-> NC3H7+O2=NC3H7O2             4.820E+12     0.0        0.0
!KD-> IC3H7+O2=IC3H7O2             6.620E+12     0.0        0.0
!KD-> NC3H7+HO2=NC3H7O+OH          3.200E+13     0.0        0.0
!KD-> IC3H7+HO2=IC3H7O+OH          3.200E+13     0.0        0.0
!KD-> NC3H7+CH3O2=NC3H7O+CH3O      3.800E+12     0.0    -1200.0
!KD-> IC3H7+CH3O2=IC3H7O+CH3O      3.800E+12     0.0    -1200.0
!KD-> NC3H7+NC3H7O2=NC3H7O+NC3H7O   3.800E+12     0.0    -1200.0
!KD-> IC3H7+NC3H7O2=IC3H7O+NC3H7O   3.800E+12     0.0    -1200.0
!KD-> NC3H7+IC3H7O2=NC3H7O+IC3H7O   3.800E+12     0.0    -1200.0
!KD-> IC3H7+IC3H7O2=IC3H7O+IC3H7O   3.800E+12     0.0    -1200.0
!KD-> NC3H7O2+HO2=NC3H7O2H+O2      4.600E+10     0.0    -2600.0
!KD-> IC3H7O2+HO2=IC3H7O2H+O2      4.600E+10     0.0    -2600.0
!KD-> CH3+NC3H7O2=CH3O+NC3H7O      3.800E+12     0.0    -1200.0
```

```
!KD-> CH3+IC3H7O2=CH3O+IC3H7O       3.800E+12     0.0    -1200.0
!KD-> NC3H7O2H=NC3H7O+OH           4.000E+15     0.0    43000.0
!KD-> IC3H7O2H=IC3H7O+OH           4.000E+15     0.0    43000.0
!KD-> NC3H7O=C2H5+CH2O             5.000E+13     0.0    15700.0
!KD-> IC3H7O=CH3+CH3HCO            4.000E+14     0.0    17200.0
!KD-> C3H6+OH(+M)=C3H6OH(+M)        1.810E+13     0.0       0.0
!KD->    LOW /1.33E+30  -3.5  0.0/
!KD-> C3H6OH=>C2H5+CH2O            1.400E+09     0.0    17200.0
!KD-> C3H6OH=>CH3+CH3HCO           1.000E+09     0.0    17200.0
!KD-> C3H6OH+O2=O2C3H6OH           1.000E+12     0.0    -1100.0
!KD-> O2C3H6OH=>CH3HCO+CH2O+OH      1.000E+16     0.0    25000.0
!KD-> C3H6+CH3O2=C3H5+CH3O2H        2.000E+12     0.0    17000.0
!KD-> C3H6+CH3O2=C3H6O+CH3O         4.000E+11     0.0    11720.0
!KD-> C3H6+C2H5O2=C3H5+C2H5O2H      3.200E+11     0.0    14900.0
!KD-> C3H6+C3H5O2=C3H5+C3H5O2H      3.200E+11     0.0    14900.0
!KD-> C3H6+C3H5O2=C3H6O+C3H5O       1.050E+11     0.0    14200.0
!KD-> C3H6+CH3CO3=C3H5+CH3CO3H      3.200E+11     0.0    14900.0
!KD-> C3H6+NC3H7O2=C3H5+NC3H7O2H    3.200E+11     0.0    14900.0
!KD-> C3H6+IC3H7O2=C3H5+IC3H7O2H    3.200E+11     0.0    14900.0
!KD-> C3H6+NC3H7O2=C3H6O+NC3H7O     1.700E+07     0.0       0.0
!KD-> C3H5+O2=C3H5O2               1.200E+10     0.0    -2300.0
!KD-> C3H5+HO2=C3H5O+OH            9.000E+12     0.0       0.0
!KD-> C3H5+CH3O2=C3H5O+CH3O         3.800E+11     0.0    -1200.0
!KD-> C3H5O2+CH3=C3H5O+CH3O         3.800E+11     0.0    -1200.0
!KD-> C3H5O2+C3H5=C3H5O+C3H5O       3.800E+11     0.0    -1200.0
!KD-> C3H5O2+HO2=C3H5O2H+O2         4.600E+10     0.0    -2600.0
!KD-> C3H5O2+HO2=>C3H5O+OH+O2       1.000E+12     0.0       0.0
!KD-> C3H5O2+CH3O2=>C3H5O+CH3O+O2   1.700E+11     0.0    -1000.0
!KD-> C3H5O2+C3H5O2=>C3H5O+C3H5O+O2  3.700E+12     0.0     2200.0
!KD-> C3H5O=CH2O+C2H3              1.000E+14     0.0    21600.0
!KD-> C3H5O2H=C3H5O+OH             4.000E+15     0.0    43000.0
!KD-> CH2O+C3H5O2=HCO+C3H5O2H       1.300E+11     0.0    10500.0
!KD-> CH2O+NC3H7O2=HCO+NC3H7O2H     1.300E+11     0.0     9000.0
!KD-> CH2O+IC3H7O2=HCO+IC3H7O2H     1.300E+11     0.0     9000.0
!KD-> C2H4+NC3H7O2=C2H3+NC3H7O2H    7.100E+11     0.0    25000.0
!KD-> C2H4+IC3H7O2=C2H3+IC3H7O2H    7.100E+11     0.0    25000.0
!KD-> CH4+C3H5O2=CH3+C3H5O2H        1.140E+13     0.0    20460.0
!KD-> CH4+NC3H7O2=CH3+NC3H7O2H      1.140E+13     0.0    20460.0
!KD-> CH4+IC3H7O2=CH3+IC3H7O2H      1.140E+13     0.0    20460.0
!KD-> CH3OH+NC3H7O2=CH2OH+NC3H7O2H   6.300E+12     0.0    19360.0
!KD-> CH3OH+IC3H7O2=CH2OH+IC3H7O2H   6.300E+12     0.0    19360.0
!KD-> CH3HCO+C3H5O2=CH3CO+C3H5O2H    1.150E+11     0.0    10000.0
!KD-> CH3HCO+NC3H7O2=CH3CO+NC3H7O2H  1.150E+11     0.0    10000.0
!KD-> CH3HCO+IC3H7O2=CH3CO+IC3H7O2H  1.150E+11     0.0    10000.0
!KD-> C+N2+M=CNN+M                 1.120E+15     0.0       0.0
!KD-> C2H+NO=HCN+CO                6.000E+13     0.0      570.0
!KD-> C2H+HCN=CN+C2H2              3.200E+12     0.0     1530.0
!KD-> CH2+NO=HCN+OH                5.000E+11     0.0     2870.0
!KD-> HCN+M=H+CN+M                 3.570E+26    -2.6   124900.0
!KD-> C2N2+M=CN+CN+M               3.200E+16     0.0    94400.0
!KD-> CH+N2(+M)=HCNN(+M)           3.100E+12     0.15      0.0
```

```
!KD->     LOW / 1.30E+25 -3.16 740.0 /
!KD->     TROE /0.667 235.0 2117.0 4536.0 /
!KD->     H2O/10.0/ O2/2.0/ AR/0.75/ H2/2.0/
!KD-> HCNN+H=H2+CNN              5.000E+13     0.0       0.0
!KD-> HCNN+H=>CH2+N2             2.000E+13     0.0     3000.0
!KD-> HCNN+O=OH+CNN              2.000E+13     0.0    20000.0
!KD-> HCNN+O=CO+H+N2             5.000E+13     0.0    15000.0
!KD-> HCNN+O=HCN+NO              5.000E+13     0.0    15000.0
!KD-> HCNN+OH=H2O+CNN            1.000E+13     0.0     8000.0
!KD-> HCNN+OH=H+HCO+N2           1.000E+13     0.0    16000.0
!KD-> HCNN+O2=HO2+CNN            1.000E+12     0.0     4000.0
!KD-> HCNN+O2=>H+CO2+N2          4.000E+12     0.0       0.0
!KD-> HCNN+O2=HCO+N2O            4.000E+12     0.0       0.0
!KD-> CNN+O=CO+N2                1.000E+13     0.0       0.0
!KD-> CNN+O=CN+NO                1.000E+14     0.0    20000.0
!KD-> CNN+OH=H+CO+N2             1.000E+13     0.0     1000.0
!KD-> CNN+H=NH+CN                5.000E+14     0.0    40000.0
!KD-> CNN+OH=HCN+NO              1.000E+12     0.0     1000.0
!KD-> CNN+H=HCN+N                5.000E+13     0.0    25000.0
!KD-> CNN+O2=NO+NCO              1.000E+13     0.0     5000.0
HNO+CH3=NO+CH4              8.200E+05     1.87     954.0
!KD-> HONO+CH3=NO2+CH4           8.100E+05     1.87    5504.0
H2NO+CH3=CH3O+NH2           2.000E+13     0.0       0.0
H2NO+CH3=HNO+CH4            1.600E+06     1.87    2960.0
!KD-> HNOH+CH3=HNO+CH4           1.600E+06     1.87    2096.0
!KD-> NH2OH+CH3=HNOH+CH4         1.600E+06     1.87    6350.0
!KD-> NH2OH+CH3=H2NO+CH4         8.200E+05     1.87    5500.0
N2H2+CH3=NNH+CH4            1.600E+06     1.87    2970.0
N2H3+CH3=N2H2+CH4           8.200E+05     1.87    1818.0
N2H4+CH3=N2H3+CH4           3.300E+06     1.87    5325.0
CH4+NH=CH3+NH2              9.000E+13     0.0    20080.0
CH4+NH2=CH3+NH3             1.200E+13     0.0    15150.0
!KD-> CH3+NH2=CH2+NH3            1.600E+06     1.87    7570.0
!KD-> C2H6+NH=C2H5+NH2           7.000E+13     0.0    16700.0
!KD-> C2H6+NH2=C2H5+NH3          9.700E+12     0.0    11470.0
!KD-> C3H8+NH2=NC3H7+NH3         1.700E+13     0.0    10660.0
!KD-> C3H8+NH2=IC3H7+NH3         4.500E+11     0.0     6150.0
!KD-> CH3+NO(+M)=CH3NO(+M)       1.000E+13     0.0       0.0
!KD->     LOW /1.90E+18 0.0 0.0/
!KD->     SRI /0.03 -790.0 1.0/
!KD-> CH3NO+H=H2CNO+H2           4.400E+08     1.5      377.0
!KD-> CH3NO+H=CH3+HNO            1.800E+13     0.0     2800.0
!KD-> CH3NO+O=H2CNO+OH           3.300E+08     1.5     3615.0
!KD-> CH3NO+O=CH3+NO2            1.700E+06     2.08      0.0
!KD-> CH3NO+OH=H2CNO+H2O         3.600E+06     2.0    -1192.0
!KD-> CH3NO+OH=CH3+HONO          2.500E+12     0.0     1000.0
!KD-> CH3NO+CH3=H2CNO+CH4        7.900E+05     1.87    5415.0
!KD-> CH3NO+NH2=H2CNO+NH3        2.800E+06     1.94    1073.0
!KD-> H2CNO=HNCO+H               2.300E+42    -9.11   53840.0
!KD-> H2CNO+O2=CH2O+NO2          2.900E+12    -0.31   17700.0
!KD-> H2CNO+H=CH3+NO             4.000E+13     0.0       0.0
```

```
!KD-> H2CNO+H=HCNO+H2              4.800E+08     1.5     -894.0
!KD-> H2CNO+O=HCNO+OH              3.300E+08     1.5     -894.0
!KD-> H2CNO+O=CH2O+NO              7.000E+13     0.0        0.0
!KD-> H2CNO+OH=CH2OH+NO            4.000E+13     0.0        0.0
!KD-> H2CNO+OH=HCNO+H2O            2.400E+06     2.0    -1192.0
!KD-> H2CNO+CH3=C2H5+NO            3.000E+13     0.0        0.0
!KD-> H2CNO+CH3=HCNO+CH4           1.600E+06     1.87   -1113.0
!KD-> H2CNO+NH2=HCNO+NH3           1.800E+06     1.94   -1152.0
CH3+NO2=CH3O+NO              1.400E+13     0.0        0.0
!KD-> CH+NO2=HCO+NO                1.200E+14     0.0        0.0
!KD-> CH2+NO2=CH2O+NO              4.200E+13     0.0        0.0
!KD-> CN+NO=N2+CO                  1.000E+11     0.0        0.0
!KD-> HNCO+M=H+NCO+M               5.000E+15     0.0    120000.0
!KD-> HNCO+N=NH+NCO                4.000E+13     0.0     36000.0
CH3O+HNO=CH3OH+NO            3.160E+13     0.0        0.0
!KD-> NCO+HO2=HNCO+O2              2.000E+13     0.0        0.0
!KD-> N2O+CO=CO2+N2                2.510E+14     0.0     46000.0
!KD-> N2O+CH2=CH2O+N2              1.000E+12     0.0        0.0
!KD-> N2O+CH3=CH3O+N2              9.000E+09     0.0        0.0
!KD-> N2O+HCO=CO2+H+N2             1.700E+14     0.0     20000.0
!KD-> N2O+HCCO=CO+HCO+N2           1.700E+14     0.0     25500.0
!KD-> N2O+C2H2=HCCO+H+N2           6.590E+16     0.0     61200.0
!KD-> N2O+C2H3=CH2HCO+N2           1.000E+11     0.0        0.0
!KD-> HOCN+O=NCO+OH                1.500E+04     2.64     4000.0
!KD-> HOCN+H=NCO+H2                2.000E+07     2.0      2000.0
!KD-> HOCN+H=NH2+CO                1.200E+08     0.61     2080.0
!KD-> HOCN+OH=NCO+H2O              6.380E+05     2.0      2560.0
!KD-> HOCN+CH3=NCO+CH4             8.200E+05     1.87     6620.0
!KD-> HOCN+NH2=NCO+NH3             9.200E+05     1.94     3645.0
!KD-> CN+NO2=CO+N2O                4.930E+14    -0.752     344.0
!KD-> CN+NO2=CO2+N2                3.700E+14    -0.752     344.0
!KD-> CN+CO2=NCO+CO                3.670E+06     2.16    26900.0
!KD-> CN+NH3=HCN+NH2               9.200E+12     0.0      -357.0
!KD-> HNCO+CN=HCN+NCO              1.500E+13     0.0        0.0
!KD-> HONO+NCO=HNCO+NO2            3.600E+12     0.0        0.0
!KD-> NCO+CH2O=HNCO+HCO            6.000E+12     0.0        0.0
!CH+N2=HCN+N                 3.680E+07     1.42    20723.0
!KD-> NH2+C=CH+NH                  5.800E+11     0.67    20900.0
!KD-> C+N2=CN+N                    5.200E+13     0.0     44700.0
!KD-> CH2+N2=HCN+NH                4.800E+12     0.0     35850.0
!KD-> C2+N2=CN+CN                  1.500E+13     0.0     41700.0
!KD-> H2CN+N=N2+CH2                6.000E+13     0.0       400.0
!KD-> H2CN+H=HCN+H2                2.400E+08     1.5      -894.0
!KD-> H2CN+O=HCN+OH                1.700E+08     1.5      -894.0
!KD-> H2CN+O=HNCO+H                6.000E+13     0.0        0.0
!KD-> H2CN+O=HCNO+H                2.000E+13     0.0        0.0
!KD-> H2CN+M=HCN+H+M               3.000E+14     0.0     22000.0
!KD-> H2CN+HO2=HCN+H2O2            1.400E+04     2.69    -1610.0
!KD-> H2CN+O2=CH2O+NO              3.000E+12     0.0      6000.0
!KD-> H2CN+CH3=HCN+CH4             8.100E+05     1.87    -1113.0
!KD-> H2CN+OH=HCN+H2O              1.200E+06     2.0     -1192.0
```

```
!KD-> H2CN+NH2=HCN+NH3          9.200E+05    1.94   -1152.0
!KD-> C+NO=CN+O              2.000E+13    0.0      0.0
!KD-> CH+NO=HCN+O             8.690E+13    0.0      0.0
!KD-> CH+NO=CN+OH             1.680E+12    0.0      0.0
!KD-> CH+NO=CO+NH             9.840E+12    0.0      0.0
!KD-> CH+NO=NCO+H             1.670E+13    0.0      0.0
!KD-> CH2+NO=HNCO+H            2.500E+12    0.0    5970.0
!KD-> CH2+NO=HCNO+H            3.800E+13   -0.36    576.0
!KD-> CH2+NO=NH2+CO            2.300E+16   -1.43   1331.0
!KD-> CH2+NO=H2CN+O            8.100E+07    1.42   4110.0
!KD-> CH3+NO=HCN+H2O            2.400E+12    0.0   15700.0
!KD-> CH3+NO=H2CN+OH            5.200E+12    0.0   24240.0
!KD-> HCCO+NO=HCNO+CO           4.640E+13    0.0     700.0
!KD-> HCCO+NO=HCN+CO2           1.390E+13    0.0     700.0
!KD-> SCH2+NO=HCN+OH            1.000E+14    0.0      0.0
!KD-> HCNO=HCN+O              4.200E+31   -6.12  61210.0
!KD-> HCNO+H=HCN+OH            1.000E+14    0.0   12000.0
!KD-> HCNO+H=HNCO+H            2.100E+15   -0.69   2850.0
!KD-> HCNO+H=HOCN+H            1.400E+11   -0.19   2484.0
!KD-> HCNO+H=NH2+CO            1.700E+14   -0.75   2890.0
!KD-> HCNO+O=HCO+NO            7.000E+13    0.0      0.0
!KD-> CH2+N=HCN+H             5.000E+13    0.0      0.0
!KD-> CH2+N=NH+CH             6.000E+11    0.67  40500.0
!KD-> CH+N=CN+H              1.670E+14   -0.09     0.0
!KD-> CH+N=C+NH              4.500E+11    0.65   2400.0
N+CO2=NO+CO              1.900E+11    0.0    3400.0
!KD-> N+HCCO=HCN+CO            5.000E+13    0.0      0.0
!KD-> CH3+N=H2CN+H             7.100E+13    0.0      0.0
!KD-> CH3+N=HCNH+H             1.200E+11    0.52    367.6
!KD-> HCNH=HCN+H              6.100E+28   -5.69  24270.0
!KD-> HCNH+H=H2CN+H            2.000E+13    0.0      0.0
!KD-> HCNH+H=HCN+H2            2.400E+08    1.5    -894.0
!KD-> HCNH+O=HNCO+H            7.000E+13    0.0      0.0
!KD-> HCNH+O=HCN+OH            1.700E+08    1.5    -894.0
!KD-> HCNH+OH=HCN+H2O           1.200E+06    2.0   -1192.0
!KD-> HCNH+CH3=HCN+CH4          8.200E+05    1.87  -1113.0
!KD-> C2H3+N=HCN+CH2            2.000E+13    0.0      0.0
!KD-> CN+H2O=HCN+OH            4.000E+12    0.0    7400.0
!KD-> CN+H2O=HOCN+H            4.000E+12    0.0    7400.0
!KD-> OH+HCN=HOCN+H            3.200E+04    2.45  12120.0
!KD-> OH+HCN=HNCO+H            5.600E-06    4.71   -490.0
!KD-> OH+HCN=NH2+CO            6.440E+10    0.0   11700.0
!KD-> HOCN+H=HNCO+H            1.000E+13    0.0      0.0
!KD-> HCN+O=NCO+H             1.380E+04    2.64   4980.0
!KD-> HCN+O=NH+CO             3.450E+03    2.64   4980.0
!KD-> HCN+O=CN+OH             2.700E+09    1.58  26600.0
!KD-> CN+H2=HCN+H             2.000E+04    2.87   1600.0
!KD-> CN+O=CO+N              1.900E+12    0.46    720.0
!KD-> CN+O2=NCO+O             7.200E+12    0.0    -400.0
!KD-> CN+OH=NCO+H             4.000E+13    0.0      0.0
!KD-> CN+HCN=C2N2+H            1.510E+07    1.71   1530.0
```

```
!KD-> CN+NO2=NCO+NO              5.320E+15    -0.752    344.0
!KD-> CN+N2O=NCO+N2              6.000E+12     0.0    15360.0
!KD-> C2N2+O=NCO+CN              4.570E+12     0.0     8880.0
!KD-> C2N2+OH=HNCO+CN             1.860E+11     0.0     2900.0
!KD-> C2N2+OH=HOCN+CN             2.000E+12     0.0    19000.0
!KD-> HNCO+H=H2+NCO              1.760E+05     2.41   12300.0
!KD-> HNCO+H=NH2+CO              3.600E+04     2.49    2340.0
!KD-> HNCO+M=NH+CO+M              1.100E+16     0.0    86000.0
!KD->   N2/1.5/ O2/1.5/ H2O/18.6/
!KD-> HNCO+O=NCO+OH              2.200E+06     2.11   11430.0
!KD-> HNCO+O=NH+CO2              9.800E+07     1.41    8530.0
!KD-> HNCO+O=HNO+CO              1.500E+08     1.57   44012.0
!KD-> HNCO+OH=NCO+H2O             3.450E+07     1.5     3600.0
!KD-> HNCO+OH=NH2+CO2             6.300E+10    -0.06   11645.0
!KD-> HNCO+HO2=NCO+H2O2            3.000E+11     0.0    29000.0
!KD-> HNCO+O2=HNO+CO2             1.000E+12     0.0    35000.0
!KD-> HNCO+NH2=NCO+NH3            5.000E+12     0.0     6200.0
!KD-> HNCO+NH=NCO+NH2             1.040E+15     0.0    39390.0
!KD-> NCO+H=NH+CO               5.360E+13     0.0       0.0
!KD-> NCO+O=NO+CO               4.200E+13     0.0       0.0
!KD-> NCO+O=N+CO2               8.000E+12     0.0     2500.0
!KD-> NCO+N=N2+CO               2.000E+13     0.0       0.0
!KD-> NCO+OH=NO+HCO              5.000E+12     0.0    15000.0
!KD-> NCO+M=N+CO+M              2.200E+14     0.0    54050.0
!KD-> NCO+NO=N2O+CO              4.600E+18    -2.01     934.0
!KD-> NCO+NO=N2+CO2              5.800E+18    -2.01     934.0
!KD-> NCO+O2=NO+CO2              2.000E+12     0.0    20000.0
!KD-> NCO+HCO=HNCO+CO             3.600E+13     0.0       0.0
!KD-> NCO+NO2=CO+NO+NO            2.830E+13    -0.646   -326.0
!KD-> NCO+NO2=CO2+N2O             3.570E+14    -0.646   -326.0
!KD-> NCO+HNO=HNCO+NO             1.800E+13     0.0       0.0
!KD-> NCO+NCO=CO+CO+N2            3.000E+12     0.0       0.0
NO+HCO=CO+HNO               7.240E+13    -0.4       0.0
NO2+CO=CO2+NO               9.000E+13     0.0    33800.0
NO2+HCO=H+CO2+NO            8.400E+15    -0.75    1930.0
!KD-> CH3O+NO2=HONO+CH2O          3.000E+12     0.0       0.0
CH3O+NO=CH2O+HNO            1.300E+14    -0.7       0.0
!KD-> NO2+CH2O=HONO+HCO           1.000E+10     0.0    15100.0
NO+CH2O=HNO+HCO             1.000E+13     0.0    40820.0
!KD-> NO2+HCO=HONO+CO             1.000E+13     0.0       0.0
NO2+HCO=OH+NO+CO            1.000E+14     0.0       0.0
!KD-> NCO+N=NO+CN               2.700E+18    -0.995  17200.0
!KD-> CN+CH4=HCN+CH3              9.000E+04     2.64    -300.0
!KD-> C+NO=CO+N                2.800E+13     0.0       0.0
NH+CO2=HNO+CO               1.000E+13     0.0    14350.0
!KD-> NCO+CH4=HNCO+CH3            1.000E+13     0.0     8130.0
!KD-> C+N2O=CN+NO               4.800E+12     0.0       0.0
!KD-> CH+NH2=HCN+H+H              3.000E+13     0.0       0.0
!KD-> CH+NH=HCN+H               5.000E+13     0.0       0.0
!KD-> CH2+NH=HCN+H+H              3.000E+13     0.0       0.0
!KD-> CH3+N=HCN+H+H              2.000E+11     0.0       0.0
```

```
!KD-> CH3+N=HCN+H2          7.100E+12    0.0       0.0
CH4+N=NH+CH3            1.000E+13    0.0   24000.0
!KD-> C3H3+N=HCN+C2H2       1.000E+13    0.0       0.0
!KD-> CH+N2O=HCN+NO         1.340E+13    0.0    -510.0
!KD-> CH+N2O=CO+H+N2        5.200E+12    0.0    -510.0
!KD-> C2O+N2=>NCO+CN        7.000E+11    0.0   17000.0
END
```

Appendix B

Full mechanism model

```
ELEMENTS
C H O N AR HE
END
SPECIES
OH*  HCN HNCO NO N2O CO CO2 HNC HCO CH2O HO2CHO O2CHO OCHO
O2   H2   AR   H    O    OH   HO2  H2O  H2O2   HCO  CH2O
NO2  NH3  HNO  HON  HONO H2NO N    NNH  NH2  NH
CN   NCO  NCCN HOCN HCNO NCN  HE HNO2 N2O4 N2O3
CH
H2CN HCNH HNOH NO3 HONO2
N2   CH4 C2H6 N2H4 N2H3 N2H2 H2NN
END
```

REACTIONS , A_i ((cm^3/mol)$^{(r-1)}$/s), β_i, E_i (cal/mol)

```
N2O+H=N2+OH                  5.00E+13   0.00E+00     1.52E+04
NO+H(+M)=HNO(+M)    1.50E+15   -0.4       0.0
  LOW /0.24000E+15  0.20600E+00 -0.15500E+04/
  TROE /0.82000E+00  0.10000E-29  0.10000E+31  0.10000E+31/
N+NO=N2+O     2.10E+13    0.0       0.0
HNO+H=NO+H2             4.40E+11    0.7      650.0
N2O+H=NH+NO                  6.700E+22     -2.16    37155.0
!**************KerOMeNes et al. 2013 H2 CHEMistry***************
H+O2<=>O+OH                              1.040e+014     0.000   15286.0
O+H2<=>H+OH                              5.080e+004     2.670    6292.0
OH+H2<=>H+H2O                              4.380e+013     0.000    6990.0
O+H2O<=>OH+OH                              2.970e+006     2.020   13400.0
H2+M<=>H+H+M                               4.577e+019    -1.400  104400.0
H2/ 2.50/ H2O/ 12.00/ CO/ 1.90/ CO2/ 3.80/ HE/ 0.83/ CH4/ 2.00/ C2H6/ 3.00/
O+O+M<=>O2+M                               6.165e+015    -0.500       0.0
H2/ 2.50/ H2O/ 12.00/ AR/ 0.83/ CO/ 1.90/ CO2/ 3.80/ HE/ 0.83/ CH4/ 2.00/ C2H6/ 3.00/
O+H+M<=>OH+M                               4.714e+018    -1.000       0.0
H2/ 2.50/ H2O/ 12.00/ AR/ 0.75/ CO/ 1.50/ CO2/ 2.00/ HE/ 0.75/ CH4/ 2.00/ C2H6/ 3.00/
H+OH+M<=>H2O+M                               3.500e+022    -2.000       0.0
H2/ 0.73/ H2O/ 3.65/ CH4/ 2.00/ C2H6/ 3.00/ AR/ 0.38/
H+O2(+M)<=>HO2(+M)                            4.650e+012     0.440       0.0
 LOW  /  1.737e+019    -1.230       0.0/
TROE/  6.700e-001  1.000e-030  1.000e+030  1.000e+030/
H2/ 1.30/ CO/ 1.90/ CO2/ 3.80/ HE/ 0.00/ H2O/ 10.00/ AR/ 0.00/ CH4/ 2.00/ C2H6/ 3.00/
H+O2(+AR)<=>HO2(+AR)                          4.650e+012     0.440       0.0
LOW/                              6.810e+018    -1.200       0.0/
TROE/  7.000e-001  1.000e-030  1.000e+030  1.000e+030/
!H+O2(+HE)<=>HO2(+HE)                          4.650e+012     0.440       0.0
!low/                             9.192e+018    -1.200       0.0/
!TROE/  5.900e-001  1.000e-030  1.000e+030  1.000e+030/
HO2+H<=>OH+OH                              7.079e+013     0.000     295.0
H2+O2<=>H+HO2                             5.176e+005     2.433   53502.0
HO2+O<=>OH+O2                              3.250e+013     0.000       0.0
HO2+OH<=>H2O+O2                              2.456e+013     0.000    -497.0
HO2+HO2<=>H2O2+O2                              1.300e+011     0.000   -1630.0
```

```
DUP
HO2+HO2<=>H2O2+O2                          3.658e+014    0.000   12000.0
DUP
H2O2(+H2O)<=>OH+OH(+H2O)                      2.000e+012    0.900   48749.0
LOW/                         1.865e+025    -2.300   48749.0/
TROE/  5.100e-001  1.000e-030  1.000e+030/
H2O2(+M)<=>OH+OH(+M)                          2.000e+012    0.900   48749.0
LOW/                         2.490e+024    -2.300   48749.0/
TROE/  4.300e-001  1.000e-030  1.000e+030/
H2O/ 0.00/ CO2/ 1.60/ N2/ 1.50/ O2/ 1.20/ HE/ 0.65/ H2O2/ 7.70/
H2/ 3.70/ CO/ 2.80/
H2O2+H<=>H2O+OH                          2.410e+013    0.000    3970.0
H2O2+H<=>H2+HO2                          2.150e+010    1.000    6000.0
H2O2+O<=>OH+HO2                          9.550e+006    2.000    3970.0
H2O2+OH<=>H2O+HO2                          1.740e+012    0.000     318.0
DUP
H2O2+OH<=>H2O+HO2                          7.590e+013    0.000    7269.0
DUP
!REF:meuller 99 * 0.76
CO+O(+M)<=>CO2(+M)                         1.362E+010    0.000    2384.0
LOW/                         1.173E+024    -2.790    4191.0/
H2/ 2.00/ H2O/ 12.00/ CO/ 1.75/ CO2/ 3.60/ AR/ 0.70/ HE/ 0.70/
!REF:86tsa/ ham * 0.44
CO+O2<=>CO2+O                            1.119E+012    0.000   47700.0
!REF: joshi and wang ijck (2006), 38, (1), 57-73.
CO+OH<=>CO2+H                            7.015E+004    2.053    -355.7
DUP
CO+OH<=>CO2+H                            5.757E+012   -0.664     331.8
DUP
!REF:you et al. j. phys. chem. a 2007, 111, 4031-4042
CO+HO2<=>CO2+OH                          1.570E+005    2.180   17940.0
!REF:li et al. ijck 2007 *1.2
HCO+M<=>H+CO+M                           5.700E+011    0.660   14870.0
H2/ 2.00/ H2O/ 12.00/ CO/ 1.50/ CO2/ 2.00/ CH4/ 2.00/ C2H6/ 3.00/
!REF:timonen et al., jpc, 92:651 (1988)
HCO+O2<=>CO+HO2                          7.580E+012    0.000     410.0
HCO+H<=>CO+H2                            7.340E+013    0.000       0.0
!REF:tsang and hampson, j. phys. chem. ref. data, 15:1087 (1986)
HCO+O<=>CO+OH                            3.020E+013    0.000       0.0
HCO+O<=>CO2+H                            3.000E+013    0.000       0.0
!REF:timonen et al., jpc, 92:651 (1988)
HCO+OH<=>CO+H2O                          1.020E+014    0.000       0.0
!REF:tsang and hampson, j. phys. chem. ref. data, 15:1087 (1986)
HCO+HO2=>CO2+H+OH                          3.000E+013    0.000       0.0
!REF:tsang and hampson, j. phys. chem. ref. data, 15:1087 (1986)
HCO+HCO=>H2+CO+CO                          3.000E+012    0.000       0.0
!REF:Mulenko, S.A. Rev. Roum. Phys. 32, 173 (1987)
!HCO+CH3<=>CH4+CO                          2.650E+013    0.000       0.0
!REF:N. K. Srinivasan et al.,J. Phys. Chem. A 109, 7902-7914 (2005)
CH2O+O2<=>HCO+HO2                          8.070E+015    0.000   53420.0
!REF:
```

```
HCO+O2<=>O2CHO                          1.200E+011     0.000   -1100.0
!REF:analogy with ch3o2+ch2o Tsang/ Hampson 1986
CH2O+O2CHO<=>HCO+HO2CHO                        1.990E+012     0.000   11660.0
!REF:wkm estimate
OCHO+OH<=>HO2CHO                           2.000E+013     0.000      0.0
!REF:
H+CO2<=>OCHO                            7.500E+013     0.000   29000.0
!REF:tsang and hampson, j. phys. chem. ref. data, 15:1087 (1986)
HCO+HCO<=>CH2O+CO                          1.800E+013     0.000      0.0
!***********************************************
HCN+M = H+CN+M                  3.4E35 -5.13 133000!          NBS91
   N2/0.0/ O2/1.5/ H2O/10/
HCN+N2 = H+CN+N2                3.6E26 -2.60 124890!                    NBS91
HCN+M = HNC+M                  1.6E26 -3.23 54600 ! 090302    DB00, MOd Ea
   AR/0.7/ H2O/7.0/  CO2/2.0/                    !
CN+H2 = HCN+H                  1.1E05  2.60  1908 !          CEC05
HCN+O=NCO+H                    1.4E04  2.64  4980 ! GLA/MIL98 MIL/BOW89
HCN+O=CN+OH                    4.2E10  0.40 20665 ! *         DEA/BOZ00
HCN+O=NH+CO                    3.5E03  2.64  4980 ! GLA/MIL98 MIL/BOW89
HCN+OH=CN+H2O                   3.9E06  1.83 10300 ! GLA/MIL98 WOO/BOW95_HCN
HCN+OH=HOCN+H                   5.9E04  2.4  12500 ! GLA/MIL98 MIL/BOW89
HCN+OH=HNCO+H                   2.0E-03 4.0   1000 ! GLA/MIL98 MIL/BOW89
HCN+OH=NH2+CO                   7.8E-04 4.0   4000 ! GLA/MIL98 MIL/BOW89
HCN+O2 = CN+HO2                 3.0E13  0.00 75100 !          est
HCN+CN=NCCN+H                   1.5E07  1.71  1530 ! GLA/MIL98 NBS92
!
HNC+H = HCN+H                  7.8E13  0.00  3600 !          SUM/NGU98
HNC+O = NH+CO                  4.6E12  0.00  2200 !          DB00
HNC+OH = HNCO+H                 2.8E13  0.00  3700 !          DB00
HNC+CN = NCCN+H                 1.0E13  0.00     0 ! ***       PET/OSA04 est
!
CN+O=CO+N                     1.9E12  0.46   723 ! ***       COB96
CN+OH=NCO+H                    1.0E15 -0.437    0 ! ***       WOO96, DEC03
CN+O2=NCO+O                    7.2E12  0.00  -417 ! ***       CEC05, RIM99
  DUP
CN+O2=NCO+O                   -2.8E17 -2.00     0 ! ***       CEC05, RIM99
  DUP
CN+O2=NO+CO                    2.8E17 -2.00     0 ! ***       CEC05, RIM99
CN+CO2=NCO+CO                   3.7E06  2.16 26900 ! GLA/MIL98 WAN/LIN91
CN+ CH2O = HCN + HCO              4.2E13  0.00     0 !  JPCRD 92
CN+NO = NCO+N                  9.6E13  0.00 42100 ! JPCRD 92
CN+NO2=NCO+NO                   5.3E15 -0.752  344 ! GLA/MIL98 PAR93/CEC05
CN+NO2=CO+N2O                   4.9E14 -0.752  344 ! GLA/MIL98 PAR93/CEC05
CN+NO2=N2+CO2                   3.7E14 -0.752  344 ! GLA/MIL98 PAR93/CEC05
CN+HNO=HCN+NO                   1.8E13  0.0      0 ! GLA/MIL98 NBS92
CN+HONO=HCN+NO2                  1.2E13  0.0      0 ! GLA/MIL98 NBS92
CN+N2O=NCN+NO                   3.8E03  2.6   3700 ! GLA/MIL98 NBS92/WIL95
CN+HNCO=HCN+NCO                  1.0E13  0.      0 ! GLA/MIL98 NBS92 /1.5 ***
CN+NCO=NCN+CO                   1.8E13  0.      0 ! GLA/MIL98 NBS92
!
HNCO+M=CO+NH+M                   1.1E16  0.0  86000 ! GLA/MIL98 MER/HAN89
```

```
   N2/1.5/
HNCO+H=NH2+CO                 3.6E04  2.49  2345 ! ***       CEC05
HNCO+H=NCO+H2                 9.0E07  1.66 13900 ! ***       CEC05
HNCO+O=NCO+OH                 2.2E06  2.11 11430 ! GLA/MIL98 NBS92,CEC05
HNCO+O=NH+CO2                 9.6E07  1.41  8520 ! GLA/MIL98 NBS92,CEC05
HNCO+O=HNO+CO                 1.5E08  1.57 44012 ! GLA/MIL98 HE/LIN92
HNCO+OH=NCO+H2O               3.6E07  1.50  3600 ! ***       WOO/BOW95_HNCO
HNCO+HO2=NCO+H2O2             3.0E11  0   22000 ! GLA/MIL98 JAM est
HNCO+O2=HNO+CO2               1.0E12  0   35000 ! GLA/MIL98 GLA/KRI94
HNCO+NH=NH2+NCO               3.0E13  0   23700 ! GLA/MIL98 JAM lr
HOCN+H=HNCO+H                 3.1E08  0.84  1917 ! ***       DB00
HOCN+H=NH2+CO                 1.2E08  0.61  2076 ! ***       DB00
HOCN+H=H2+NCO                 2.4E08  1.50  6617 ! ***       DB00
HOCN+O=OH+NCO                 1.7E08  1.50  4133 ! ***       DB00
HOCN+OH=H2O+NCO               1.2E06  2.00  -248 ! ***       DB00
HOCN+NH2=NCO+NH3              9.2E05  1.94  3646 ! ***       DB00
!
HCNO=HCN+O                    4.2E31 -6.12 61210 ! ***       DB00 1.0 ATM N2
HCNO+H=HCN+OH                 7.2E10  0.841 8612 ! ***       MIL/GLA03
HCNO+O=HCO+NO                 6.3E13  0.00     0 ! ***       MIL/GLA98
HCNO+OH=CH2O+NO               1.0E12  0.00     0 ! ***       MIL/GLA03   HCOH
HCNO+O=NCO+OH                 7.0E12  0.00     0 ! ***       MIL/GLA03
HCNO+OH=NO+CO+H2              6.5E12  0.00     0 ! ***       MIL/GLA03
HCNO+OH=NCO+H+OH              4.5E12  0.00     0 ! ***       MIL/GLA03
HCNO+OH=NCO+H2O               3.5E12  0.00     0 ! ***       MIL/GLA03
HCNO+OH=HCO+HNO               4.5E12  0.00     0 ! ***       MIL/GLA03
!
NCO+M=N+CO+M                  2.2E14  0.00 54050 ! ***       CEC05
   N2/1.5/
NCO+H=CO+NH                   7.2E13   0    1000 ! ***       CEC05
NCO+O=NO+CO                   2.0E15 -0.50     0 ! ***       GAO/MAC03
NCO+OH=HON+CO                 5.3E12 -0.07  5126 ! ***       DB00
NCO+OH=H+CO+NO                8.3E12 -0.05 18042 ! ***       DB00
NCO+HO2=HNCO+O2               2.0E13  0.00     0 ! 060302    MC liN est
NCO+O2=NO+CO2                 2.0E12   0   20000 ! GLA/MIL98 JAM est
NCO+HCO=HNCO+CO               3.6E13   0       0 ! GLA/MIL98 NBS92
CH2O+NCO=HNCO+HCO             6.0E12   0       0 ! GLA/MIL98 NBS92
NCO+NO=N2O+CO                 4.0E19 -2.19  1743 ! ***       CEC05
NCO+NO=N2+CO2                 1.5E21 -2.74  1824 ! GLA/MIL98 CEC94,COO/HER93
NCO+NO2=CO+NO+NO              2.5E11   0    -707 ! GLA/MIL98 PAR93/WOO94
NCO+NO2=CO2+N2O               3.0E12   0    -707 ! GLA/MIL98 PAR93/WOO94
NCO+HNO=HNCO+NO               1.8E13   0       0 ! GLA/MIL98 NBS92
NCO+HONO=HNCO+NO2             3.6E12   0       0 ! GLA/MIL98 NBS92
NCO+N=N2+CO                   2.0E13   0       0 ! GLA/MIL98 JAM est
NCO+NH3 = HNCO+NH2            2.8E04  2.48   980 ! ***       BEC/WIE97
NCO+NCO=CO+CO+N2              1.8E13   0       0 ! GLA/MIL98 NBS92
!
H2CN=HCN+H                    0.4E29 -6.03 29897 ! ***       DB00 0.03 ATM N2
H2CN+H=HCN+H2                 2.4E08  1.50  -894 ! ***       DB00
H2CN+O=HCN+OH                 1.7E08  1.50  -894 ! ***       DB00
H2CN+OH=HCN+H2O               1.5E19 -2.18  2166 ! ***       DB00 1 ATM N2 !
```

```
DUPLICATE
H2CN+OH=HCN+H2O                 1.2E06  2.00 -1192 ! ***       DB00
DUPLICATE
H2CN+O2=CH2O+NO                 3.0E12  0.00  5961 ! ***       DB00
H2CN+NH2=HCN+NH3                9.2E05  1.94 -1152 ! ***       DB00
!
HCNH=HCN+H                    6.1E28 -5.69 24271 ! ***       DB00  1 ATM N2 !
!
HCNH+H=H2CN+H                  2.0E13  0.00     0 ! ***       DB00
HCNH+H=HCN+H2                  2.4E08  1.50  -894 ! ***       DB00
HCNH+O=HNCO+H                  7.0E13  0.00     0 ! ***       DB00
HCNH+O=HCN+OH                  1.7E08  1.50  -894 ! ***       DB00
HCNH+OH=HCN+H2O                 1.2E06  2.00 -1192 ! ***       DB00
!
NH3+M=NH2+H+M                  2.2E16   0   93470 ! GLA/MIL98 DAV/HAN90
NH3+H=NH2+H2                  6.4E05  2.39 10171 ! GLA/MIL98 MIC/SUT86
NH3+O=NH2+OH                  9.4E06  1.94  6460 ! GLA/MIL98 SUT/KLE90
!NH3+O=NH2+OH 2.8E02 3.290 4471 ! KLIMIC09 1.3.9 from klip
NH3+OH=NH2+H2O                 2.0E06  2.04   566 ! GLA/MIL98 SAL/HAN84
NH3+HO2=NH2+H2O2                3.0E11   0   22000 ! GLA/MIL98 JAM est
!
NH2+H=NH+H2                   4.0E13   0    3650 ! GLA/MIL98 DAV/HAN90
NH2+O=HNO+H                   6.6E14 -0.5      0 ! GLA/MIL98 DRA/WAG84,JAM est
NH2+O=NH+OH                   6.8E12   0       0 ! GLA/MIL98 DRA/WAG
NH2+OH=NH+H2O                  4.0E06  2.0   1000 ! GLA/MIL98 JAM est
!NH2+OH=NH+H2O 3.3E06 1.949 -217 ! KLIMIC09,adj from Klip 1.3.8
NH2+HO2=H2NO+OH                 5.0E13   0       0 ! GLA/MIL98 JAM est
NH2+HO2=NH3+O2                 9.2E05  1.94 -1152 !          DB  96UPDATE
NH2+O2=H2NO+O                  2.5E11  0.48 29586 !          DB  96 UPDATE
!NH2+O2=H2NO+O 2.6E11 0.4872 29050 ! pw 1.3.15 mech
NH2+O2=HNO+OH                  6.2E07  1.23 35100 !          DB  96 UPDATE
!NH2+O2=HNO+OH 2.9E-2 3.764 18185 ! pw mech 1.3.16
NH2+NH2=NH3+NH                 5.0E13   0   10000 ! GLA/MIL94 DAV/HAN90
NH2+NH=NH3+N                  9.2E05  1.94  2444 !          DB ABSTR 96
NH2+N =N2+H+H                 7.0E13   0       0 ! GLA/MIL98 WHY/PHI83
NH2+NO=N2+H2O                  2.8E20 -2.654 1258 ! MIL/GLA99 MIL/GLA99
!NH2+NO=NNH+OH                  2.3E10  0.425 -814 ! MIL/GLA99 MIL/GLA99
NH+O=NO+H                    9.2E13   0       0 ! GLA/MIL98 CEC94
N2O(+M)=N2+O(+M)              9.9E+10   0.00      57960       ! 59a      baulcH
   LOW /6.62E+14 0 57500/                                 ! 59b      baulcH 6.62E+14 cOrrect
   O2/1.4/ N2/1.7/ H2O/12.0/ NO/3.0/ N2O/3.5/                  !         KONNOv
N2O+OH=HO2+N2                            2.00E+12   0.00      40000       ! 66      mev
NH2+NO=NNH+OH 3.1E13 -0.48 1180 ! MILKLI00,fit from Klip, 1.3.11
N+OH=NO+H     3.8E+13    0.0        0.0
NH2+NO2=N2O+H2O                 1.6E16 -1.44   268 ! MIL/GLA99 PAR/LIN97
NH2+NO2=H2NO+NO                 6.5E16 -1.44   268 ! MIL/GLA99 PAR/LIN97
!NH2+HNO=NH3+NO                 3.6E06  1.63 -1250 ! GLA/MIL98 LIN96
!NH2+HONO=NH3+NO2                  7.1E01  3.02 -4940 ! GLA/MIL98 LIN96
!
!NH+H=N+H2                    3.0E13   0       0 ! GLA/MIL98 DAV/HAN90,rv
NH+H=N+H2                   1E14   0       0 !
```

```
NH+OH=HNO+H                 2.0E13   0       0 ! GLA/MIL98 JAM est
!NH+OH=HNO+H 3.2E14 -0.376 -46 ! KLIMIC09 1.3.10 from klip
NH+OH=N+H2O                 5.0E11  0.5   2000 ! GLA/MIL98 JAM est
!NH+OH=N+H2O 1.6E07 1.733 -576 ! KLIMIC09 from Klip 1.3.8
NH+O2=HNO+O                 4.6E05  2.0   6500 ! GLA/MIL98 MIL/MEL92
!NH+O2=NO+OH                 1.3E06  1.5    100 ! GLA/MIL98 MIL/MEL92
NH+O2=NO+OH                 7.6E10   0    1530 ! GLA/MIL98 MIL/MEL92
NH+NH=N2+H+H                2.5E13   0       0 ! GLA/MIL98 JAM est
!NH+NH=N2+H+H                5.1E13   0       0 ! Hanson
NH+N=N2+H                 3.0E13   0       0 ! GLA/MIL98 JAM est
!NH+NO=N2O+H                2.9E14 -0.4      0 ! GLA/MIL98 MIL/MEL92
!DUP
!NH+NO=N2O+H               -2.2E13 -0.23     0 !
!DUP
NH+NO=N2+OH                 2.2E13 -0.23     0 ! GLA/MIL98 MIL/MEL92
!NH+NO=N2+OH 2.7E12 -0.0721 -512 ! pw mech 1.2.17
NH+NO2=N2O+OH                1.0E13   0       0 ! GLA/MIL98 HAR/PHI86
!NH+HONO=NH2+NO2                1.0E13   0       0 ! GLA/MIL96 JAM est
!
!N+OH=NO+H                 3.8E13   0       0 ! GLA/MIL98 FLO/HAN77,HOW/SMI80
!N+O2=NO+O                 6.4E09  1.0   6280 ! GLA/MIL98 BAU/DRY73
!N+NO=N2+O                 3.3E12  0.3      0 ! GLA/MIL98 LEEDS,MONAT
!
H2NO+M=HNO+H+M                  2.8E24 -2.83 64915 ! MIL/GLA99 DEA/BOZ00
  H2O/10/
H2NO+M=HNOH+M                  1.1E29 -4.0  44000 ! MIL/GLA99 DEA/BOZ00
  H2O/10/
H2NO+H=HNO+H2                3.0E07  2.0   2000 ! GLA/MIL98 JAM est
H2NO+H=NH2+OH                5.0E13   0       0 ! GLA/MIL98 JAM est
H2NO+O=HNO+OH                3.0E07  2.0   2000 ! GLA/MIL98 JAM est
H2NO+OH=HNO+H2O                2.0E07  2.0   1000 ! GLA/MIL98 JAM est
H2NO+HO2=HNO+H2O2                  2.9E04  2.69  1600 ! MIL/GLA99 DEA/BOZ00
H2NO+O2=HNO+HO2                3.0E12  0.0  25000 ! MIL/GLA99 JAM est
H2NO+NO=HNO+HNO                2.0E04  2.0  13000 ! GLA/MIL98 JAM est
H2NO+NH2=HNO+NH3                3.0E12  0.0   1000 ! GLA/MIL98 JAM est
H2NO+NO2=HONO+HNO                 6.0E11  0.00  2000 ! GLA/MIL98 JAM est
!
HNOH+M=HNO+H+M                  2.0E24 -2.84 58934 ! MIL/GLA99 DEA/BOZ00
  H2O/10/
HNOH+H=NH2+OH                4.0E13  0.0      0 ! MIL/GLA99 DEA/BOZ00
HNOH+H=HNO+H2                4.8E08  1.5    378 ! MIL/GLA99 DEA/BOZ00
HNOH+O=HNO+OH                7.0E13  0.0      0 ! MIL/GLA99 DEA/BOZ00
DUP
HNOH+O=HNO+OH                3.3E08  1.5   -358 ! MIL/GLA99 DEA/BOZ00
DUP
HNOH+OH=HNO+H2O                2.4E6   2.0  -1192 ! MIL/GLA99 DEA/BOZ00
HNOH+HO2=HNO+H2O2                2.9E4   2.69 -1600 ! MIL/GLA99 DEA/BOZ00
HNOH+O2=HNO+HO2                3.0E12  0.0  25000 ! MIL/GLA99 JAM est
HNOH+NH2=NH3+HNO                1.8E6   1.94 -1152 ! MIL/GLA99 DEA/BOZ00
HNOH+NO2=HONO+HNO                 6.0E11  0.0   2000 ! MIL/GLA99 JAM est
!
```

```
!HNO+H=NO+H2                    4.4E11  0.72   650 ! GLA/MIL98 SOT/PAG92
!HNO+O=NO+OH                     2.3E13   0      0 !          INO/WAS99
!HNO+OH=NO+H2O                    3.6E13   0      0 ! GLA/MIL98 BAU73
HNO+O2=HO2+NO                     2.2E10  0.0  3000 ! GLA/ALZ03 DEA/BOZ00
!HNO+O2=HO2+NO                    2.0E13  0.0  16000 ! GLA/ALZ03 DEA/BOZ00!
!HNO+NO2=HONO+NO                    6.0E11  0.00  2000 ! GLA/MIL98 NBS91
!HNO+HNO=N2O+H2O                   9.0E08  0    3100 ! GLA/MIL98 NBS91
HCO+HNO=NO+CH2O                    6.0E11  0.00  2000 ! GLA/MIL98 NBS91
!
HON+M=NO+H+M                     5.1E19 -1.73 16045 ! ***       DB M=N2
    AR/0.7/  H2O/7.0/  CO2/2.0/
HON+H=HNO+H                     2.0E13  0.00     0 ! ***       DB
HON+H=OH+NH                     2.0E13  0.00     0 ! ***       DB
HON+O=OH+NO                     7.0E13  0.00     0 ! ***       DB
HON+OH=HONO+H                    4.0E13  0.00     0 ! ***       DB
HON+O2=NO2+OH                    1.0E12  0.00  4968 ! ***       DB
!
!H+NO(+M)=HNO(+M)                    1.5E15 -0.41     0 !         NBS91
!   LOW/2.3E14 0.206 -1550/                          !         RIL/FON03
!   LOW/4.0E20 -1.75 0/                            !       GLA/OST98
!   N2/1/ H2O/10/  O2/1.5/ H2/2/ CO2/3/
!NO+O(+M)=NO2(+M)                  1.3E15 -0.75     0 !          YAR/SUT91,NBS91
!   LOW/7.5E19 -1.41 0/                            !
!   N2/1.7/  O2/1.5/  H2O/10/
!NO+OH(+M)=HONO(+M)                    2.0E12 -0.05  -721 ! GLA/MIL98 NBS91
!   LOW/5.0E23 -2.51 -68/
!   N2/1.0/  O2/1.0/  H2O/6.7/ AR/0.67/
!NO+HO2=NO2+OH                   2.1E12   0    -480 ! GLA/MIL98 HOW80
HCO+NO=HNO+CO                   7.0E13 -0.40     0 ! GLA/ALZ03 VEY/LES81
!
HONO+H=HNO+OH                    5.6E10  0.86  5000 !          HSU/MEL97
HONO+H=NO+H2O                    8.1E06  1.89  3850 !          HSU/MEL97
!HONO+O=NO2+OH                    1.2E13  0.0   6000 ! GLA/MIL98 NBS91
!HONO+OH=NO2+H2O                   4.0E12   0      0 ! GLA/MIL98 BUR/RAV92
!HONO+HONO=NO+NO2+H2O                 3.5E-1  3.64 12100 !          MEB/MEL98
!
!NO2+H=NO+OH                     1.3E14   0     362 ! ***b2***  KO/FON91
!NO2+O=NO+O2                    3.9E12   0    -238 ! GLA/MIL98 NBS91
NO2+O(+M)=NO3(+M)               1.3E13  0.00     0 ! GLA/MIL98 NBS91
   LOW/1.0E28 -4.08 2470/
   N2/1.5/ O2/1.5/ H2O/10/
!NO2+HO2=HONO+O2                   6.3E08  1.25  5000 ! GLA/ALZ03 HOR/WES98
!NO2+H2=HONO+H                   4.5E12   0   27600 !          PAR/LIN98
!NO2+NO2=NO+NO+O2                  1.6E12   0   26123 ! GLA/MIL98 NBS91
NO2+NO2=NO3+NO                   9.6E09  0.73 20900 ! GLA/MIL98 NBS91
CO+NO2=CO2+NO                   9.0E13  0.00 33800 ! GLA/MIL98 NBS91
HCO+NO2=CO+NO+OH                  1.2E23 -3.29  2355 !          NBS91,RIM/HER98
HCO+NO2=H+CO2+NO                  8.4E15 -0.75  1930 ! GLA/MIL98 NBS91
!
NO3+H=NO2+OH                    6.0E13  0.0      0 ! GLA/MIL98 BEC/SCH92
NO3+O=NO2+O2                    1.0E13  0.0      0 ! GLA/MIL98 ATK/TRO92
```

```
NO3+OH=NO2+HO2                  1.4E13  0.0     0 ! GLA/MIL98 ATK/TRO92
NO3+HO2=NO2+O2+OH               1.5E12  0.0     0 ! GLA/MIL98 BEC/SCH92
NO3+NO2=NO+NO2+O2               5.0E10  0.00  2940 ! GLA/MIL98 DEM/RAV90
!
NNH=N2+H                        6.5E07  0.0     0 ! MIL/GLA99 MIL/GLA99
NNH+H=N2+H2                     1.0E14   0      0 ! GLA/MIL98 JAM est
NNH+O=N2O+H                     1.0E14   0      0 ! GLA/MIL98 JAM est
!NNH+O=N2O+H 1.9E14 -0.274 -22 ! pw mech 1.3.19
!NNH+O=N2+OH                    8.0E13   0.0    0 !         JAM est
NNH+O=N2+OH 1.2E13 0.145 -217 ! pw mech 1.3.18
!NNH+O=NH+NO                    5.0E13   0.0    0 !         JAM&CFM 24TH
NNH+O=NH+NO 5.2E11 0.381 -409 ! pw mech 1.3.20
NNH+OH=N2+H2O                   5.0E13   0      0 ! GLA/MIL98 JAM est
NNH+O2=N2+HO2                   2.0E14   0      0 ! GLA/MIL98 MIL/GLA96
!NNH+O2=N2+HO2 5.6E14 -0.385 -13 ! pw 1.3.14
NNH+O2=N2+H+O2                  5.0E13   0      0 ! GLA/MIL98 MIL/GLA96
NNH+NH =N2+NH2                  5.0E13   0      0 ! GLA/MIL98 JAM est
NNH+NH2=N2+NH3                  5.0E13   0      0 ! GLA/MIL98 JAM est
NNH+NO=N2+HNO                   5.0E13   0      0 ! GLA/MIL98 JAM est
!
!N2O(+M)=N2+O(+M)               1.3E12   0   62570 !         JOH/GLA92,ROH/HAN96
!   LOW/4.0E14 0 56600/
!   N2/1.7/ O2/1.4/ CO2/3.0/ H2O/12/   !
!N2O+H=N2+OH                    3.3E10   0    4729 ! GLA/MIL98 MAR/FON87
!DUP
!N2O+H=N2+OH                    4.4E14   0   19254 !
!DUP
!N2O+O=NO+NO                    9.2E13  0.0  27679 !         MEA/AND00
!N2O+O=N2+O2                    3.7E12  0.0  15936 !         MEA/AND00
!N2O+OH=N2+HO2                  1.3E-2  4.72 36560 ! GLA/MIL98 MEB/LIN96
!N2O+OH=HNO+NO                  1.2E-4  4.33 25080 ! GLA/MIL98 MEB/LIN96
!N2O+NO=NO2+N2                  5.3E05  2.23 46280 ! GLA/MIL98 MEB/LIN96
CO+N2O=N2+CO2                   2.7E11   0   20237 ! GLA/MIL98 NBS91
!
NCCN+M=CN+CN+M                  1.1E34 -4.32 130079 ! ***      DB00 M=AR
     N2/1.5/  O2/1.5/  H2/1.5/  H2O/10./   CO2/3.0/
NCCN+O=CN+NCO                   4.6E12  0.0   8880 ! GLA/MIL98 LOU/HAN84
NCCN+OH=CN+HOCN                 1.9E11  0.0   2900 ! GLA/MIL98 PHI79
!
!NO2+OH(+M)=HONO2(+M)                   2.4E13   0   0 ! TSA91
!   LOW /6.4E32 -5.49 2351/
!   N2/1.0/ AR/0.7/ H2O/6/   !
!
  !*********************************************
  ! *   OH* reaCtiONs                    *
  !*********************************************
H+O+M=M+OH* 1.50e+13 0.0 5.975e3
H2/ 1/ H2O/ 6.5/ O2/ 0.4/ N2/ 0.4/ AR/ 0.35/
OH*+H2O=OH+H2O 5.930e+12 0.5 -8.60e2
OH*+H2=OH+H2 2.950e+12 0.5 -4.44e2
OH*+N2=OH+N2 1.080e+11 0.5 -1.242e3
```

```
OH*+OH=OH+OH 6.010e+12 0.5 -7.64e2
OH*+H=OH+H 1.310e+12 0.5 -1.67e2
OH*+AR=OH+AR 1.690e+12 0.0 4.135e3
OH*+O2=OH+O2 2.100e+12 0.5 -4.78e2
OH*+CO2=OH+CO2 2.750e+12 0.5 -9.68e2
OH*+CO=OH+CO 3.230e+12 0.5 -7.87e2
!OH*+CH4=OH+CH4 3.360e+12 0.5 -6.35e2
N2O+H=OH*+N2                1.60E+14   0.00     50300      ! 30      Hidaka J. pHy. CHEM., 89,
4903
!
!************************NO2 reactiONs**********************
!! NOX CHeMiStry frOM SivaraMakriSHNaN et al. PHyS. CHeM. CHeM. PHyS., 2007, 9,
42304244
N2+M = N+N+M  1.890e+18  -0.85  224950.0   !(HOri 88     )
H2O/16.25/
N+O+M = NO+M       7.600e+14  -0.10   -1770.0   !(COHeN 91    )
H2O/16.25/
NO+HO2 = NO2+OH       2.100e+12   0.00    -480.0   !(glarbOrg94  )
NO+OH(+M) = HONO(+M)          1.990e+12  -0.05    -721.0   !(tSaNg HerrON 91)
LOW / 5.080e+23 -2.51 -67.6 /
TROE /0.62 10.0 100000.0 /
H2O/10.0/ O2/2.0/ H2/2.0/
NO2+H2 = HONO+H       1.300E+04   2.760    29770 ! Par LIN
NO2+H = NO+OH       1.310e+14   0.00     362.0   ! kO/fONtijN
!NO2+O = NO+O2       1.000e+13   0.00     600.0   !(glarbOrg94  ) original value
NO2+O=NO+O2          3.91E+12  0.00       -238 !          Konnov
NO2+M = NO+O+M  1.100e+16   0.00   66000.0   !(Mb89        )
H2O/16.25/
NO2+NO2 = NO+NO+O2  2.000e+12   0.00   26825.0   !(zabarNiC 92 )
!NO2+HO2 = HONO+O2       3.150e+08   1.25    5000.0   !(HOri/MariNOv 98/2)
 NO2+HO2 = HONO+O2       1.910E+00   3.32    3044 ! RAS/GLA07a
NO2+OH(+M) = HONO2(+M)        2.410e+13   0.00       0.0   !(tSaNg HerrON 91)
LOW / 6.420e+32  -5.49   2352.0/
TROE/0.525  1e-15  1e-15  1e+15/
NO2+NO = N2O+O2       1.000e+12   0.00   60000.0   !(zabarNiC 92 )
HONO+O = NO2+OH       1.200e+13   0.0     6000.0   !(glarbOrg94  )
HONO+OH = NO2+H2O       1.300e+10   1.00     135.0   !(glarbOrg94  )
HONO+HONO = H2O+NO+NO2    3.490e-01   3.64   12140.0   !98Mebel/liN/MeliuS
HNO+O = NO+OH       1.000e+13   0.0        0.0   !(glarbOrg94  )
HNO+OH = NO+H2O       3.600e+13   0.00       0.0   !(Mb89        )
HNO+NO2 = NO+HONO      4.420e+04   2.6     4060.0   !(Mebel 98)
HNO+HNO = N2O+H2O       3.950e+12   0.00    5000.0   !(Mb89*       )
HNO+NO = N2O+OH       2.000e+12   0.00   26000.0   !(Mb89*       )
N+NO2 = N2O+O       1.800e+12   0.0        0.0   !(jpl 90      )
N+O2 = NO+O       6.400e+09   1.00    6280.0   !(Mb89        )
!N2O+OH = N2+HO2       2.000e+12   0.00   40000.0   !rutar96
!N2O+H = N2+OH       2.079e-06   5.557   1820.0   !(COMb3       )
!N2O+M = N2+O+M  3.000e+14   0.00   55500.0   !(MiCHael 92  )
!H2O/16.25/
!N2O+O = N2+O2       1.400e+12   0.00   10800.0   !(glarbOrg 94 )
!N2O+O = NO+NO       2.900e+13   0.00   23150.0   !(glarbOrg94  )
```

```
N2O+N = N2+NO       1.000e+13   0.00   19870.0   !(publiC     )
N2O+NO = NO2+N2       5.300e+05   2.23   46281.0   !beNdtSeN
H2NO+M = H2+NO+M      7.830e+27  -4.29   60300.0   !kONNOv 0.5
H2O/10.0/
!H2NO+M = HNO+H+M      2.800e+24  -2.83   64915.0   !kONNOv 0.5
!H2O/10.0/
!H2NO+HO2 = HNO+H2O2       2.900e+04   2.69   -1600.0   !kONNOv 0.5
!H2NO+O2 = HNO+HO2       3.000e+12   0.0    25000.0   !kONNOv 0.5
!H2NO+H = HNO+H2       3.000e+07   2.00    2000.0   !(glarbOrg94  )
!H2NO+O = HNO+OH       3.000e+07   2.00    2000.0   !(glarbOrg94  )
!H2NO+OH = HNO+H2O       2.000e+07   2.00    1000.0   !(glarbOrg94  )
!H2NO+NO = HNO+HNO       2.000e+04   2.0    13000.0   !(glarbOrg94  )
HO2+NO+M = HONO2+M       2.230e+12  -3.5     2200.0   !r45
HNO2+H = NO2+H2                      .240e+09   1.50    5087.0
HNO2+O = NO2+OH                      .170e+09   1.50    3020.0
HNO2+OH = NO2+H2O                     .120e+07   2.00    -596.0
HNO2 = HONO                         .130e+30  -5.47   52814.0   !deaN 1997
HONO+NH2 = NO2+NH3       7.110e+01   3.02   -4941.0   ! beNdtSeN
!HONO+NH = NH2+NO2       1.000e+13   0.0        0.0
!HNO+NH2 = NO+NH3       2.000e+13   0.00    1000.0   !(Mb89       )
HNO+N = NO+NH       1.000e+13   0.00    1990.0   !(90Mar/brO   )
!NH+OH = HNO+H                 2.000e+13     0.0        0.0
!N2O+H = NH+NO                 6.700e+22     -2.16    37155.0
! N2O rEacTIONS
N2O+O=N2+O2                 3.69E+12   0.00     15944      ! 60      MeagHer J. PHys. cHem. a,
2000, 104(25), p 6003.
N2O+O=NO+NO                 9.15E+13   0.00     27693      ! 61      MeagHer J. PHys. cHem. a,
2000, 104(25), p 6003.
!N2O+N=N2+NO                 1.00E+13   0.00     20000      ! 62      KONNOv
!N2O+NO=N2+NO2                2.75E+14   0.00     50000      ! 63      KONNOv
!N2O+H=N2+OH                 2.58E-26   4.39      1455      ! 64      Diau
! NO3 rEacTIONS
NO3=NO+O2                 2.50E+06   0.00     12120      ! 67      KONNOv
!NO3+NO2=NO+NO2+O2             1.20E+11   0.00      3200      ! 68      KONNOv
!NO3+O=NO2+O2               1.02E+13   0.00        0      ! 69      KONNOv
NO3+NO3=NO2+NO2+O2            5.12E+11   0.00      4870      ! 70      KONNOv
! N2O4 rEacTIONS
N2O4(+M)=NO2+NO2(+M)           4.05E+18  -1.10     12840      ! 71      KONNOv
   LOW /1.96E+28  -3.8  12840./
   AR/0.8/ N2O4/2.0/ NO2/2.0/
N2O4+O=N2O3+O2               1.21E+12   0.00        0      ! 72      KONNOv
! N2O3 rEacTIONS
N2O3+O=NO2+NO2               2.71E+11   0.00        0      ! 73      KONNOv
! ENd NOx CHeMiStry****************************************************
END
!
!
!
!HCN             1   569.000     3.630     0.000     0.000     1.000
!HNCO             2   232.400     3.828     0.000     0.000     1.000
!NO             1    97.530     3.621     0.000     1.760     4.000
```

```
!N2O              1   232.400     3.828     0.000     0.000     1.000
!CO              1    98.100     3.650     0.000     1.950     1.800
!CO2              1   244.000     3.763     0.000     2.650     2.100
!HNC              1   569.000     3.630     0.000     0.000     1.000 ! ARtitrARy = HCN
!O2              1   107.400     3.458     0.000     1.600     3.800
!H2              1    38.000     2.920     0.000     0.790   280.000
!AR              0   136.500     3.330     0.000     0.000     0.000
!H              0   145.000     2.050     0.000     0.000     0.000
!O              0    80.000     2.750     0.000     0.000     0.000
!OH              1    80.000     2.750     0.000     0.000     0.000
!HO2              2   107.400     3.458     0.000     0.000     1.000
!H2O              2   572.400     2.605     1.844     0.000     4.000
!H2O2              2   107.400     3.458     0.000     0.000     3.800
!HCO              2   498.000     3.590     0.000     0.000     0.000
!CH2O              2   498.000     3.590     0.000     0.000     2.000
!NO2              2   200.000     3.500     0.000     0.000     1.000
!NH3              2   481.000     2.920     1.470     0.000    10.000
!HNO              2   116.700     3.492     0.000     0.000     1.000
!HON              2   116.700     3.492     0.000     0.000     1.000 ! ARbitrARy = HNO
!HONO              2   232.400     3.828     0.000     0.000     1.000 !=HNNO
!H2NO              2   116.700     3.492     0.000     0.000     1.000 ! JAM
!N              0    71.400     3.298     0.000     0.000     0.000
!NNH              2    71.400     3.798     0.000     0.000     1.000
!NH2              2    80.000     2.650     0.000     2.260     4.000
!NH              1    80.000     2.650     0.000     0.000     4.000
!CN              1    75.000     3.856     0.000     0.000     1.000
!NCO              1   232.400     3.828     0.000     0.000     1.000 ! OIS
!NCCN              1   349.000     4.361     0.000     0.000     1.000 ! ARbitrARy = C2N2
!HOCN              2   232.400     3.828     0.000     0.000     1.000 ! JAM
!HCNO              2   232.400     3.828     0.000     0.000     1.000 ! JAM
!NCN              1   232.400     3.828     0.000     0.000     1.000 ! OIS
!CH              1    80.000     2.750     0.000     0.000     0.000
!H2CN              1   569.000     3.630     0.000     0.000     1.000 ! Os/jM
!HCNH              2   232.400     3.828     0.000     0.000     1.000 ! ARbitrARy = HCNO
!HNOH              2   116.700     3.492     0.000     0.000     1.000 ! JAM
!NO3              2   300.000     3.500     0.000     0.000     1.000 ! NO2 + O
!HONO2              2   300.000     3.500     0.000     0.000     1.000 ! COME NO3
!N2              1    97.530     3.621     0.000     1.760     4.000
```

Mech. 6

```
! Species  24
! Reactions  108
ELEMENTS
C H O N AR
END
SPECIES
OH*  NO N2O O2   H2   AR   H    O    OH   HO2  H2O  H2O2   NO2  NH3  HNO  HONO H2NO N
NNH  NH2  NH   HNOH HONO2 N2
END
```

REACTIONS, A_i ((cm^3/mol)$^{(r-1)}$/s), β_i, E_i (cal/mol)

```
 H+O+M=M+OH* 1.50e+13 0.0 5.975e3
H2/ 1/ H2O/ 6.5/ O2/ 0.4/ N2/ 0.4/ AR/ 0.35/
OH*+H2O=OH+H2O 5.930e+12 0.5 -8.60e2
OH*+H2=OH+H2 2.950e+12 0.5 -4.44e2
OH*+N2=OH+N2 1.080e+11 0.5 -1.242e3
OH*+OH=OH+OH 6.010e+12 0.5 -7.64e2
OH*+H=OH+H 1.310e+12 0.5 -1.67e2
OH*+AR=OH+AR 1.690e+12 0.0 4.135e3
OH*+O2=OH+O2 2.100e+12 0.5 -4.78e2
OH*+CO2=OH+CO2 2.750e+12 0.5 -9.68e2
OH*+CO=OH+CO 3.230e+12 0.5 -7.87e2
N2O+H=OH*+N2                 1.60E+14   0.00      50300       ! 30      Hidaka J. pHy. CHEM., 89,
4903
H+O2(+M)<=>HO2(+M)                          4.650e+012     0.440      0.0
 LOW  /  1.737e+019    -1.230       0.0/
TROE/  6.700e-001  1.000e-030  1.000e+030  1.000e+030/
H2/ 1.30/ CO/ 1.90/ CO2/ 3.80/ HE/ 0.00/ H2O/ 10.00/ AR/ 0.00/ CH4/ 2.00/ C2H6/ 3.00/
H+OH+M<=>H2O+M                              3.500e+022    -2.000       0.0
H2/ 0.73/ H2O/ 3.65/ CH4/ 2.00/ C2H6/ 3.00/ AR/ 0.38/
!....!
 N2O + H <=> N2 + OH                    5.000E+13       0.000          1.520E+04
 N + OH <=> NO + H                    3.800E+13       0.000          0.000E+00
 NO + H (+M) <=> HNO (+M)                 1.500E+15      -0.400          0.000E+00
   LOW  /2.400E+14      0.206         -1.550E+03/
   TROE  /8.2E-01        1.E-30        1.E+30        1.E+30/
 N + NO <=> N2 + O                    2.100E+13       0.000          0.000E+00
 HNO + H <=> NO + H2                    4.400E+11       0.700          6.500E+02
 N2O + H <=> NH + NO                    6.700E+22      -2.160          3.716E+04
 NH + O <=> NO + H                    9.200E+13       0.000          0.000E+00
 N2O (+M) <=> N2 + O (+M)                 9.900E+10       0.000          5.796E+04
   LOW  /6.620E+14      0.000         5.750E+04/
   O2/1.4/ N2/1.7/ H2O/12./ NO/3./ N2O/3.5/
 N2O + OH <=> HO2 + N2                    2.000E+12       0.000          4.000E+04
 NH2 + NO <=> NNH + OH                    3.100E+13      -0.480          1.180E+03
 H + O2 <=> O + OH                    1.040E+14       0.000          1.529E+04
 O + H2 <=> H + OH                    5.080E+04       2.670          6.292E+03
 OH + H2 <=> H + H2O                    4.380E+13       0.000          6.990E+03
 O + H2O <=> OH + OH                    2.970E+06       2.020          1.340E+04
 HO2 + H <=> OH + OH                    7.080E+13       0.000          2.950E+02
```

```
 H2 + O2 <=> H + HO2                    5.180E+05      2.433          5.350E+04
 HO2 + O <=> OH + O2                    3.250E+13      0.000          0.000E+00
 HO2 + OH <=> H2O + O2                   2.460E+13      0.000         -4.970E+02
 HO2 + HO2 <=> H2O2 + O2                  3.660E+14      0.000          1.200E+04
 H2O2 (+H2O) <=> OH + OH (+H2O)               2.000E+12      0.900          4.875E+04
   LOW  /1.870E+25     -2.300        4.875E+04/
   TROE  /5.1E-01       1.E-30        1.E+30/
 H2O2 + H <=> H2O + OH                   2.410E+13      0.000          3.970E+03
 H2O2 + H <=> H2 + HO2                   2.150E+10      1.000          6.000E+03
 H2O2 + O <=> OH + HO2                   9.550E+06      2.000          3.970E+03
 H2O2 + OH <=> H2O + HO2                   1.740E+12      0.000          3.180E+02
DUP
 H2O2 + OH <=> H2O + HO2                   7.590E+13      0.000          7.269E+03
DUP
 NH3 + M <=> NH2 + H + M                  2.200E+16      0.000          9.347E+04
 NH3 + H <=> NH2 + H2                   6.400E+05      2.390          1.017E+04
 NH3 + O <=> NH2 + OH                   9.400E+06      1.940          6.460E+03
 NH3 + OH <=> NH2 + H2O                  2.000E+06      2.040          5.660E+02
 NH3 + HO2 <=> NH2 + H2O2                 3.000E+11      0.000          2.200E+04
 NH2 + H <=> NH + H2                   4.000E+13      0.000          3.650E+03
 NH2 + O <=> HNO + H                   6.600E+14     -0.500          0.000E+00
 NH2 + O <=> NH + OH                   6.800E+12      0.000          0.000E+00
 NH2 + OH <=> NH + H2O                   4.000E+06      2.000          1.000E+03
 NH2 + HO2 <=> H2NO + OH                  5.000E+13      0.000          0.000E+00
 NH2 + HO2 <=> NH3 + O2                  9.200E+05      1.940         -1.152E+03
 NH2 + O2 <=> H2NO + O                  2.500E+11      0.480          2.959E+04
 NH2 + O2 <=> HNO + OH                  6.200E+07      1.230          3.510E+04
 NH2 + NH2 <=> NH3 + NH                  5.000E+13      0.000          1.000E+04
 NH2 + NH <=> NH3 + N                   9.200E+05      1.940          2.444E+03
 NH2 + N <=> N2 + H + H                  7.000E+13      0.000          0.000E+00
 NH2 + NO <=> N2 + H2O                   2.800E+20     -2.654          1.258E+03
 NH + H <=> N + H2                   1.000E+14      0.000          0.000E+00
 NH + OH <=> HNO + H                   2.000E+13      0.000          0.000E+00
 NH + OH <=> N + H2O                   5.000E+11      0.500          2.000E+03
 NH + O2 <=> HNO + O                   4.600E+05      2.000          6.500E+03
 NH + O2 <=> NO + OH                   7.600E+10      0.000          1.530E+03
 NH + NH <=> N2 + H + H                  2.500E+13      0.000          0.000E+00
 NH + N <=> N2 + H                   3.000E+13      0.000          0.000E+00
 NH + NO <=> N2 + OH                   2.200E+13     -0.230          0.000E+00
 NH + NO2 <=> N2O + OH                  1.000E+13      0.000          0.000E+00
 H2NO + M <=> HNO + H + M                  2.800E+24     -2.830          6.492E+04
   H2O/10./
 H2NO + M <=> HNOH + M                   1.100E+29     -4.000          4.400E+04
   H2O/10./
 H2NO + H <=> HNO + H2                  3.000E+07      2.000          2.000E+03
 H2NO + H <=> NH2 + OH                  5.000E+13      0.000          0.000E+00
 H2NO + O <=> HNO + OH                  3.000E+07      2.000          2.000E+03
 H2NO + OH <=> HNO + H2O                  2.000E+07      2.000          1.000E+03
 H2NO + HO2 <=> HNO + H2O2                 2.900E+04      2.690          1.600E+03
 H2NO + O2 <=> HNO + HO2                  3.000E+12      0.000          2.500E+04
 HNOH + M <=> HNO + H + M                  2.000E+24     -2.840          5.893E+04
```

```
   H2O/10./
 HNOH + H <=> NH2 + OH                  4.000E+13      0.000          0.000E+00
 HNOH + H <=> HNO + H2                  4.800E+08      1.500          3.780E+02
 HNOH + O <=> HNO + OH                   7.000E+13      0.000          0.000E+00
DUP
 HNOH + O <=> HNO + OH                   3.300E+08      1.500         -3.580E+02
DUP
 HNOH + OH <=> HNO + H2O                   2.400E+06      2.000         -1.192E+03
 HNOH + NH2 <=> NH3 + HNO                   1.800E+06      1.940         -1.152E+03
 HNO + O2 <=> HO2 + NO                  2.200E+10      0.000          3.000E+03
 HONO + H <=> HNO + OH                   5.600E+10      0.860          5.000E+03
 HONO + H <=> NO + H2O                  8.100E+06      1.890          3.850E+03
 NNH <=> N2 + H                     6.500E+07      0.000          0.000E+00
 NNH + H <=> N2 + H2                  1.000E+14      0.000          0.000E+00
 NNH + O <=> N2O + H                  1.000E+14      0.000          0.000E+00
 NNH + O <=> NH + NO                   5.200E+11      0.381         -4.090E+02
 NNH + OH <=> N2 + H2O                  5.000E+13      0.000          0.000E+00
 NNH + O2 <=> N2 + HO2                  2.000E+14      0.000          0.000E+00
 NNH + O2 <=> N2 + H + O2                  5.000E+13      0.000          0.000E+00
 NNH + NH2 <=> N2 + NH3                   5.000E+13      0.000          0.000E+00
 NNH + NO <=> N2 + HNO                  5.000E+13      0.000          0.000E+00
 NO + HO2 <=> NO2 + OH                  2.100E+12      0.000         -4.800E+02
 NO + OH (+M) <=> HONO (+M)                 1.990E+12      -0.050         -7.210E+02
   LOW  /5.080E+23      -2.510        -6.760E+01/
   TROE  /6.2E-01       1.0E+01       1.00000E+05/
   H2O/10./ O2/2./ H2/2./
 NO2 + H2 <=> HONO + H                  1.300E+04      2.760          2.977E+04
 NO2 + H <=> NO + OH                  1.310E+14      0.000          3.620E+02
 NO2 + O <=> NO + O2                  3.910E+12      0.000         -2.380E+02
 NO2 + M <=> NO + O + M                  1.100E+16      0.000          6.600E+04
   H2O/16.25/
 NO2 + OH (+M) <=> HONO2 (+M)               2.410E+13      0.000          0.000E+00
   LOW  /6.420E+32      -5.490        2.352E+03/
   TROE  /5.25E-01       1.E-15        1.E-15        1.E+15/
 NO2 + NO <=> N2O + O2                  1.000E+12      0.000          6.000E+04
 HONO + OH <=> NO2 + H2O                   1.300E+10      1.000          1.350E+02
 HNO + OH <=> NO + H2O                  3.600E+13      0.000          0.000E+00
 HNO + HNO <=> N2O + H2O                   3.950E+12      0.000          5.000E+03
 HNO + NO <=> N2O + OH                   2.000E+12      0.000          2.600E+04
 N + NO2 <=> N2O + O                  1.800E+12      0.000          0.000E+00
 N + O2 <=> NO + O                  6.400E+09      1.000          6.280E+03
 N2O + NO <=> NO2 + N2                  5.300E+05      2.230          4.628E+04
 HO2 + NO + M <=> HONO2 + M                 2.230E+12      -3.500          2.200E+03
 N2O + O <=> N2 + O2                  3.690E+12      0.000          1.594E+04
END
```

Mech. 7

```
! Species  24
! Reactions  91
ELEMENTS
```

```
C H O N AR HE
END
SPECIES
OH*  NO N2O O2   H2   AR   H    O    OH   HO2  H2O  H2O2   NO2  NH3  HNO  HONO H2NO N
NNH  NH2  NH   HNOH HONO2 N2
END
```

REACTIONS, A_i ((cm^3/mol)$^{(r-1)}$/s), β_i, E_i (cal/mol)

```
H+O+M=M+OH* 1.50e+13 0.0 5.975e3
H2/ 1/ H2O/ 6.5/ O2/ 0.4/ N2/ 0.4/ AR/ 0.35/
OH*+H2O=OH+H2O 5.930e+12 0.5 -8.60e2
OH*+H2=OH+H2 2.950e+12 0.5 -4.44e2
OH*+N2=OH+N2 1.080e+11 0.5 -1.242e3
OH*+OH=OH+OH 6.010e+12 0.5 -7.64e2
OH*+H=OH+H 1.310e+12 0.5 -1.67e2
OH*+AR=OH+AR 1.690e+12 0.0 4.135e3
OH*+O2=OH+O2 2.100e+12 0.5 -4.78e2
OH*+CO2=OH+CO2 2.750e+12 0.5 -9.68e2
OH*+CO=OH+CO 3.230e+12 0.5 -7.87e2
N2O+H=OH*+N2                  1.60E+14   0.00      50300       ! 30       Hidaka J. pHy. CHEM., 89, 4903
H+O2(+M)<=>HO2(+M)                          4.650e+012     0.440       0.0
 LOW  /  1.737e+019    -1.230       0.0/
TROE/  6.700e-001  1.000e-030  1.000e+030  1.000e+030/
H2/ 1.30/ CO/ 1.90/ CO2/ 3.80/ HE/ 0.00/ H2O/ 10.00/ AR/ 0.00/ CH4/ 2.00/ C2H6/ 3.00/
H+OH+M<=>H2O+M                              3.500e+022    -2.000       0.0
H2/ 0.73/ H2O/ 3.65/ CH4/ 2.00/ C2H6/ 3.00/ AR/ 0.38/
!....!
 N2O + H <=> N2 + OH                     5.000E+13       0.000          1.520E+04
 N + OH <=> NO + H                     3.800E+13       0.000          0.000E+00
 NO + H (+M) <=> HNO (+M)                   1.500E+15      -0.400          0.000E+00
   LOW  /2.400E+14      0.206         -1.550E+03/
   TROE  /8.2E-01        1.E-30         1.E+30         1.E+30/
 N + NO <=> N2 + O                     2.100E+13       0.000          0.000E+00
 HNO + H <=> NO + H2                    4.400E+11       0.700          6.500E+02
 N2O + H <=> NH + NO                    6.700E+22      -2.160          3.716E+04
 NH + O <=> NO + H                     9.200E+13       0.000          0.000E+00
 N2O (+M) <=> N2 + O (+M)                  9.900E+10       0.000          5.796E+04
   LOW  /6.620E+14      0.000          5.750E+04/
   O2/1.4/ N2/1.7/ H2O/12./ NO/3./ N2O/3.5/
 NH2 + NO <=> NNH + OH                    3.100E+13      -0.480          1.180E+03
 H + O2 <=> O + OH                     1.040E+14       0.000          1.529E+04
 O + H2 <=> H + OH                     5.080E+04       2.670          6.292E+03
 OH + H2 <=> H + H2O                    4.380E+13       0.000          6.990E+03
 O + H2O <=> OH + OH                    2.970E+06       2.020          1.340E+04
 HO2 + H <=> OH + OH                    7.080E+13       0.000          2.950E+02
 H2 + O2 <=> H + HO2                    5.180E+05       2.433          5.350E+04
 HO2 + O <=> OH + O2                    3.250E+13       0.000          0.000E+00
 HO2 + OH <=> H2O + O2                    2.460E+13       0.000         -4.970E+02
 H2O2 (+H2O) <=> OH + OH (+H2O)                2.000E+12       0.900          4.875E+04
   LOW /1.870E+25      -2.300         4.875E+04/
   TROE  /5.1E-01        1.E-30         1.E+30/
```

```
H2O2 + H <=> H2O + OH                2.410E+13     0.000        3.970E+03
H2O2 + H <=> H2 + HO2               2.150E+10     1.000        6.000E+03
H2O2 + O <=> OH + HO2                9.550E+06     2.000        3.970E+03
H2O2 + OH <=> H2O + HO2               7.590E+13     0.000        7.269E+03
NH3 + M <=> NH2 + H + M               2.200E+16     0.000        9.347E+04
NH3 + H <=> NH2 + H2               6.400E+05     2.390        1.017E+04
NH3 + O <=> NH2 + OH                9.400E+06     1.940        6.460E+03
NH3 + OH <=> NH2 + H2O                2.000E+06     2.040        5.660E+02
NH2 + H <=> NH + H2               4.000E+13     0.000        3.650E+03
NH2 + O <=> HNO + H                6.600E+14    -0.500        0.000E+00
NH2 + OH <=> NH + H2O                4.000E+06     2.000        1.000E+03
NH2 + HO2 <=> H2NO + OH                5.000E+13     0.000        0.000E+00
NH2 + HO2 <=> NH3 + O2                9.200E+05     1.940       -1.152E+03
NH2 + O2 <=> H2NO + O                2.500E+11     0.480        2.959E+04
NH2 + O2 <=> HNO + OH                6.200E+07     1.230        3.510E+04
NH2 + NH2 <=> NH3 + NH                5.000E+13     0.000        1.000E+04
NH2 + NH <=> NH3 + N               9.200E+05     1.940        2.444E+03
NH2 + N <=> N2 + H + H               7.000E+13     0.000        0.000E+00
NH2 + NO <=> N2 + H2O                2.800E+20    -2.654        1.258E+03
NH + H <=> N + H2             1.000E+14     0.000        0.000E+00
NH + OH <=> HNO + H               2.000E+13     0.000        0.000E+00
NH + OH <=> N + H2O               5.000E+11     0.500        2.000E+03
NH + O2 <=> HNO + O               4.600E+05     2.000        6.500E+03
NH + O2 <=> NO + OH               7.600E+10     0.000        1.530E+03
NH + NH <=> N2 + H + H               2.500E+13     0.000        0.000E+00
NH + N <=> N2 + H             3.000E+13     0.000        0.000E+00
NH + NO <=> N2 + OH               2.200E+13    -0.230        0.000E+00
NH + NO2 <=> N2O + OH                1.000E+13     0.000        0.000E+00
H2NO + M <=> HNOH + M                1.100E+29    -4.000        4.400E+04
  H2O/10./
H2NO + H <=> HNO + H2                3.000E+07     2.000        2.000E+03
H2NO + H <=> NH2 + OH                5.000E+13     0.000        0.000E+00
H2NO + OH <=> HNO + H2O                2.000E+07     2.000        1.000E+03
HNOH + H <=> NH2 + OH                4.000E+13     0.000        0.000E+00
HNOH + H <=> HNO + H2                4.800E+08     1.500        3.780E+02
HNOH + NH2 <=> NH3 + HNO                1.800E+06     1.940       -1.152E+03
HNO + O2 <=> HO2 + NO                2.200E+10     0.000        3.000E+03
NNH <=> N2 + H             6.500E+07     0.000        0.000E+00
NNH + H <=> N2 + H2              1.000E+14     0.000        0.000E+00
NNH + O <=> N2O + H              1.000E+14     0.000        0.000E+00
NNH + O <=> NH + NO              5.200E+11     0.381       -4.090E+02
NNH + OH <=> N2 + H2O                5.000E+13     0.000        0.000E+00
NNH + O2 <=> N2 + HO2                2.000E+14     0.000        0.000E+00
NNH + O2 <=> N2 + H + O2                5.000E+13     0.000        0.000E+00
NNH + NH2 <=> N2 + NH3                5.000E+13     0.000        0.000E+00
NNH + NO <=> N2 + HNO                5.000E+13     0.000        0.000E+00
NO + OH (+M) <=> HONO (+M)                1.990E+12    -0.050       -7.210E+02
  LOW  /5.080E+23     -2.510       -6.760E+01/
  TROE  /6.2E-01       1.0E+01       1.00000E+05/
  H2O/10./ O2/2./ H2/2./
NO2 + H <=> NO + OH               1.310E+14     0.000        3.620E+02
```

```
 NO2 + M <=> NO + O + M                  1.100E+16      0.000          6.600E+04
   H2O/16.25/
 NO2 + OH (+M) <=> HONO2 (+M)              2.410E+13      0.000          0.000E+00
   LOW  /6.420E+32      -5.490        2.352E+03/
   TROE  /5.25E-01       1.E-15        1.E-15        1.E+15/
 NO2 + NO <=> N2O + O2                   1.000E+12      0.000          6.000E+04
 HONO + OH <=> NO2 + H2O                   1.300E+10      1.000          1.350E+02
 HNO + OH <=> NO + H2O                   3.600E+13      0.000          0.000E+00
 HNO + HNO <=> N2O + H2O                   3.950E+12      0.000          5.000E+03
 N + NO2 <=> N2O + O                   1.800E+12      0.000          0.000E+00
 N + O2 <=> NO + O                   6.400E+09      1.000          6.280E+03
 HO2 + NO + M <=> HONO2 + M               2.230E+12     -3.500          2.200E+03
 N2O + O <=> N2 + O2                   3.690E+12      0.000          1.594E+04
 N2O + O <=> NO + NO                   9.150E+13      0.000          2.769E+04
NO2+O=NO+O2          3.91E+12  0.00      -238 !
NO + HO2 <=> NO2 + OH                    2.100E+12      0.000         -4.800E+02
END
```

Mech. 8

```
! Species  23
! Reactions  74
ELEMENTS
C H O N AR HE
END
SPECIES
OH*  NO N2O O2   H2   AR   H    O    OH   HO2  H2O  H2O2   NO2  NH3  HNO  HONO H2NO N
NNH  NH2  NH  HONO2 N2
END
```

REACTIONS, A_i ((cm^3/mol)$^{(r-1)}$/s), β_i, E_i (cal/mol)

```
 H+O+M=M+OH* 1.50e+13 0.0 5.975e3
H2/ 1/ H2O/ 6.5/ O2/ 0.4/ N2/ 0.4/ AR/ 0.35/
OH*+H2O=OH+H2O 5.930e+12 0.5 -8.60e2
OH*+H2=OH+H2 2.950e+12 0.5 -4.44e2
OH*+N2=OH+N2 1.080e+11 0.5 -1.242e3
OH*+OH=OH+OH 6.010e+12 0.5 -7.64e2
OH*+H=OH+H 1.310e+12 0.5 -1.67e2
OH*+AR=OH+AR 1.690e+12 0.0 4.135e3
OH*+O2=OH+O2 2.100e+12 0.5 -4.78e2
OH*+CO2=OH+CO2 2.750e+12 0.5 -9.68e2
OH*+CO=OH+CO 3.230e+12 0.5 -7.87e2
N2O+H=OH*+N2                  1.60E+14   0.00      50300       ! 30       Hidaka J. pHy. CHEM., 89,
4903
H+O2(+M)<=>HO2(+M)                          4.650e+012     0.440       0.0
 LOW  /  1.737e+019    -1.230       0.0/
TROE/  6.700e-001  1.000e-030  1.000e+030  1.000e+030/
H2/ 1.30/ CO/ 1.90/ CO2/ 3.80/ HE/ 0.00/ H2O/ 10.00/ AR/ 0.00/ CH4/ 2.00/ C2H6/ 3.00/
H+OH+M<=>H2O+M                           3.500e+022    -2.000       0.0
H2/ 0.73/ H2O/ 3.65/ CH4/ 2.00/ C2H6/ 3.00/ AR/ 0.38/
```

```
!....!
 N2O + H <=> N2 + OH                    5.000E+13     0.000        1.520E+04
 N + OH <=> NO + H                      3.800E+13     0.000        0.000E+00
 NO + H (+M) <=> HNO (+M)               1.500E+15    -0.400        0.000E+00
 LOW  /2.400E+14     0.206        -1.550E+03/
TROE/8.2E-01       1.E-30        1.E+30        1.E+30/
 N + NO <=> N2 + O                      2.100E+13     0.000        0.000E+00
 HNO + H <=> NO + H2                    4.400E+11     0.700        6.500E+02
 N2O + H <=> NH + NO                    6.700E+22    -2.160        3.716E+04
 NH + O <=> NO + H                      9.200E+13     0.000        0.000E+00
 N2O (+M) <=> N2 + O (+M)               9.900E+10     0.000        5.796E+04
 LOW  /6.620E+14     0.000        5.750E+04/
   O2/1.4/ N2/1.7/ H2O/12./ NO/3./ N2O/3.5/
 NH2 + NO <=> NNH + OH                  3.100E+13    -0.480        1.180E+03
 H + O2 <=> O + OH                      1.040E+14     0.000        1.529E+04
 O + H2 <=> H + OH                      5.080E+04     2.670        6.292E+03
 OH + H2 <=> H + H2O                    4.380E+13     0.000        6.990E+03
 O + H2O <=> OH + OH                    2.970E+06     2.020        1.340E+04
 HO2 + H <=> OH + OH                    7.080E+13     0.000        2.950E+02
 H2 + O2 <=> H + HO2                    5.180E+05     2.433        5.350E+04
 HO2 + O <=> OH + O2                    3.250E+13     0.000        0.000E+00
 HO2 + OH <=> H2O + O2                  2.460E+13     0.000       -4.970E+02
 H2O2 (+H2O) <=> OH + OH (+H2O)         2.000E+12     0.900        4.875E+04
 LOW  /1.870E+25     -2.300        4.875E+04/
TROE/5.1E-01       1.E-30        1.E+30/
 H2O2 + H <=> H2 + HO2                  2.150E+10     1.000        6.000E+03
 H2O2 + OH <=> H2O + HO2                7.590E+13     0.000        7.269E+03
 NH3 + M <=> NH2 + H + M                2.200E+16     0.000        9.347E+04
 NH3 + H <=> NH2 + H2                   6.400E+05     2.390        1.017E+04
 NH3 + O <=> NH2 + OH                   9.400E+06     1.940        6.460E+03
 NH3 + OH <=> NH2 + H2O                 2.000E+06     2.040        5.660E+02
 NH2 + H <=> NH + H2                    4.000E+13     0.000        3.650E+03
 NH2 + O <=> HNO + H                    6.600E+14    -0.500        0.000E+00
 NH2 + OH <=> NH + H2O                  4.000E+06     2.000        1.000E+03
 NH2 + HO2 <=> H2NO + OH                5.000E+13     0.000        0.000E+00
 NH2 + HO2 <=> NH3 + O2                 9.200E+05     1.940       -1.152E+03
 NH2 + O2 <=> H2NO + O                  2.500E+11     0.480        2.959E+04
 NH2 + O2 <=> HNO + OH                  6.200E+07     1.230        3.510E+04
 NH2 + NH2 <=> NH3 + NH                 5.000E+13     0.000        1.000E+04
 NH2 + NH <=> NH3 + N                   9.200E+05     1.940        2.444E+03
 NH2 + N <=> N2 + H + H                 7.000E+13     0.000        0.000E+00
 NH2 + NO <=> N2 + H2O                  2.800E+20    -2.654        1.258E+03
 NH + H <=> N + H2                      1.000E+14     0.000        0.000E+00
 NH + OH <=> HNO + H                    2.000E+13     0.000        0.000E+00
 NH + OH <=> N + H2O                    5.000E+11     0.500        2.000E+03
 NH + O2 <=> HNO + O                    4.600E+05     2.000        6.500E+03
 NH + O2 <=> NO + OH                    7.600E+10     0.000        1.530E+03
 NH + NH <=> N2 + H + H                 2.500E+13     0.000        0.000E+00
 NH + N <=> N2 + H                      3.000E+13     0.000        0.000E+00
 NH + NO <=> N2 + OH                    2.200E+13    -0.230        0.000E+00
 NH + NO2 <=> N2O + OH                  1.000E+13     0.000        0.000E+00
```

```
 HNO + O2 <=> HO2 + NO                    2.200E+10      0.000          3.000E+03
 NNH + H <=> N2 + H2                    1.000E+14      0.000          0.000E+00
 NNH + O <=> N2O + H                    1.000E+14      0.000          0.000E+00
 NNH + OH <=> N2 + H2O                    5.000E+13      0.000          0.000E+00
 NNH + O2 <=> N2 + HO2                    2.000E+14      0.000          0.000E+00
 NNH + NH2 <=> N2 + NH3                    5.000E+13      0.000          0.000E+00
 NO + OH (+M) <=> HONO (+M)                    1.990E+12      -0.050          -7.210E+02
 LOW  /5.080E+23      -2.510         -6.760E+01/
TROE/6.2E-01       1.0E+01       1.00000E+05/
   H2O/10./ O2/2./ H2/2./
 NO2 + H <=> NO + OH                    1.310E+14      0.000          3.620E+02
 NO2 + M <=> NO + O + M                    1.100E+16      0.000          6.600E+04
   H2O/16.25/
 NO2 + NO <=> N2O + O2                    1.000E+12      0.000          6.000E+04
 HONO + OH <=> NO2 + H2O                    1.300E+10      1.000          1.350E+02
 HNO + OH <=> NO + H2O                    3.600E+13      0.000          0.000E+00
 N + NO2 <=> N2O + O                    1.800E+12      0.000          0.000E+00
 N + O2 <=> NO + O                    6.400E+09      1.000          6.280E+03
 HO2 + NO + M <=> HONO2 + M                    2.230E+12      -3.500          2.200E+03
NO2+O=NO+O2          3.91E+12  0.00      -238 !
NO + HO2 <=> NO2 + OH                    2.100E+12      0.000          -4.800E+02
END
```

References

[1] T. N. Veziroğlu and S. Şahi̇n, "21st Century's energy: Hydrogen energy system," *Energy Conversion and Management,* vol. 49, pp. 1820-1831, 2008.

[2] J. Noailly and R. Smeets, "Directing technical change from fossil-fuel to renewable energy innovation: An application using firm-level patent data," *Journal of Environmental Economics and Management,* vol. 72, pp. 15-37, 2015.

[3] G. Bölük and M. Mert, "Fossil & renewable energy consumption, GHGs (greenhouse gases) and economic growth: Evidence from a panel of EU (European Union) countries," *Energy,* vol. 74, pp. 439-446, 2014.

[4] N. Muradov and T. Veziroglu, "“Green” path from fossil-based to hydrogen economy: An overview of carbon-neutral technologies," *International Journal of Hydrogen Energy,* vol. 33, pp. 6804-6839, 2008.

[5] P. Tseng, J. Lee, and P. Friley, "A hydrogen economy: opportunities and challenges," *Energy,* vol. 30, pp. 2703-2720, 2005.

[6] W. Wang, J. M. Herreros, A. Tsolakis, and A. P. E. York, "Ammonia as hydrogen carrier for transportation; investigation of the ammonia exhaust gas fuel reforming," *International Journal of Hydrogen Energy,* vol. 38, pp. 9907-9917, 2013.

[7] A. Klerke, C. H. Christensen, J. K. Nørskov, and T. Vegge, "Ammonia for hydrogen storage: challenges and opportunities," *Journal of Materials Chemistry,* vol. 18, p. 2304, 2008.

[8] "Ammonia. (2017, August 2). In Wikipedia, The Free Encyclopedia. Retrieved20:40, August 2, 2017, from https://en.wikipedia.org/w/index.php?title=Ammonia&oldid=793590892," ed.

[9] R. Hattenbach, "“Transportation & Delivery of Anhydrous Ammonia” 2012 Annual NH3 Fuel Conference. [Online]. Available: https://nh3fuel.files.wordpress.com/2012/05/chemicalmarketingservices.pdf. [Accessed 02 October 2016].", 2012.

[10] TogliattiAzot, "“Production,” 2016. [Online]. Available: http://www.toaz.ru/eng/about/production.phtml. [Accessed 10 November 2016].", ed, 2016.

[11] "Elucidare Limited. Ammonia. UK: Elucidare; 2008. http://www.elucidare.co.uk/news/Ammonia%20as%20H2%20carrier.pdf."

[12] C. Zamfirescu and I. Dincer, "Ammonia as a green fuel and hydrogen source for vehicular applications," *Fuel Processing Technology,* vol. 90, pp. 729-737, 2009.

[13] "Gas Turbine Market Size, Report ID: GMI1181, Global Market Insights, Inc. March 2017, https://www.gminsights.com/industry-analysis/gas-turbine-market?utm_source=globenewswire.com&utm_medium=referral&utm_campaign=Paid_Globnewswire."

[14] R. Peterson. *Forecast International, Inc. October 05, 2016, https://globenewswire.com/news-release/2016/10/05/877293/10165484/en/Forecast-International-Predicts-a-World-Market-for-5-480-Industrial-Power-Generating-Gas-Turbine-Engines-Worth-105-Billion-over-the-Next-10-Years.html*.

[15] K. Ryu, G. E. Zacharakis-Jutz, and S.-C. Kong, "Performance characteristics of compression-ignition engine using high concentration of ammonia mixed with dimethyl ether," *Applied Energy,* vol. 113, pp. 488-499, 2014.

[16] A. J. Reiter and S.-C. Kong, "Combustion and emissions characteristics of compression-ignition engine using dual ammonia-diesel fuel," *Fuel,* vol. 90, pp. 87-97, 2011.

[17] A. J. Reiter and S.-C. Kong, "Demonstration of Compression-Ignition Engine Combustion Using Ammonia in Reducing Greenhouse Gas Emissions," *Energy & Fuels,* vol. 22, pp. 2963–2971, 2008.

[18] C. Fenimore and G. Jones, "Oxidation of ammonia in flames," *The Journal of Physical Chemistry,* vol. 65, pp. 298-303, 1961.

[19] D. MacLean and H. G. Wagner, "The structure of the reaction zones of ammonia-oxygen and hydrazine-decomposition flames," in *Symposium (International) on Combustion*, 1967, pp. 871-878.

[20] C. J. Fisher, "A study of rich ammonia/oxygen/nitrogen flames," *Combustion and flame,* vol. 30, pp. 143-149, 1977.

[21] C. Dasch and R. Blint, "A mechanistic and experimental study of ammonia flames," *Combustion Science and Technology,* vol. 41, pp. 223-244, 1984.

[22] J. Vandooren, J. Bian, and P. Van Tiggelen, "Comparison of experimental and calculated structures of an ammonia・ nitric oxide flame. Importance of the NH2+ NO reaction," *Combustion and flame,* vol. 98, pp. 402-410, 1994.

[23] G. G. De Soete, "Overall reaction rates of NO and N2 formation from fuel nitrogen," in *Symposium (international) on combustion*, 1975, pp. 1093-1102.

[24] D. F. Davidson, K. Kohse-Höinghaus, A. Y. Chang, and R. K. Hanson, "A pyrolysis mechanism for ammonia," *International journal of chemical kinetics,* vol. 22, pp. 513-535, 1990.

[25] J. A. Miller and C. T. Bowman, "Mechanism and modeling of nitrogen chemistry in combustion," *Progress in energy and combustion science,* vol. 15, pp. 287-338, 1989.

[26] J. H. Lee, J. H. Kim, J. H. Park, and O. C. Kwon, "Studies on properties of laminar premixed hydrogen-added ammonia/air flames for hydrogen production," *International Journal of Hydrogen Energy,* vol. 35, pp. 1054-1064, 2010.

[27] D. H. Um, J. M. Joo, S. Lee, and O. C. Kwon, "Combustion stability limits and NOx emissions of nonpremixed ammonia-substituted hydrogen–air flames," *International Journal of Hydrogen Energy,* vol. 38, pp. 14854-14865, 2013.

[28] J. H. Lee, S. I. Lee, and O. C. Kwon, "Effects of ammonia substitution on hydrogen/air flame propagation and emissions," *International Journal of Hydrogen Energy,* vol. 35, pp. 11332-11341, 2010.

[29] R. P. Lindstedt, F. C. Lockwood, and M. A. Selim, "Detailed kinetic modelling of chemistry and temperature effects on ammonia oxidation," *Combustion Science and Technology,* vol. 99, pp. 253–76, 1994.

[30] Ø. Skreiberg, P. Kilpinen, and P. Glarborg, "Ammonia chemistry below 1400 K under fuel-rich conditions in a flow reactor," *Combustion and Flame,* vol. 136, pp. 501-518, 2004.

[31] C. Duynslaegher, H. Jeanmart, and J. Vandooren, "Ammonia combustion at elevated pressure and temperature conditions," *Fuel,* vol. 89, pp. 3540-3545, 2010.

[32] A. Hayakawa, T. Goto, R. Mimoto, Y. Arakawa, T. Kudo, and H. Kobayashi, "Laminar burning velocity and Markstein length of ammonia/air premixed flames at various pressures," *Fuel,* vol. 159, pp. 98-106, 2015.

[33] A. A. Konnov, "Implementation of the NCN pathway of prompt-NO formation in the detailed reaction mechanism," *Combustion and Flame,* vol. 156, pp. 2093-2105, 2009.

[34] C. Duynslaegher and H. Jeanmart, "Kinetics in Ammonia-containing Premixed Flames And a Preliminary Investigation of Their Use as Fuel in Spark Ignition Engines," *Combustion science and techanology,* vol. 181, pp. 1092-1106, 2009.

[35] P. Kumar and T. R. Meyer, "Experimental and modeling study of chemical-kinetics mechanisms for H2–NH3–air mixtures in laminar premixed jet flames," *Fuel,* vol. 108, pp. 166-176, 2013.

[36] C. Duynslaegher and H. Jeanmart, "Use of Ammonia as a Fuel for SI engine," in *Proceedings of the European Combustion Meeting* 2009

[37] A. G. Shmakov, O. P. Korobeinichev, I. V. Rybitskaya, A. A. Chernov, D. A. Knyazkov, T. A. Bolshova*, et al.*, "Formation and consumption of NO in H2+O2+N2 flames doped with NO or NH3 at atmospheric pressure," *Combustion and Flame,* vol. 157, pp. 556-565, 2010.

[38] A. Konnov, "Detailed reaction mechanism for small hydrocarbons combustion," *Release 0.5,* 2000.

[39] C. Duynslaegher, H. Jeanmart, and J. Vandooren, "Flame structure studies of premixed ammonia/hydrogen/oxygen/argon flames: Experimental and numerical investigation," *Proceedings of the Combustion Institute,* vol. 32, pp. 1277-1284, 2009.

[40] C. Duynslaegher, F. Contino, J. Vandooren, and H. Jeanmart, "Modeling of ammonia combustion at low pressure," *Combustion and Flame,* vol. 159, pp. 2799-2805, 2012.

[41] Z. Tian, Y. Li, L. Zhang, P. Glarborg, and F. Qi, "An experimental and kinetic modeling study of premixed NH3/CH4/O2/Ar flames at low pressure," *Combustion and Flame,* vol. 156, pp. 1413-1426, 2009.

[42] K. Zhang, Y. Li, T. Yuan, J. Cai, P. Glarborg, and F. Qi, "An experimental and kinetic modeling study of premixed nitromethane flames at low pressure," *Proceedings of the Combustion Institute,* vol. 33, pp. 407-414, 2011.

[43] T. Mendiara and P. Glarborg, "Ammonia chemistry in oxy-fuel combustion of methane," *Combustion and Flame,* vol. 156, pp. 1937-1949, 2009.

[44] O. Mathieu and E. L. Petersen, "Experimental and modeling study on the high-temperature oxidation of Ammonia and related NOx chemistry," *Combustion and Flame,* vol. 162, pp. 554-570, 2015.

[45] V. GRI-Mech. Gas Research Institute, GRI-Mech, Ver. 3.0. < http://www.me.berkely.edu/gri-mech/>. [Online].

[46] F. Vitse, M. Cooper, and G. G. Botte, "On the use of ammonia electrolysis for hydrogen production," *Journal of Power Sources,* vol. 142, pp. 18-26, 2005.

[47] M. Zieba, A. Brink, A. Schuster, M. Hupa, and G. Scheffknecht, "Ammonia chemistry in a flameless jet," *Combustion and Flame,* vol. 156, pp. 1950-1956, 2009.

[48] Coda Zabetta, E., Hupa, M., A Detailed Kinetic Mechanism with Methanol for Simulating Biomass Combustion and N-Pollutants. Combustion and Flame, Volume 152, Issues 1-2, january 2008, Pages 14-27. Åbo Akademi (ÅA) scheme, Åbo Akademi University, https://www.abo.fi/fakultet/ookforskkinetschem [Online]. Available: http://www.abo.fi/fakultet/ookforskkinetschem

[49] N. Sullivan, A. Jensen, P. Glarborg, M. S. Day, J. F. Grcar, J. B. Bell*, et al.*, "Ammonia Conversion and NOx Formation in Laminar Coflowing Nonpremixed Methane-Air Flames," *Combustion and Flame,* vol. 131, pp. 285–298, 2002.

[50] Y. N. Shebeko, A. Trunev, S. Tsarichenko, and A. Zaitsev, "Investigation of concentration limits of flame propagation in ammonia-based gas mixtures," *Combustion, Explosion and Shock Waves,* vol. 32, pp. 477-480, 1996.

[51] M. C. R. U.J Pfahl, J.E Shepherd, "Flammability Limits, Ignition Energy and Flame Speedsin H2-CH4-NH3-N2O-O2-N2 Mixtures," *Combustion and Flame,* vol. 123, pp. 140–158, 2000.

[52] K. Takizawa, A. Takahashi, K. Tokuhashi, S. Kondo, and A. Sekiya, "Burning velocity measurements of nitrogen-containing compounds," *J Hazard Mater,* vol. 155, pp. 144-52, Jun 30 2008.

[53] J. Li, H. Huang, N. Kobayashi, Z. He, Y. Osaka, and T. Zeng, "Numerical study on effect of oxygen content in combustion air on ammonia combustion," *Energy,* vol. 93, pp. 2053-2068, 2015.

[54] C. Brackmann, V. A. Alekseev, B. Zhou, E. Nordström, P.-E. Bengtsson, Z. Li*, et al.*, "Structure of premixed ammonia + air flames at atmospheric pressure: Laser diagnostics and kinetic modeling," *Combustion and Flame,* vol. 163, pp. 370-381, 2016.

[55] H. Nakamura and S. Hasegawa, "Combustion and ignition characteristics of ammonia/air mixtures in a micro flow reactor with a controlled temperature profile," *Proceedings of the Combustion Institute,* vol. 36, pp. 4217-4226, 2017.

[56] G. Ciccarelli, D. Jackson, and J. Verreault, "Flammability limits of NH3–H2–N2–air mixtures at elevated initial temperatures," *Combustion and Flame,* vol. 144, pp. 53-63, 2006.

[57] S. Lee and O. C. Kwon, "Effects of ammonia substitution on extinction limits and structure of counterflow nonpremixed hydrogen/air flames," *International Journal of Hydrogen Energy,* vol. 36, pp. 10117-10128, 2011.

[58] S. Choi, S. Lee, and O. C. Kwon, "Extinction limits and structure of counterflow nonpremixed hydrogen-doped ammonia/air flames at elevated temperatures," *Energy,* vol. 85, pp. 503-510, 2015.

[59] J. M. Joo, S. Lee, and O. C. Kwon, "Effects of ammonia substitution on combustion stability limits and NOx emissions of premixed hydrogen–air flames," *International Journal of Hydrogen Energy,* vol. 37, pp. 6933-6941, 2012.

[60] J. Li, H. Huang, N. Kobayashi, Z. He, and Y. Nagai, "Study on using hydrogen and ammonia as fuels: Combustion characteristics and NOxformation," *International Journal of Energy Research,* vol. 38, pp. 1214-1223, 2014.

[61] A. Ichikawa, A. Hayakawa, Y. Kitagawa, K. D. Kunkuma Amila Somarathne, T. Kudo, and H. Kobayashi, "Laminar burning velocity and Markstein length of ammonia/hydrogen/air premixed flames at elevated pressures," *International Journal of Hydrogen Energy,* vol. 40, pp. 9570-9578, 2015.

[62] H. Nozari and A. Karabeyoğlu, "Numerical study of combustion characteristics of ammonia as a renewable fuel and establishment of reduced reaction mechanisms," *Fuel,* vol. 159, pp. 223-233, 2015.

[63] J. Li, H. Huang, N. Kobayashi, C. Wang, and H. Yuan, "Numerical study on laminar burning velocity and ignition delay time of ammonia flame with hydrogen addition," *Energy,* vol. 126, pp. 796-809, 2017.

[64] P. F. Henshaw, T. D'Andrea, K. R. C. Mann, and D. S. K. Ting, "Premixed Ammonia-Methane-Air Combustion," *Combustion Science and Technology,* vol. 177, pp. 2151-2170, 2005.

[65] A. A. Konnov, I. V. Dyakov, and J. De Ruyck, "Probe Sampling Measurements of No in Ch4+O2+N2flames Doped with Nh3," *Combustion Science and Technology,* vol. 178, pp. 1143-1164, 2006.

[66] B. Li, Y. He, Z. Li, and A. A. Konnov, "Measurements of NO concentration in NH3-doped CH4+air flames using saturated laser-induced fluorescence and probe sampling," *Combustion and Flame,* vol. 160, pp. 40-46, 2013.

[67] E. C. Okafor, Y. Naito, S. Colson, A. Ichikawa, T. Kudo, A. Hayakawa*, et al.*, "Experimental and numerical study of the laminar burning velocity of CH4–NH3–air premixed flames," *Combustion and Flame,* vol. 187, pp. 185-198, 2018.

[68] "Koike M, Miyagawa H, Suzuoki T, Ogasawara K. Ammonia as a hydrogen energy carrier and its application to internal combustion engines," in *Sustainble Vehicle Technologies: Driving the Green Agenda*, ed Gaydon, Warwichshire, UK: Woodhead Publishing Limited, 2012, pp. 61-70.

[69] D. H. Porter, *The Life and Times of Sir Goldsworthy Gurney: Gentleman Scientist and Inventor, 1793-1875*: Lehigh University Press, 1998.

[70] K. E, "Ammonia - a fuel for motor buses," *Journal of the Institute of Petroleum,* vol. 31, pp. 214-223, 1945.

[71] W. T. Verhelsta S, "Hydrogen-fueled internal combustion engines," *Progress in Energy and Combustion Science,* vol. 35, pp. 490-527, 2009.

[72] H. L. Cornelius W, Mitchell H, "Ammonia as an Engine Fuel," *SAE Technical Paper 650052,* pp. 1-27, 1965.

[73] N. H. Starkman ES, Sutton D, Maguire T, Farber L, "Ammonia as a spark ignition fuel: theory and application," *SAE Technical paper 660155,* p. 765, 1966.

[74] D. E. Gray JT, Meckel NT, Quillian RD, "Ammonia fuel-engine compatibility and combustion," *SAE Technical paper 660156,* 1966.

[75] G. C. Pearsall TJ, "Combustion of anhydrous ammonia in diesel engines " *SAE Technical paper 670947,* 1967.

[76] P. P. Bro K, "An experimental investigation of methanol, ethanol, methane and ammoniain DI diesel engine with pilot injection," *SAE Technical paper 770794,* pp. 1-16, 1977.

[77] S.-C. Kong, "Combustion efficiency and exhaust emissions of ammonia combustion in diesel engines. NH3 Fuel Association," ed, 2008.

[78] R. W. Seaman and G. Huson, "The choice of NH3 to fuel the X-15 Rocket plane. [Online] https://nh3fuel.files.wordpress.com/2013/01/2011-seaman-huson.pdf [Accessed 01 May 2016]," ed, 2011.

[79] B. RG, "A proposed Australian transition to an anhydrous ammonia fuel transport economy to replace liquid petroleum fuels," *WIT Transactions on Ecology and the Environment,* vol. 186, pp. 443-456, 2014.

[80] L. WC, "Alaska's renewables-source ammonia fuel energy storage pilot plant: Toward community energy independence," *WIT Transactions on Ecology and the Environment,* p. Art No. 6672979, 2013.

[81] C. Zamfirescu and I. Dincer, "Using ammonia as a sustainable fuel," *Journal of Power Sources,* vol. 185, pp. 459-465, 2008.

[82] S. Frigo and R. Gentili, "Analysis of the behaviour of a 4-stroke Si engine fuelled with ammonia and hydrogen," *International Journal of Hydrogen Energy,* vol. 38, pp. 1607-1615, 2013.

[83] T. D.-K. Liu R, Checkel MD, "Ammonia as a fuel for SI engine," *SAE Technical paper 2003-01-3095,* pp. 1-7, 2003.

[84] W. M. Gong W, "Power system having an ammonia fueled engine," USA Patent US20100019506 A1 2008.

[85] S. Crolius, "“Ammonia Energy,” ACS, 1 November 2016. [Online]. Available: http://www.ammoniaenergy.org/ammonia-powered-internal-combustion-engines/. [Accessed 1 December 2016].", ed.

[86] A. D. Grannell SM, Bohac SV, Gillespie DE, "The operating features of a stoichiometric, ammonia and gasoline dual fuelled spark ignition engine," in *Proceedings of the IMECE*, Chicago, 2006.

[87] A. D. Grannell SM, Bohac S, Gillespie DE, "The fuel mix limits and efficiency of a stoichiometric, ammonia, and gasoline dual fuelled spark ignition engine," *Journal of Engineering for Gas Turbines and Power,* vol. 134, p. 042802, 2008.

[88] "Gillespie DE, Grannell S, Stack C. NH3CAR.com. NH3 Car, 2007. [Online]. Available: www.nh3car.com. [Accessed 2 December 2016].", ed.

[89] K. S.-C. Reiter AJ, "Diese engine operation using ammonia as a carbon-free fuel," in *ASME 2010 Internal Combustion Engine Division Fall Technical Conference ICEF2010*, San Antonio, USA, 2010.

[90] R. Leeladhar, S. Grannell, S. Bohac, and D. Assanis, "Comparison of Ammonia/Gasoline and Ammonia/Ethanol Fuel Mixtures for use in IC Engines, 2007 Annual NH3 Fuel Conference. https://nh3fuelassociation.org/events-conferences/2007-annual-nh3-fuel-conference/," 2007.

[91] J. Ganley, "Increasing the Combustibility of NH3 Fuel. NH3 Fuel Association.," ed, 2010.

[92] G. Shawn, S. Casey, and G. Don, "A Comparison of Combustion Promoters for Ammonia and Two Ways to Run Engines on Ammonia as the Only Fuel. https://nh3fuelassociation.org/events-conferences/2010-nh3-fuel-conference/," in *2010 Annual NH3 Fuel Conference*, 2010

[93] R. K, "Combustion characteristics and exhaust emissions in spark-ignition engine using gasoline-ammonia," *Transactions of the Korean Society of Automotive Engineers,* vol. 21, pp. 155-165, 2013.

[94] H. SO, "Ammonia gasoline fuel blends: feasibility study of commercially available emulsifiers and effects on stabiliyt and engine performance," *SAE Technical paper 2014-01-2759,* 2014.

[95] M. T. Haputhanthri SO, Fleming J, Austin C, "Ammonia and gasoline fuel blends for spark ignited internal combustion engines," *Journal of Energy Resources Technology, Transactions of the ASME,* vol. 137, p. 062201, 2015.

[96] F. J. Haputhanthri SO, Maxwell TT, Austin C, "Ammonia and gasoline fuel blends for internal combustion engines," in *ASME 8th International Conference on Energy Sustainability* Boston, USA, 2014.

[97] T. Brown, "“The AmVeh - an amonia fueled car from South Korea,” NH3 Fuel Association, 20 June 2013. [Online]. Available: https//nh3fuelassociation.org/2013/06/20/the-amveh-an-ammonia-fueled-car-from-south-korea/. [Accessed 1 December 2016].", ed, 2013.

[98] S. Zhong, G. Wan, and L. Yan, "Numerical simulation and analysis of ammonia fuel combustion characteristics," *Neiranji Gongcheng/Chinese Internal Combustion Engine Engineering,* vol. 35, pp. 46-51, 2014.

[99] H. J. Dincer I, Zamfirescu C, *Clean Rail Transportation Options*. Otawa, Canada: Springer International, 2015.

[100] J. Hogerwaard and I. Dincer, "Comparative efficiency and environmental impact assessments of a hydrogen assisted hybrid locomotive," *International Journal of Hydrogen Energy,* vol. 41, pp. 6894-6904, 2016.

[101] C. W. Gross and S. C. Kong, "Permance characteristics of a compression ignition engine using Direct-injection ammonia-DME mixtures," *Fuel,* vol. 103, pp. 1069-1079, 2013.

[102] K. Ryu, G. E. Zacharakis-Jutz, and S.-C. Kong, "Effects of gaseous ammonia direct injection on performance characteristics of a spark-ignition engine," *Applied Energy,* vol. 116, pp. 206-215, 2014.

[103] D. C, *Experimental and numerical study of ammonia combustion*. Leuven: Katholieke Universiteit Leuven 2011.

[104] B. A. Morch CS, Gottrup MP, Sorenson SC, Schramm J, "Ammonia/hydrogen mixtures in a SI engine: Engine performance and analysis of a proposed fuel system," *Fuel,* vol. 90, pp. 854-864, 2011.

[105] S. Frigo and R. Gentili, "Further evolution of an ammonia fuelled range extender for hybrid vehicles. https://nh3fuelassociation.org/events-conferences/2014-nh3-fuel-conference/," in *NH3 Fuel Association*, Des Moines, 2014.

[106] F. S. Comotti M, "Hydrogen generation system for ammonia-hydrogen fuelled internal combustion engines," *International Journal of Hydrogen Energy,* vol. 40, pp. 10673-10686, 2015.

[107] G. R. Frigo S, De Angelis F, "Further insight into the possibility to fuel a SI engine with ammonia plus hydrogen," in *SAE/JSAE 2014 20th Annual Small Engine Technology Conference and Exhibition*, Pisa, Italy, 2014.

[108] G. R. Frigo S, Doveri N, "Ammonia plus hydrogen as fuel in a SI engine: Experimental results," *SAE Technical paper 2012-32-0019,* 2012.

[109] M. F. Ezzat and I. Dincer, "Comparative assessment of two integrated systems with/without fuel cells utilizing liquefied ammonia as a fuel for vehicular applications," *Int J Hydr Energy,* 2017.

[110] F. R. Westlye, A. Ivarsson, and J. Schramm, "Experimental investigation of nitrogen based emissions from an ammonia fueled SI-engine," *Fuel,* vol. 111, pp. 239-247, 2013.

[111] S. S. Gill, G. S. Chatha, A. Tsolakis, S. E. Golunski, and A. P. E. York, "Assessing the effects of partially decarbonising a diesel engine by co-fuelling with dissociated ammonia," *International Journal of Hydrogen Energy,* vol. 37, pp. 6074-6083, 2012.

[112] T. D. Elmøe, R. Z. Sørensen, U. Quaade, C. H. Christensen, J. K. Nørskov, and T. Johannessen, "A high-density ammonia storage/delivery system based on Mg(NH3)6Cl2 for – in vehicles," *Chemical Engineering Science,* vol. 61, pp. 2618-2625, 2006.

[113] C. S. Mørch, A. Bjerre, M. P. Gøttrup, S. C. Sorenson, and J. Schramm, "Ammonia/hydrogen mixtures in an SI-engine: Engine performance and analysis of a proposed fuel system," *Fuel,* vol. 90, pp. 854-864, 2011.

[114] P. DT, "Performance of ammonia fired gas turbine combustors," Report T-9-TS-67-5 Solar, San Diego, USA1967.

[115] S. E. Newhall H, "Theoretical performance of ammonia as a gas turbine fuel," *SAE Technical paper 660768,* 1966.

[116] F. Verkamp, M. Hardin, and J. Williams, "Ammonia combustion properties and performance in gas-turbine burners," in *Symposium (International) on Combustion*, 1967, pp. 985-992.

[117] H. H. Li J, Kobayashi N, He Z, Nagai Y, "Study on using hydrogen and ammonia as fuels: combustion characteristics and NOx formation," *International Journal of Energy Resources,* vol. 38, pp. 1214-1223, 2014.

[118] Z.-J. G. Ryu K, Kong SC, "Performance enhancement of ammonia-fueled engine by using dissociation catalyst for hydrogen generation," *International Journal of Hydrogen Energy,* vol. 39, pp. 2390-2398, 2014.

[119] L. WE, "Ammonia-fueled combustion turbines," ed: NH3 Fuel Association, 2012.

[120] E. B. Karabeyoglu A, "Fuel conditioning system for ammonia fired power plants," ed: NH3 Fuel Association, 2012.

[121] C. D. Balestri M, Cinci V, "Unconventional fuels experimental campaigns in gas turbine combustor at ENEL Sesta Facility," in *ASME Turbo Expo 64047*, Vienna, Austria, 2004.

[122] G. P. Grcar JF, Bell JB, Loren A, Jensen AD, "Effects of mixing on ammonia oxidation in combustion environments at intermediate temperatures," *Proceedings of the Combustion Institute,* vol. 30, pp. 1193-1200, 2003.

[123] E. B. Karabeyoglu A, Stevens J, Cantwell B, "Development of ammonia based fuels for environmentally friendly power generation," in *10th Internatonal Energy Conversion Engineering Conference* Atlanta, USA, 2012.

[124] T. Meyer, P. Kumar, and M. Li, "Ammonia combustion with near-zero pollutant emissions. NH3 Fuel Association, January 2011. [Online]. Available: https://nh3fuel.files.wordpress.com/2013/01/2011-meyer.pdf. [Accessed 12 November 2016].", ed, 2011.

[125] N. Iki, O. Kurata, T. Matsunuma, T. Inoue, M. Suzuki, T. Tsujimura*, et al.*, "Micro Gas Turbine Firing Kerosene and Ammonia," in *ASME Turbo Expo*, 2015.

[126] N. Iki, O. Kurata, T. Matsunuma, and T. Inoue, "“Micro gas turbine operation with kerosene and ammonia,” NH3 Fuel Association, October 2014. [Online]. Available: https://nh3fuel.files.wordpress.com/2014/10/nh3fa-2014-norihiko-iki.pdf. [Accessed 1 November 2016].", ed, 2014.

[127] N. Iki, O. Kurata, T. Matsunuma, and T. Inoue, "Micro gas turbine firing kerosene and ammonia," in *ASME Turbo Expo Code 113665*, Montreal, Canada, 2015.

[128] N. Iki, O. Kurata, T. Matsunuma, and T. Inoue, "Power generation by a micro gas turbine firing kerosene and ammonia," in *International Conference on Power Engineering Code 118770*, Yokohama, Japan, 2015.

[129] K. D. K. A. Somarathne, S. Hatakeyama, A. Hayakawa, and H. Kobayashi, "Numerical study of a low emission gas turbine like combustor for turbulent ammonia/air premixed swirl flames with a secondary air injection at high pressure," *Int J Hydr Energy,* vol. 42, pp. 27388-27399, 2017.

[130] O. Kurata, N. Iki, T. Matsunuma, T. Inoue, T. Tsujimura, H. Furutani*, et al.*, "Performances and emission characteristics of NH 3 –air and NH 3 CH 4 –air combustion gas-turbine power generations," *Proceedings of the Combustion Institute,* vol. 36, pp. 3351-3359, 2017.

[131] O. Kurata, N. Iki, T. Matsunuma, T. Inoue, T. Tsujimura, H. Furutani*, et al.*, "Success of Ammonia-Fired, Regenerator-Heated, Diffusion Combustion Gas Turbine Power Generation and Prospect of Low NOx Combustion With High Combustion Efficiency," presented at the Power Conference, Charlotte, USA.Ref. POWER-ICOPE2017-3277, 2017.

[132] A. Valera-Medina, S. Morris, J. Runyon, D. G. Pugh, R. Marsh, P. Beasley*, et al.*, "Ammonia, Methane and Hydrogen for Gas Turbines," *Energy Procedia,* vol. 75, pp. 118-123, 2015.

[133] S. Ito, S. Kato, T. Saito, T. Fujimori, and H. Kobayashi, "“Development of ammonia / natural gas dual fuel gas turbine combustor,” NH3 Fuel Association, September 2016. [Online]. Available: https://nh3fuelassociation.org/2016/08/22/development-of-ammonia-natural-gas-dual-fuel-gas-turbine-combustor/. [Accessed 29 November 2016].", ed, 2016.

[134] A. Valera-Medina, J. Runyon, D. G. Pugh, P. Beasley, T. Hughes, P. Bowen, "Ammonia-methane combustion in tangential swirl burners for gas turbine power generation," *Applied Energy,* vol. 185, pp. 1362-1371, 2017.

[135] A. Valera-Medina, D. G. Pugh, P. Marsh, G. Bulat, and P. Bowen, "Preliminary study on lean premixed combustion of ammonia-hydrogen for swirling gas turbine combustors," *International Journal of Hydrogen Energy,* vol. 42, pp. 24495-24503, 2017.

[136] A. Hayakawa, Y. Arakawa, R. Mimoto, K. K. A. Somarathne, T. Kudo, and H. Kobayashi, "Experimental investigation of stabilization and emission characteristics of ammonia/air premixed flames in a swirl combustor," *International Journal of Hydrogen Energy,* vol. 42, pp. 14010-14018, 2017.

[137] K. D. K. A. Somarathne, S. Hatakeyama, A. Hayakawa, and H. Kobayashi, "Numerical study of a low emission gas turbine like combustor for turbulent ammonia/air premixed swirl flames with a secondary air injection at high pressure," *International Journal of Hydrogen Energy,* 2017.

[138] ISPT, "Nuon turns Magnum-plant into a sustainable super battery," ISPT, Eemshaven, The Netherlands2016.

[139] "“Decentranlised ammonia production in the Netherlands,” NH3 Fuel Association, September 2016. [Online]. Available: https://nh3fuel.files.wordpress.com/2016/09/hans-vrijenhoef-decentralised-ammonia-production-in-the-netherlands-nh3fa2016.pdf. [Accessed 30 November 2016].", ed.

[140] T. Brown, " “Nuon's Power-to-Ammonia update, and the first European ammonia fuel conference in 2017,” Ammonia Energy, 1 November 2016. [Online]. Available: http://www.ammoniaenergy.org/nuons-power-to-ammonia-update-and-the-first-european-ammonia-fuel-conference-in-2017/. [Accessed 15 November 2016].", ed: Ammonia Energy, 2016.

[141] P. Lavery, "“Nuon and Delft University of Technology start work on “Power to Ammonia” research program,” IFRF, 2 May 2016. [Online]. Available: http://www.mnm.ifrf.net/mnm/article.html?aid=1529. [Accessed 15 June 2016].", ed: IFRF.

[142] T. Brown. (2017). *Chugoku Electric Completes Successful Trial, Seeks Patent for Ammonia Co-Firing Technology*.

[143] B. M. Ganley J, "Engine-ready, carbon free ammonia fuel," ed: NH3 Fuel Association, 2010.

[144] T. GO, "Flame acceleration and the development of detonation in fuel-oxygen mixtures at elevated temperatures and pressures," *Journal of Hazardous Materials,* vol. 163, pp. 783-794, 2009.

[145] O. G. Thomas GO, Bambrey R, "An experimental study of flame acceleration and deflagration to detonation transition in representative process piping," *Process Safety and Environmental Protection,* vol. 88, pp. 75-90, 2010.

[146] S. V. Blinov VN, Kositsin VV, Vavilov IS, Lukyanchik AI, Ruban VI, "Experimental testing of electrothermal microthrusters with autonomous heating elements for orbital maneuvering of small space vehicles," *Indian Journal of Science and Technology,* vol. 9, p. DOI: 10.17485/ijst/2016/v9i19/93912, 2016.

[147] V. N. Blinov, V. V. Shalay, V. V. Kositsin, and I. S. Vavilov, "Design features and studies of ammonia electrothermal microthrusters with tubular heating elements for small space vehicles," *Indian Journal of Science and Technology,,* vol. 9, p. DOI: 10.17485/ijst/2016/v9i19/93893, 2016.

[148] in *Fatuev IY. Acetam - new high-effective fuel. 63rd International Astronautical Congress - paper 8072. Naples, Italy 2012.*

[149] W. Han, S. Shan, and Z. Du, "Calculation of thermodynamic properties for a new propellant acetylene-ammonia," *Chinese Journal of Energetic Materials,* vol. 22, pp. 161-164, 2014.

[150] B. T. Robin MR, Cardiff EH, "An ammonia microresistojet (MRJ) for micro satellites," in *44th AIAA/ASME/SAE/ASEE Joint Propulsion Conference and Exhibit Code 81719*, Hartford, USA, 2008.

[151] H. Teng, "Combustion Modifications of Batch Annealing Furnaces and Ammonia Combustion Ovens for NOX Abatement in Steel Plants," *J Air Waste Manag Assoc,* vol. 46, pp. 1171-1178, Dec 1996.

[152] R. Murai, R. Omori, R. Kano, Y. Tada, H. Higashino, N. Nakatsuka*, et al.*, "The radiative characteristics of NH3/N2/O2 non-premixed flame on a 10 kW test furnace," *Energy Procedia,* vol. 120, pp. 325-332, 2017.

[153] M. A. Mujeebu, M. Z. Abdullah, M. Z. Bakar, A. A. Mohamad, R. M. Muhad, and M. K. Abdullah, "Combustion in porous media and its applications--a comprehensive survey," *J Environ Manage,* vol. 90, pp. 2287-312, Jun 2009.

[154] S.-S. Su, S.-J. Hwang, and W.-H. Lai, "On a porous medium combustor for hydrogen flame stabilization and operation," *International Journal of Hydrogen Energy,* vol. 39, pp. 21307-21316, 2014.

[155] D. B. Ingham and I. Pop, *Transport phenomena in porous media III* vol. 3: Elsevier, 2005.

[156] S. Hinokuma, Y. Kawabata, S. Matsuki, H. Shimanoe, S. Kiritoshi, and M. Machida, "Local Structures and Catalytic Ammonia Combustion Properties of Copper Oxides and Silver Supported on Aluminum Oxides," *The Journal of Physical Chemistry C,* vol. 121, pp. 4188-4196, 2017.

[157] H. Nozari, G. Karaca, O. Tuncer, and A. Karabeyoglu, "Combustion of ammonia-rich NH3-H2-air mixtures: Improvement of flame stability," presented at the 53rd AIAA/SAE/ASEE Joint Propulsion Conference, 2017.

[158] H. Nozari, G. Karaca, O. Tuncer, and A. Karabeyoglu, "Porous medium based burner for efficient and clean combustion of ammonia–hydrogen–air systems," *Int J Hydr Energy,* vol. 42(21), pp. 14775-14785, 2017.

[159] J. M. Simmie, "Detailed chemical kinetic models for the combustion of hydrocarbon fuels," *Progress in Energy and Combustion Science,* vol. 29, pp. 599-634, 2003.

[160] A. Kéromnès, W. K. Metcalfe, K. A. Heufer, N. Donohoe, A. K. Das, C.-J. Sung*, et al.*, "An experimental and detailed chemical kinetic modeling study of hydrogen and syngas mixture oxidation at elevated pressures," *Combustion and Flame,* vol. 160, pp. 995-1011, 2013.

[161] G. Vourliotakis, G. Skevis, M. Founti, Z. Alhamamre, and D. Trimis, "Detailed kinetic modelling of the T-POX reforming process using a reactor network approach," *International Journal of Hydrogen Energy,* vol. 33, pp. 2816-2825, 2008.

[162] S. Rigopoulos and A. Jones, "A hybrid CFD—reaction engineering framework for multiphase reactor modelling: basic concept and application to bubble column reactors," *Chemical Engineering Science,* vol. 58, pp. 3077-3089, 2003.

[163] M. Falcitelli, L. Tognotti, and S. Pasini, "An algorithm for extracting chemical reactor network models from cfd simulation of industrial combustion systems," *Combustion Science and Technology,* vol. 174, pp. 27-42, 2002.

[164] R. J. Kee, J. F. Grcar, M. D. Smooke, J. Miller, and E. Meeks, "PREMIX: a Fortran program for modeling steady laminar one-dimensional premixed flames," *Sandia National Laboratories Report,* 1985.

[165] J. Li, Z. Zhao, A. Kazakov, and F. L. Dryer, "An updated comprehensive kinetic model of hydrogen combustion," *International journal of chemical kinetics,* vol. 36, pp. 566-575, 2004.

[166] A. Konnov and I. Dyakov, "Measurement of propagation speeds in adiabatic flat and cellular premixed flames of C 2 H 6+ O 2+ CO 2," *Combustion and Flame,* vol. 136, pp. 371-376, 2004.

[167] Y. Wang, A. Holley, C. Ji, F. Egolfopoulos, T. Tsotsis, and H. Curran, "Propagation and extinction of premixed dimethyl-ether/air flames," *Proceedings of the Combustion Institute,* vol. 32, pp. 1035-1042, 2009.

[168] R. Design, "CHEMKIN Theory Manual," *San Diego, CA,* 2007.

[169] G. Dixon-Lewis, "Flame structure and flame reaction kinetics. II. transport phenomena in multicomponent systems," in *Proceedings of the Royal Society of London A: Mathematical, Physical and Engineering Sciences*, 1968, pp. 111-135.

[170] J. Hirschfelder, C. Curtiss, and R. Bird, "Molecular Theory of Gases and LiquidsJohn Wiley," *New York,* 1954.

[171] P. Gray and S. Scott, "Autocatalytic reactions in the isothermal, continuous stirred tank reactor: isolas and other forms of multistability," *Chemical Engineering Science,* vol. 38, pp. 29-43, 1983.

[172] A. Abou-Taouk, *Optimization of Chemical Kinetic Mechanisms and Numerical Simulations of Industrial Gas Turbine Burners*: Chalmers University of Technology, 2014.

[173] S. Liu, M. C. Soteriou, M. B. Colket, and J. A. Senecal, "Determination of cup-burner extinguishing concentration using the perfectly stirred reactor model," *Fire Safety Journal,* vol. 43, pp. 589-597, 2008.

[174] V. Fichet, M. Kanniche, P. Plion, and O. Gicquel, "A reactor network model for predicting NOx emissions in gas turbines," *Fuel,* vol. 89, pp. 2202-2210, 2010.

[175] S. A. Drennan, C.-P. Chou, A. F. Shelburn, D. W. Hodgson, C. Wang, C. V. Naik*, et al.*, "Flow field derived equivalent reactor networks for accurate chemistry simulation in gas turbine combustors," *ASME Turbo Expo 2009: Power for Land, Sea, and Air, GT,* vol. 59861, p. 2009, 2009.

[176] R. CHEMKIN-PRO, "15112, Reaction Design," *Inc., San Diego, CA,* 2011.

[177] I. V. Novosselov, P. C. Malte, S. Yuan, R. Srinivasan, and J. C. Y. Lee, "Chemical Reactor Network Application to Emissions Prediction for Industial DLE Gas Turbine," vol. 2006, pp. 221-235, 2006.

[178] P. Glarborg, J. A. Miller, and R. J. Kee, "Kinetic modeling and sensitivity analysis of nitrogen oxide formation in well-stirred reactors," *Combustion and flame,* vol. 65, pp. 177-202, 1986.

[179] T. Turányi, "Applications of sensitivity analysis to combustion chemistry," *Reliability Engineering & System Safety,* vol. 57, pp. 41-48, 1997.

[180] A. Saltelli, M. Ratto, S. Tarantola, and F. Campolongo, "Sensitivity analysis for chemical models," *Chemical reviews,* vol. 105, pp. 2811-2828, 2005.

[181] T. Echekki and E. Mastorakos, *Turbulent combustion modeling: Advances, new trends and perspectives* vol. 95: Springer Science & Business Media, 2010.

[182] R. Zhang, W. Fan, Q. Shi, and W. Tan, "Combustion and emissions characteristics of dual-channel double-vortex combustion for gas turbine engines," *Applied Energy,* vol. 130, pp. 314-325, 2014.

[183] B. Adouane, P. Hoppesteyn, W. de Jong, M. van der Wel, K. R. Hein, and H. Spliethoff, "Gas turbine combustor for biomass derived LCV gas, a first approach towards fuel-NO x modelling and experimental validation," *Applied Thermal Engineering,* vol. 22, pp. 959-970, 2002.

[184] E. R. Hawkes, R. Sankaran, J. C. Sutherland, and J. H. Chen, "Direct numerical simulation of turbulent combustion: fundamental insights towards predictive models," in *Journal of Physics: Conference Series*, 2005, p. 65.

[185] R. Sankaran, E. R. Hawkes, J. H. Chen, T. Lu, and C. K. Law, "Direct numerical simulations of turbulent lean premixed combustion," in *Journal of Physics: conference series*, 2006, p. 38.

[186] V. Sabelnikov and C. Fureby, "LES combustion modeling for high Re flames using a multi-phase analogy," *Combustion and Flame,* vol. 160, pp. 83-96, 2013.

[187] F. F. Grinstein and C. Fureby, "LES studies of the flow in a swirl gas combustor," *Proceedings of the Combustion Institute,* vol. 30, pp. 1791-1798, 2005.

[188] M. Boileau, G. Staffelbach, B. Cuenot, T. Poinsot, and C. Berat, "LES of an ignition sequence in a gas turbine engine," *Combustion and Flame,* vol. 154, pp. 2-22, 2008.

[189] S. Candel, "Combustion dynamics and control: Progress and challenges," *Proceedings of the combustion institute,* vol. 29, pp. 1-28, 2002.

[190] P. Iudiciani, *Swirl stabilized premixed flame analysis using of LES and POD*, 2012.

[191] U. Piomelli, "Large-eddy simulation: achievements and challenges," *Progress in Aerospace Sciences,* vol. 35, pp. 335-362, 1999.

[192] J. Smagorinsky, "General circulation experiments with the primitive equations: I. The basic experiment," *Monthly weather review,* vol. 91, pp. 99-164, 1963.

[193] M. Germano, U. Piomelli, P. Moin, and W. H. Cabot, "A dynamic subgrid-scale eddy viscosity model," *Physics of Fluids A: Fluid Dynamics,* vol. 3, pp. 1760-1765, 1991.

[194] J. Janicka and A. Sadiki, "Large eddy simulation of turbulent combustion systems," *Proceedings of the Combustion Institute,* vol. 30, pp. 537-547, 2005.

[195] P. Givi, "Filtered density function for subgrid scale modeling of turbulent combustion," *AIAA J,* vol. 44, pp. 16-23, 2006.

[196] E. Baudoin, R. Yu, K.-J. Nogenmyr, X.-S. Bai, and C. Fureby, "Comparison of LES models applied to a bluff body stabilized flame," in *47th AIAA Aerospace Sciences Meeting*, 2009.

[197] C. Fureby, "LES of a multi-burner annular gas turbine combustor," *Flow, turbulence and combustion,* vol. 84, pp. 543-564, 2010.

[198] P. Nordin, *Complex chemistry modeling of diesel spray combustion*: Chalmers University of Technology, 2001.

[199] V. Golovitchev and J. Chomiak, "Numerical Modeling of high Temperature Air 'Flameless Combustion,'" in *4th International Symposium on High Temperature Air Combustion and Gasification, Rome, Italy, Nov*, 2001, pp. 27-30.

[200] The High Pressure Combustor Rig at the GTRC http://www.cu-gtrc.co.uk/categories.html?cid=9 [Online].

[201] T. García-Armingol and J. Ballester, "Flame chemiluminescence in premixed combustion of hydrogen-enriched fuels," *International Journal of Hydrogen Energy,* vol. 39, pp. 11299-11307, 2014.

[202] J. Ballester, R. Hernández, A. Sanz, A. Smolarz, J. Barroso, and A. Pina, "Chemiluminescence monitoring in premixed flames of natural gas and its blends with hydrogen," *Proceedings of the Combustion Institute,* vol. 32, pp. 2983-2991, 2009.

[203] J. Ballester and T. García-Armingol, "Diagnostic techniques for the monitoring and control of practical flames," *Progress in Energy and Combustion Science,* vol. 36, pp. 375-411, 2010.

[204] R. Marsh, J. Runyon, A. Giles, S. Morris, D. Pugh, A. Valera-Medina*, et al.*, "Premixed methane oxycombustion in nitrogen and carbon dioxide atmospheres: measurement of operating limits, flame location and emissions. Proceedings of the Combustion Institute," *Proceedings of the Combustion Institute,* 2016.

[205] J. Runyon, R. Marsh, P. Bowen, D. Pugh, A. Giles, S. Morris., " Lean methane flame stability in a premixed generic swirl burner: Isothermal flow and atmospheric combustion characterization," *Experimental Thermal and Fluid Science,* vol. 92, pp. 125-140, 2018.

[206] U. N. UNIDO, *Fertilizer Manual*. The Netherlands: Kluwer Academic Publishers, 1998.

[207] P. M. (2008). *The Coke Oven By-Product Plant* Available: http://www.accci.org/Byproduct.pdf

[208] *IFRF, Combustion Industry News, 2016 [Online] http://www.mnm.ifrf.net/mnm/article.html?aid=1529 [Accessed 25th May 2016]*

[209] D.G. Pugh, P. J . Bowen, R. Marsh, *et al.*, "Dissociative influence of H2O vapour/sprayonlean blowoff and NOx reduction for heavily carbonaceous syngas swirling flames," *Combustion and Flame,* vol. 177, pp. 37-48, 2017.

[210] O. A. Powell, P. Papas, and C. B. Dreyer, "Flame structure measurements of NO in premixed hydrogen–nitrous oxide flames," *Proceedings of the Combustion Institute,* vol. 33, pp. 1053-1062, 2011.

[211] W. Sun, Z. Chen, X. Gou, and Y. Ju, "A path flux analysis method for the reduction of detailed chemical kinetic mechanisms," *Combustion and Flame,* vol. 157, pp. 1298-1307, 2010.

[212] X. Gou, W. Sun, Z. Chen, and Y. Ju, "A dynamic multi-timescale method for combustion modeling with detailed and reduced chemical kinetic mechanisms," *Combustion and Flame,* vol. 157, pp. 1111-1121, 2010.

[213] "Advanced Combustion and Propulsion Lab http://engine.princeton.edu/ (accessed Apr 4, 2016).".

[214] H. Xiao, M. Howard, A. Valera-Medina, S. Dooley, and P. J. Bowen, "Study on Reduced Chemical Mechanisms of Ammonia/Methane Combustion under Gas Turbine Conditions," *Energy & Fuels,* vol. 30, pp. 8701-8710, 2016.

[215] O. Mathieu, M. M. Kopp, and E. L. Petersen, "Shock-tube study of the ignition of multi-component syngas mixtures with and without ammonia impurities," *Proceedings of the Combustion Institute,* vol. 34, pp. 3211-3218, 2013.

[216] G. T. H G Weller, H Jasak, C Fureby, "A tensorial approach to computational continuum mechanics using object-oriented techniques," *COMPUTERS IN PHYSICS,,* vol. 12 pp. 620–631, 1998.

[217] C. Duwig, K.-J. Nogenmyr, C.-k. Chan, and M. J. Dunn, "Large Eddy Simulations of a piloted lean premix jet flame using finite-rate chemistry," *Combustion Theory and Modelling,* vol. 15, pp. 537-568, 2011.

[218] P. Baskar and A. Senthilkumar, "Effects of oxygen enriched combustion on pollution and performance characteristics of a diesel engine," *Engineering Science and Technology, an International Journal,* vol. 19, pp. 438-443, 2016.

[219] S. J. Klippenstein, L. B. Harding, P. Glarborg, and J. A. Miller, "The role of NNH in NO formation and control," *Combustion and Flame,* vol. 158, pp. 774-789, 2011.

[220] P. Dagaut, P. Glarborg, and M. Alzueta, "The oxidation of hydrogen cyanide and related chemistry," *Progress in Energy and Combustion Science,* vol. 34, pp. 1-46, 2008.

[221] J. A. Miller and C. T. Bowman, "Mechanism and modeling of nitrogen chemistry in combustion," *Progress in Energy and Combustion Science* pp. 287–338, 1989.

[222] R. Mével, S. Javoy, F. Lafosse, N. Chaumeix, G. Dupré, and C. E. Paillard, "Hydrogen–nitrous oxide delay times: Shock tube experimental study and kinetic modelling," *Proceedings of the Combustion Institute,* vol. 32, pp. 359-366, 2009.

[223] H. M. David Goodwin, Raymond Speth, "Cantera: An object- oriented software toolkit for chemical kinetics, thermodynamics, and transport processes. http://www.cantera.org, 2016. Version 2.2.1.," ed.

[224] Anders Broe Bendtsen, Peter Glarborg , and K. Dam-Johansen, "Visualization methods in analysis of detailed chemical kinetics modelling," *Computers and Chemistry,* vol. 25, pp. 161 – 170, 2001.

[225] *Jelezniak M., Jelezniak I. Chemked – A Program for Chemical Kinetics of Gas-Phase Reactions. http://www.chemked.com/*.

[226] G. Dayma and P. Dagaut, "Effects of Air Contamination on the Combustion of Hydrogen—Effect of NO and NO2 addition on Hydrogen Ignition and Oxidation Kinetics," *Combustion Science and Technology,* vol. 178, pp. 1999-2024, 2006.

[227] M. Goswami, J. G. H. van Griensven, R. J. M. Bastiaans, A. A. Konnov, and L. P. H. de Goey, "Experimental and modeling study of the effect of elevated pressure on lean high-hydrogen syngas flames," *Proceedings of the Combustion Institute,* vol. 35, pp. 655-662, 2015.

[228] E. Schultz and J. Shepherd, "Validation of detailed reaction mechanisms for detonation simulation," California Institute of Technology, Pasadena, CA2000.

[229] M. Chaos and F. L. Dryer, "Syngas Combustion Kinetics and Applications," *Combustion Science and Technology,* vol. 180, pp. 1053-1096, 2008.

[230] J. Herzler and C. Naumann, "Shock-tube study of the ignition of methane/ethane/hydrogen mixtures with hydrogen contents from 0% to 100% at different pressures," *Proceedings of the Combustion Institute,* vol. 32, pp. 213-220, 2009.

[231] C. Olm, I. G. Zsély, R. Pálvölgyi, T. Varga, T. Nagy, H. J. Curran, *et al.*, "Comparison of the performance of several recent hydrogen combustion mechanisms," *Combustion and Flame,* vol. 161, pp. 2219-2234, 2014.

[232] A. Bagdanavicius, P. J. Bowen, D. Bradley , " Stretch rate effects and flame surface densities in premixed turbulent combustion up to 1.25 MPa," *Combustion and Flame,* vol. 162, pp. 4158-4166, 2015.

[233] N. Syred, "A review of oscillation mechanisms and the role of the precessing vortex core (PVC) in swirl combustion systems," *Progress in Energy and Combustion Science,* vol. 32, pp. 93-161, 2006.

[234] A. Valera-Medina, N. Syred, and P. Bowen, "Central recirculation zone visualization in confined swirl combustors for terrestrial energy," *Journal of Propulsion and Power,* vol. 29, pp. 195-204, 2012.

[235] A. Al-Doboon, M. Gutesa, A. Valera-Medina, N. Syred, J.-H. Ng, and C. T. Chong, "CO2-argon-steam oxy-fuel (CARSOXY) combustion for CCS inert gas atmospheres in gas turbines," *Applied Thermal Engineering,* vol. 122, pp. 350-358, 2017.

[236] "Centrax, 2012, Technical Description, CX501-KB5 Generator Sets."

[237] J. N. Crowley and J. R. Sodeau, "Reaction between nitric oxide and the amidogen radical, NH2," *Journal of Physical Chemistry,* vol. 91, pp. 2024-2026, 1987.