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Emissions of Nitrogen-based Fuel Combustion in Swirl Burner

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Abstract

To provide a first insight into combustion characteristics of ammonia-based fuel in gas turbine engines for power generation, a generic swirl burner is tested with ammonia/hydrogen mixtures in this study. Based on the Computational Fluid Dynamics (CFD) simulation results, Chemical Reaction Network (CRN) model is developed to study the NOx emission characteristics of different ammonia/hydrogen mixtures in a gas turbine swirl burner. The NOx emission results predicted by the CRN model using Konnov's mechanism have shown satisfactory agreement with the experimental data. The parameter study are then performed to estimate the effect of pressure, inlet temperature and equivalence ratio. Areas are identified which more attention for model development and emission need control in future studies.

Keywords: Ammonia/hydrogen combustion; Gas Turbine; Chemical Reactor Network; NOx

1. Introduction

With a stronger need to reduce environmental pollution and carbon emissions caused by conventional fossil fuels, ammonia was suggested to be a possible alternative fuel for future energy system[1]. As a carbon free chemical,

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ammonia has a high content of hydrogen atom but remarkable advantages than hydrogen in terms of storage, transport, distribution problems. In this background, interest in utilizing ammonia as a kind of green fuel is becoming stronger. Some fundamental investigations of ammonia combustion have already provided preliminary knowledge of the potential of using ammonia as fuel. However, to meet the demands of electrical grids, responsive and larger power generators will be required. Thus as a result, considering the pressure to reduce carbon dioxide emission and finite resources of fossil fuels, using ammonia combustion for power generation is an interesting proposition.

Applications of ammonia as fuel have already been widely studied in internal combustion engines recently. Frigo et al. [2] used hydrogen obtained from ammonia by catalytic reforming in a 4-stroke SI engine. A general decrement in engine performance is observed in respect to the original gasoline version. Ryu et al. [3] investigated gasoline–ammonia of a spark-ignition engine in terms of the combustion characteristics and exhaust emissions with direct injection. CO emissions are decreased but emissions of NOx and HC are increased when ammonia is used. Direct injection of gaseous ammonia is proven feasible engine combustion. Reiter et al. [4] demonstrated the feasibility of ammonia combustion in compression-ignition diesel engines. In this work, using ammonia to replace diesel fuel and biodiesel are both tested in which a maximum energy replacement of 95% was achieved. There are also some studies on improving understanding of ammonia-based fuels for gas turbine. For instance, Norihiko et al. performed demonstration test using a micro gas turbine system firing kerosene with 30% decrease of kerosene by supplying ammonia gas. Valera-Medina et al. [5] studied a generic swirl burner with ammonia and hydrogen/methane. Stabilized flames were achieved while NOx and CO were considerably lower at high equivalence ratios >1.10. To successfully utilize ammonia in gas turbine engines for power generation, a detailed understanding of ammonia combustion in gas turbine combustor is necessary. Academia has shown some development in the understanding of these systems, but this is limited. Considering the benefit of hydrogen yielding no carbon dioxide, this research appraises ammonia/hydrogen as the fuel for application in gas turbine combustion.

The previous studies on utilizing ammonia suggested that NOx emission is one of the most important concern for ammonia combustion in gas turbine combustor. Therefore the challenge of accurate NOx emission prediction is important for the design and analyses of gas turbine combustor using ammonia-based fuel. Computational fluid dynamics (CFD) based methodology alongside detailed chemistry is a way can help to capture accurate information for the prediction of NOx emissions, turbulent reacting flows, combustion dynamics, autoignition, etc. However, the large numbers of species and reactions in detailed mechanisms can lead to huge computational cost which makes it almost impossible to conduct CFD simulation with detailed chemistry for practical complex combustion system like a gas turbine combustor. Instead, Chemical Reactor Network (CRN) model which has been also used in combustion system simulation is capable of using detailed chemical kinetic mechanism and costs quite small computational source [6]. Especially, it is found to be a valuable tool for the evaluation of pollutant formation in gas turbine system [7]. In this kind of method, a flow field is divided into an ensemble of connected zones and each zone is representative of a homogeneous chemical reaction compartment. Then using the flow field information as a start point, the CRN structure can be determined. This kind of approach simplifies the flow representation but remains an accurate description of the kinetics. In this way the CRN model can have good prediction performance but cost much less computational time. Therefore it is supposed to be suitable for the study of NOx emission of ammonia combustion in gas turbine.

In this study, a generic swirl burner was investigated with ammonia/hydrogen mixtures to provide a first insight into combustion performance. A CFD-based CRN model is developed to study the NOx emission characteristics of ammonia/hydrogen mixtures and provide deep insight into the NOx formation chemistry. The parameter study was also performed to investigate influence of pressure, inlet temperature and equivalence ratio.

Nomenclature

LES	Large Eddy Simulation
PaSR	Partially Stirred Reactor
CRN	Chemical Reaction Network

CFD	Computational Fluid Dynamics

2. Numerical simulation

2.1. Computational fluid dynamics model

In the present study, the 3D CFD simulation was firstly performed for ammonia/hydrogen combustion in a swirl burner. As Large Eddy Simulation(LES) is increasingly becoming a reliable CFD approach for gas turbines, providing a compromise between the benefits and disadvantages of the RANS (Reynolds-averaged Navier-Stokes equations) and DNS(Direct numerical simulation) approaches[8], it is utilised in this study. The simulation was implemented by using finite control volume technique under the OpenFOAM2.3.1 platform [9]. The governing equations were solved implicitly using the finite volume method in which a 2nd order scheme was employed for time stepping and spatial discretisation. No-slip boundary conditions were set for the gaseous phase at the wall. The pressure−velocity coupling was obtained using the SIMPLEC algorithm. The mole ratio of ammonia to hydrogen is 1:1. The mass flux of the ammonia/hydrogen/air mixture was 15.777g/s. The flame simulated was under ambient pressure with equivalence ratio of 0.523. a reduced Konnov's mechanism by [10] was used in the 3D simulation. More details about the configuration and numerical set up can be found in previous work [11].

Figs. 1-3 show the profile of time-averaged distributions of temperature, velocity, NO concentration of axial section. The CFD results can provide an overview of the entire field. As the simulation is axisymmetric, only half the column is plotted. As illustrated by the flow field in Fig. 1, the premixed fuel/air mixture is introduced through a swirl injector with high velocity. In the combustor, two recirculation zones are founded: a coherent central recirculation zone (CRZ) and an external recirculation zone(ERZ) have been formed in the system, stabilising the flame under the conditions analysed,. Temperatures were observed in the range of 300 to 2000K, as in industrial systems, Fig. 2. NO production takes place across the boundaries of the flame, Fig. 3. This expected behaviour is a consequence of the high temperatures of combustion and recombination of species. As expected, high NO concentration produced at the nozzle is then diluted downstream of the post flame zone.

Fig. 1. Axial velocity profile

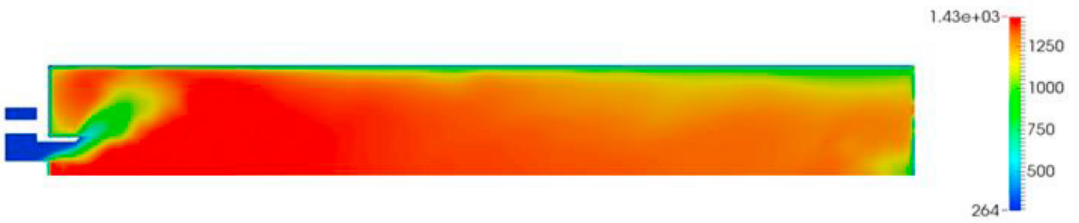

Fig. 2. Temperature profile

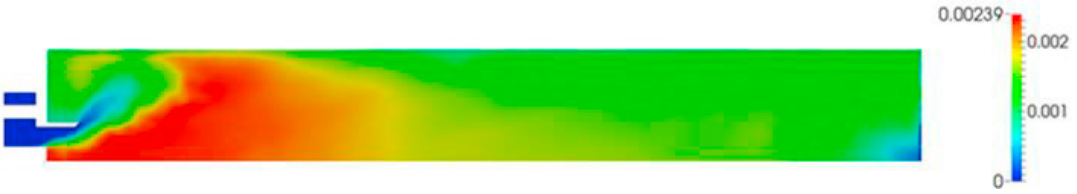

Fig. 3. NO mass fraction profile

2.2. CFD based chemical reactor network model

Based on the insights gained from CFD modelling results, a Chemical reactor network (CRN) model was employed to represent the combustion procedure in the combustor by dividing it into several distinct zones. To determine the number and the shape of the zones is the first thing for the construction of the CRN model. The number of the zones will determine the complexity of the CRN model and the shape of the zones will influence the volume and the mass flux between connected zones. For the swirl combustor in this study, it is preliminarily divided to central recirculation zone (CRZ), the external recirculation zone (ERZ), the flame zone and the post flame zone.. The mass flux between different adjacent zones are also be determined by the flow field information. The residence time for each reactor could be estimated based on the average velocity at different positions.

Since the flow is divided into homogenous zones, for each zone, the type of an elementary reactor can be represented with a Perfect Stirred Reactor(PSR) for the strong turbulence in the combustor. Fig. 4. shows the schematic CRN model. Full Konnov mechanism was used to simulate ammonia combustion chemistry occurring in the swirl combustor with the CRN model.

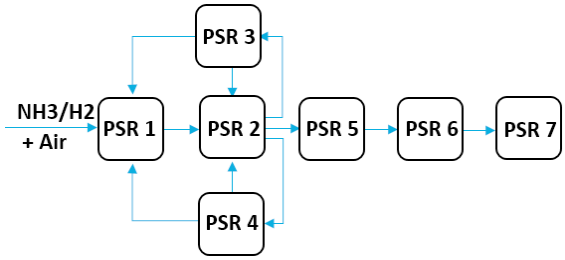

Fig. 4. Structure of CRN model (PSR1-flame zone 1, PSR2-flame zone 2, PSR3-external recirculation zone, PSR4-Central recirculation zone, PSR5-immediate post-flame zone, PSR6- main post-flame zone, PSR7- dilution post-flame zone)

3. Results and discussion

3.1. CRN model verification

In the present investigation NOx emission is chosen to be the index for the validation of the CRN model. The simulation prediction results against experimental data are illustrated in Fig. 5. Close agreement can be observed between the CRN prediction and experimental test. As expected, the CRN model is able to predict the trends of NOx emission satisfactorily using full Konnov, but the calculation time is only several seconds.

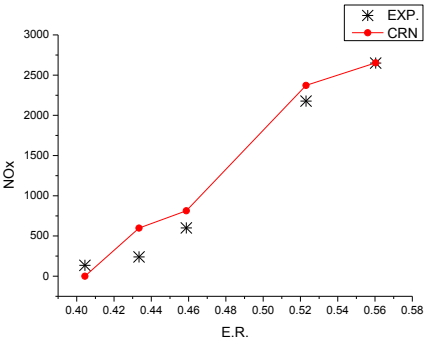

Fig. 5. Validation of CRN model Experiments as in [12]

3.2. NOx emission characteristics

To investigate the combustion characteristics of ammonia-based fuel for gas turbine use, ammonia/hydrogen mixtures with different equivalence ratios were investigated. Therefore, NOx emission predictions of different equivalence ratios were conducted to study the effect with constant pressure of 17atm and inlet temperature of 598K. As shown in Fig. 6, NOx emission increases in the lean area and decreases in the rich area with the increase of equivalence ratio. The highest NOx concentration is attained near the stoichiometric point with equivalence ratio of 0.9. This result indicates that equivalence ratio has a big impact on the NOx emission level. To achieve small NOx emission, to control equivalence ratio to slightly fuel rich condition is suggested for gas turbine use.

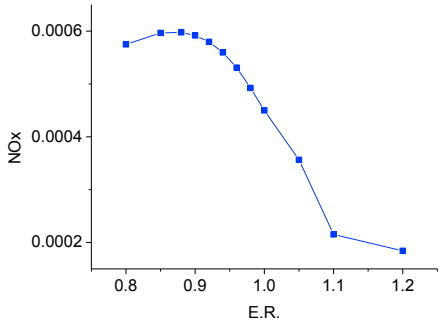

Fig. 6. NOx emissions as a function of equivalence ratio

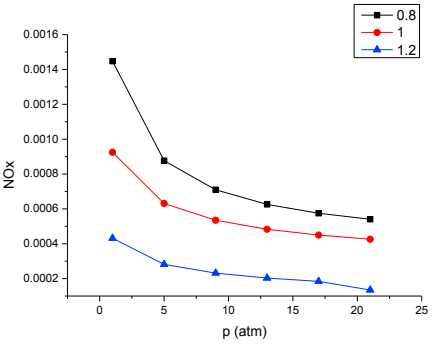

Fig. 7. NOx emissions as a function of the pressure

NOx concentration predictions were performed under different pressure conditions and different inlet temperature conditions separately, as illustrated in Fig. 7 and Fig. 8. The fuel mixture studied here is 80% ammonia and 20% hydrogen. Fig. 7 shows the NOx emissions variation with pressure for different equivalence ratios in which the inlet temperature is fixed at 598K and pressure ranges from 1 to 21atm. As can be seen, the increase of pressure has a positive effect on the reduction of NOx emissions for the swirl combustor. On the other hand, as shown in Fig. 8, NOx emissions increase slightly with the increase of inlet temperature and this effect is smaller compared to the reduction effect of pressure condition under high equivalence ratio conditions. The increase of inlet temperature leads to the increase of flame temperature Fig. 9, which contributes to the thermal NOx formation. Whist for an augmentation of pressure at constant inlet temperature, the NOx emissions decrease mainly due to the effect on fuel NOx kinetics. This indicates that fuel NOx pathways play a more important role than thermal NOx in the formation of NOx emission under the gas turbine conditions.

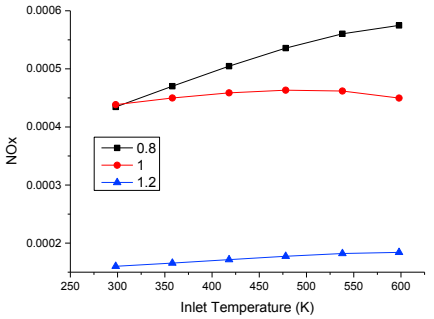

Fig. 8. NOx emissions as a function of the inlet temperature

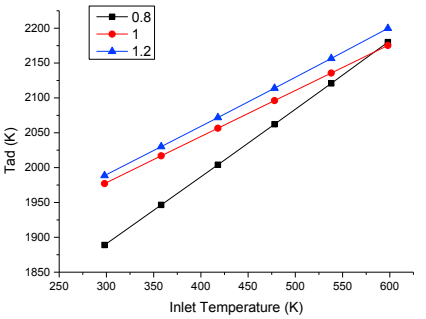

Fig. 9. Adiabatic temperature as a function of the inlet temperature

4. Conclusions

In this study, generated from preliminary CFD simulation results, a CRN model is developed to study the NOx emission characteristics of ammonia-based fuel with detailed chemistry in a generic gas turbine combustor.

The established CRN model using Konnov's mechanism is validated against NOx emission data from experiments. The methodology has shown to be effective in efficiently estimating NOx emissions with a short computational time and good accuracy.

The NOx emission prediction of different ammonia/hydrogen mixtures under real operating conditions show that higher ammonia fraction in the fuel mixture is good for NOx emission reduction. The effects of elevated pressure and inlet temperature conditions were studied using the established CRN model, which are met in real gas turbine operation. Results show that higher pressure can reduce the NOx emission whilst inlet temperature has relative quite small influence on NOx emission. Equivalence ratio has a significant effect on the NOx formation which is found to peak at E.R. of 0.9.

More research on ammonia chemistry is still needed so that the mechanism can be refined to be better suited for ammonia/hydrogen combustion and NOx emission reduction under gas turbine conditions.

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