

This is an Open Access document downloaded from ORCA, Cardiff University's institutional repository: <https://orca.cardiff.ac.uk/id/eprint/172478/>

This is the author's version of a work that was submitted to / accepted for publication.

Citation for final published version:

Zhao, Xu, Ng, Jo-Han, Mong, Guo Ren, Mashruk, Syed, Lee, Chew Tin, Fang, Xueliang, Wong, Keng Yinn, Ooi, Jong Boon, Valera Medina, Agustin and Chiong, Meng-Choung 2024. Thermochemical analysis of premixed ammonia/biogas flames in a model gas turbine swirl combustion system. Renewable Energy 236 , 121478. 10.1016/j.renene.2024.121478

Publishers page: <https://doi.org/10.1016/j.renene.2024.121478>

Please note:

Changes made as a result of publishing processes such as copy-editing, formatting and page numbers may not be reflected in this version. For the definitive version of this publication, please refer to the published source. You are advised to consult the publisher's version if you wish to cite this paper.

This version is being made available in accordance with publisher policies. See <http://orca.cf.ac.uk/policies.html> for usage policies. Copyright and moral rights for publications made available in ORCA are retained by the copyright holders.



Thermochemical Analysis of Premixed Ammonia/Biogas Flames in a Model Gas Turbine Swirl Combustion System

Xu Zhao^a, Jo-Han Ng^b, Guo Ren Mong^c, Syed Mashruk^d, Chew Tin Lee^e, Xueliang Fang^f, Keng Yinn Wong^g, Jong Boon Ooi^h, Agustin Valera-Medina^d, Meng-Choung Chiong^{a,*}

^a Department of Mechanical Engineering, Faculty of Engineering, Technology & Built Environment, UCSI University, 56000 Kuala Lumpur, Malaysia.

^b Carbon Neutrality Research Group, University of Southampton Malaysia, 79100 Iskandar Puteri, Johor, Malaysia.

^c School of Energy and Chemical Engineering, Faculty of Engineering, Xiamen University Malaysia, 43900 Selangor, Malaysia.

^d College of Physical Sciences and Engineering, Cardiff University, Wales, United Kingdom.

^e Faculty of Chemical and Energy Engineering, Universiti Teknologi Malaysia, 81310 Johor, Malaysia.

^f College of Traffic Engineering, Yangzhou Polytechnic Institute, Yangzhou 225127, China.

^g Faculty of Mechanical Engineering, Universiti Teknologi Malaysia, 81310 Johor, Malaysia.

^h Mechanical Engineering Discipline, School of Engineering, Monash University Malaysia, Jalan Lagoon Selatan, 47500 Bandar Sunway, Selangor Darul Ehsan, Malaysia.

Abstract

This study examined the premixed NH₃/biogas combustion at near stoichiometric using an experimentally validated numerical method. Raising the NH₃ wt.% in NH₃/CH₄ combustion at $\phi = 0.8$ brought up the average reaction temperature (T_{avg}) due to heat retention. Intensified by CO₂ addition, T_{avg} in NH₃/biogas increased by a factor of 1.2 compared to NH₃/CH₄. At $\phi = 1.1$, higher NH₃ and CO₂ wt.% reduced T_{avg} . The local Damköhler number (Da) was reduced marginally in the absence of CO₂ as ϕ increased from 0.8 to 1.1. Conversely, local Da grew considerably in the presence of CO₂ and was particularly sensitive to variations in the excess air ratio. Increased NH₃ wt.% promoted NO emission, primarily via $N + OH \rightarrow NO + H$ and $H + HCNO \rightarrow CH_2 + NO$ pathways. NH₃/biogas produced more NO than NH₃/CH₄ from $\phi = 0.9$ to 1.1, but as ϕ approached 1.1, NO is generally lowered. N₂O is produced mainly by $NH + NO \rightarrow N_2O + H$. Fuel-lean operation generally results in a higher N₂O than fuel-rich operation. The NH₃/biogas combustion at $\phi = 0.8$ is a potential clean fuel solution in lowering NO emissions, as compared to NH₃/CH₄ combustion.

Keywords: Ammonia; Renewable Methane; Swirl Combustion; Premixed Combustion; Biogas

*Corresponding author

Address: Faculty of Engineering, Technology & Built Environment, UCSI University, 56000 Kuala Lumpur, Malaysia.

Email : chiongmc@ucsiuniversity.edu.my ; mcchiong@outlook.com (MC Chiong)

LIST OF ABBREVIATIONS

1D	—	One-dimensional
C	—	Carbon
CH ₄	—	Methane
CO	—	Carbon monoxide
CO ₂	—	Carbon dioxide
C _x N _y	—	Compositions of CO ₂ /NH ₃
Da	—	Damköhler number
EI _{NO}	—	NO Emission Index
EI _{N₂O}	—	N ₂ O Emission Index
FGM	—	Flamelet Generated Manifold
H	—	Hydrogen radical
H ₂	—	Hydrogen
H ₂ O	—	Water vapour
HCN	—	Hydrogen cyanide
HCNO	—	Isocyanic acid
HMFR	—	High Momentum Flow Region
IRZ	—	Inner Recirculation Zone
ISL	—	Inner Shear Layer
LIF	—	Laser Induced Fluorescence
MFC	—	Mass flow controller
N	—	Nitrogen atoms
N ₂	—	Nitrogen
NH	—	Imidogen
NH ₂ *	—	Amidogen radicals
NH ₃	—	Ammonia
NO	—	Nitric oxide
NO ₂	—	Nitrogen dioxide
N ₂ O	—	Nitrous oxide
O	—	Oxygen atoms
OH	—	Hydroxyl radicals
ORZ	—	Outer Recirculation Zone
OSL	—	Outer Shear Layer
PFR	—	Plug Flow Reactor
PSR	—	Perfectly Stirred Reactor
RMSE	—	Root mean square error

LIST OF SYMBOLS

Roman Letters

K_g	—	Total number of gas-phase species
M	—	Number of materials in the surface reaction mechanism
$N_{inlet(j)}$	—	The inlet quantity for each reactor j
N_{PSR}	—	Total number of reactor modules in the reactor network
P	—	Pressure
Q_{loss}	—	Heat lost from the reactor
Q_{source}	—	Energy deposited and generated in the reactor.
$R_{r,j}$	—	Proportion of the reactor r's effluent that is recirculated back to reactor j
S_L	—	Laminar Flame Speed
S_N	—	Swirl number
STO	—	Stoichiometric proportion of the mixture
T	—	Temperature
T_{avg}	—	Average reaction zone temperature
T_0	—	Environmental temperature
U_{sys}	—	Internal energy of a system
V	—	Volume of the reactor
W_k	—	Molecular weight of species k^{th} species
Y_k	—	Mass fraction of the k^{th} species
$Y_{k,i}$	—	Mass fraction of the k^{th} species at inlet stream
a_k	—	A coefficient to ensure that the reaction rate of the flame increases monotonically
c	—	Progress variable
$c_{p,k}$	—	Specific heat at constant pressure for species k^{th}
$\bar{c}_p$	—	Average specific heat capacity of the gas
e	—	Species of electrons
eq	—	Chemical equilibrium at the flame exit
$erfc^{-1}$	—	Inverse complimentary error function
f	—	Mixture fraction
h	—	Specific enthalpy
h_f	—	Heat transfer coefficient
j	—	Number of the reactor
k^{th}	—	Number of species
$\dot{m}$	—	Outlet mass flow rate
$\dot{m}^*$	—	Inlet mass flow rate
t	—	Time
u	—	The unburned reactant at the flame input

Greek Letters

$\dot{\omega}_k$	—	The mass fraction change rate of species k th
λ	—	Heat conductivity
φ	—	Global equivalence ratio
ρ	—	The density of the fluid
χ_c	—	The scalar dissipation rate
$\chi_c(f, c)$	—	The scalar dissipation
χ_{max}	—	The maximum scalar dissipation
χ_{max}^{STO}	—	Scalar dissipation at the stoichiometric mixture fraction

LIST OF UNITS

Hz	—	Hertz
MJ/L	—	Megajoule per litre
cm	—	Centimeter
cm/s	—	Centimeter per second
g/kg	—	Gram per kilogram
kW	—	Kilowatt
mm	—	Millimeter
ppm	—	Parts per million
vol. %	—	Volume fraction
wt. %	—	Mass fraction
°	—	Degree

1.0 Introduction

Ammonia (NH_3) has been ascertained as one of the sustainable zero-carbon energy sources, owing to its high hydrogen (H_2) contents [1]. NH_3 features a lesser cost/unit of stored energy and a higher volumetric energy density than H_2 . The cost of storing pure H_2 for 182 days was higher than that of storing NH_3 by a factor of ~ 27.7 [2]. Furthermore, the volumetric energy density of NH_3 is higher than that of H_2 by ~ 4.2 MJ/L [1]. Considering these, numerous efforts have been spent to enhance the ammonia production strategy [3–5], thermo-economic analysis [6], and optimisation of the downstream supply system [7]. Nonetheless, NH_3 -based thermal power generation systems do have drawbacks [8], such as high nitric oxide (NO) and lower reactivity [9,10]. Developing new combustion strategies and technologies is essential to expedite the adoption of green NH_3 in the power generation industry. To improve the combustion of neat NH_3 , adding methane (CH_4) has been proposed as a potential solution.

Valera-Medina et al. [11] examined the swirl combustion of premixed NH_3/CH_4 . As the global equivalence ratio (ϕ) increased to > 1.1 , the NO emissions were practically diminished, mainly due to a large portion of the NO being consumed by the amidogen radicals (NH_2^*). In fuel-lean operation, the NO was produced primarily by the reactions among nitrogen atoms (N), imidogen (NH), and oxygen atoms (O). Somarathne et al. [12] found that when the NH_3 energy proportion was increased by $\sim 40\%$, NO emissions from the combustion of non-premixed NH_3/CH_4 experienced a substantial increase of nearly three orders of magnitude. Another relevant study reported that the combustion of non-premixed NH_3/CH_4 in excess air showed promising results in mitigating NO emissions [13].

An et al. [14] examined the premixed $\text{NH}_3/\text{CH}_4/\text{air}$ swirl flames via a numerical approach. The species residential time scale in the inner recirculation zone (IRZ) was identified to have influential effects on the formation of NO, prolonged local residence time led to a high NO production in the IRZ. The formation of hydroxyl radicals (OH) and NO was also closely

linked to elevated temperatures [14]. Furthermore, the elevated swirl number led to a noticeable increase in the lean blow-off limit in an NH_3/CH_4 swirl flame [15]. The authors identified four distinctive macrostructures that initiated the fuel-lean flame blow-off when lowering the flame global equivalence ratio [15]. Zhang et al. [16] reported that a high swirl flow intensity results in flame root extinguishing. On the contrary, low-intensity swirl flow failed to form the central recirculation zone that is essential for flame stabilisation. In all, a medium swirl number of ~ 0.76 was to be ideal for limiting NO emissions while ensuring flame stability.

Füzesi et al. [17] reported that the emission of nitrous oxide (N_2O) from the combustion of NH_3/CH_4 swirl was practically transformed into NO at the combustor outlet, and the levels of carbon monoxide (CO) remained consistently low across all cases. Furthermore, the NO emissions were found doubled with the elevation of NH_3 concentration from 20% to 50%. Wei et al. [18] examined the impact of acoustic excitation on the dynamics of $\text{CH}_4/\text{NH}_3/\text{air}$ swirling flame. Their study unveiled that the flame exhibits a distinctive layered V-shape with periodic fluctuations for an acoustic excitation frequency of ~ 70 Hz, and it transformed into an inverted cone shape at a high-frequency acoustic excitation frequency of ~ 270 Hz. At a flame excitation frequency of ~ 120 Hz, the NO and CO were found to be lowered by ~ 203 ppm (from ~ 700 ppm) and ~ 170 ppm (from ~ 300 ppm), respectively. Nonetheless, elevated thermoacoustic excitation frequency can disrupt the flame structure, causing a sharp escalation in CO emission. Mashruk et al. [19] examined ternary fuel combustion that comprised of containing NH_3 , CH_4 , and H_2 at varying concentrations. It was reported that the $\text{CH}_4/\text{NH}_3/\text{H}_2$ blend in 20/55/25 volumetric fraction inhibited flashback and resulted in considerably low emissions when operated at a slight fuel-rich equivalence ratio of 1.2. Furthermore, it was also found that hydrogen radical (H) and heat losses have tremendous effects in reducing the N_2O [20].

Wang et al. [21] compared the partially premixed NH_3/CH_4 swirl flames and premixed NH_3/CH_4 swirl flames. The flow field of the partially premixed swirl flame showed the dearth

of the recirculating flow structure that is found in the premixed swirl flames, yet the effect on flame stabilisation was only trivial. When compared with the premixed operation, the partially premixed flame exhibited substantial NO and CO emissions reduction by at least a factor of 2 at $\phi \sim 0.65$. In another study, Wang et al. [22] customised swirl burner was employed to examine the impact of residence time scale on premixed $\text{NH}_3/\text{CH}_4/\text{air}$ emissions. Elevating the swirl number effectively lowers the NO, nitrogen dioxide (NO_2), and N_2O emissions. NO formation was confined to the main reaction zone of the swirling flame, particularly up to 60 mm height for this burner. Extending the length of the combustor reduced the concentrations of NO_2 and N_2O without increasing the NO concentration noticeably. A positive correlation between NO and OH laser-induced fluorescence (LIF) intensities was observed.

There is an increasing effort in examining the swirl combustion of NH_3/CH_4 . Nonetheless, the study on the swirl combustion of $\text{NH}_3/\text{biogas}$ is comparatively scarce. Biogas is a type of renewable methane that is typically produced via anaerobic digestion and consists of mainly CH_4 (50-75%) and carbon dioxide (CO_2 , 25-50%) [23], where the removal of CO_2 from the biogas requires additional effort [24]. Despite its renewability, a substantially large amount of CO_2 in the fuel mixture could pose new challenges to combustion operations. To date, the effect of CO_2 in the biogas on the thermochemical, turbulent-reaction, and emissions characteristics of $\text{NH}_3/\text{biogas}$ swirl flame at the near stoichiometric operations remains undetermined. By using an NH_3/CH_4 swirl flame as the baseline, the present study extends on previous work [25] by examining the swirl combustion characteristics of $\text{NH}_3/\text{biogas}$ at near stoichiometric operations.

2.0 Research method

2.1 Experimental setup

The experimental work was performed using a generic gas turbine premixed swirl burner (Figure 1a & b) to obtain emissions data for numerical model validation in the subsequent subsection. CH₄ and CO₂ were blended inside the fuel mixer to form biogas. The biogas was then directed to the plenum to mix up with the air to form a homogeneous flammable mixture. The mass flow rate of CH₄, CO₂, and air were regulated using Sierra mass flow controllers (MFC) to set up the flame at 7 kW input thermal power. An axial swirler with 6 straight vanes (thickness 1.5 mm) oriented at 45° from the axial centreline axis was laid at the burner exit to generate swirling flow with a geometric swirl number (S_N) of ~ 0.84 . The swirl flame was established at the burner outlet by igniting the flammable mixture. A biogas composition of 30% CO₂ and 70% CH₄ by mass was chosen for this study. A KANE Quintox 905 gas analyser was used to measure exhaust gas emissions at the outlet of the quartz tube. The range of the NO was 0-5000 ppm with a resolution of 1 ppm. The uncertainty for NO emission <100 ppm was ± 5 ppm, while the uncertainty for NO emission >100 ppm was $\pm 5\%$. The propagated error for NO in this experiment was found to be $\pm 7.5\%$.

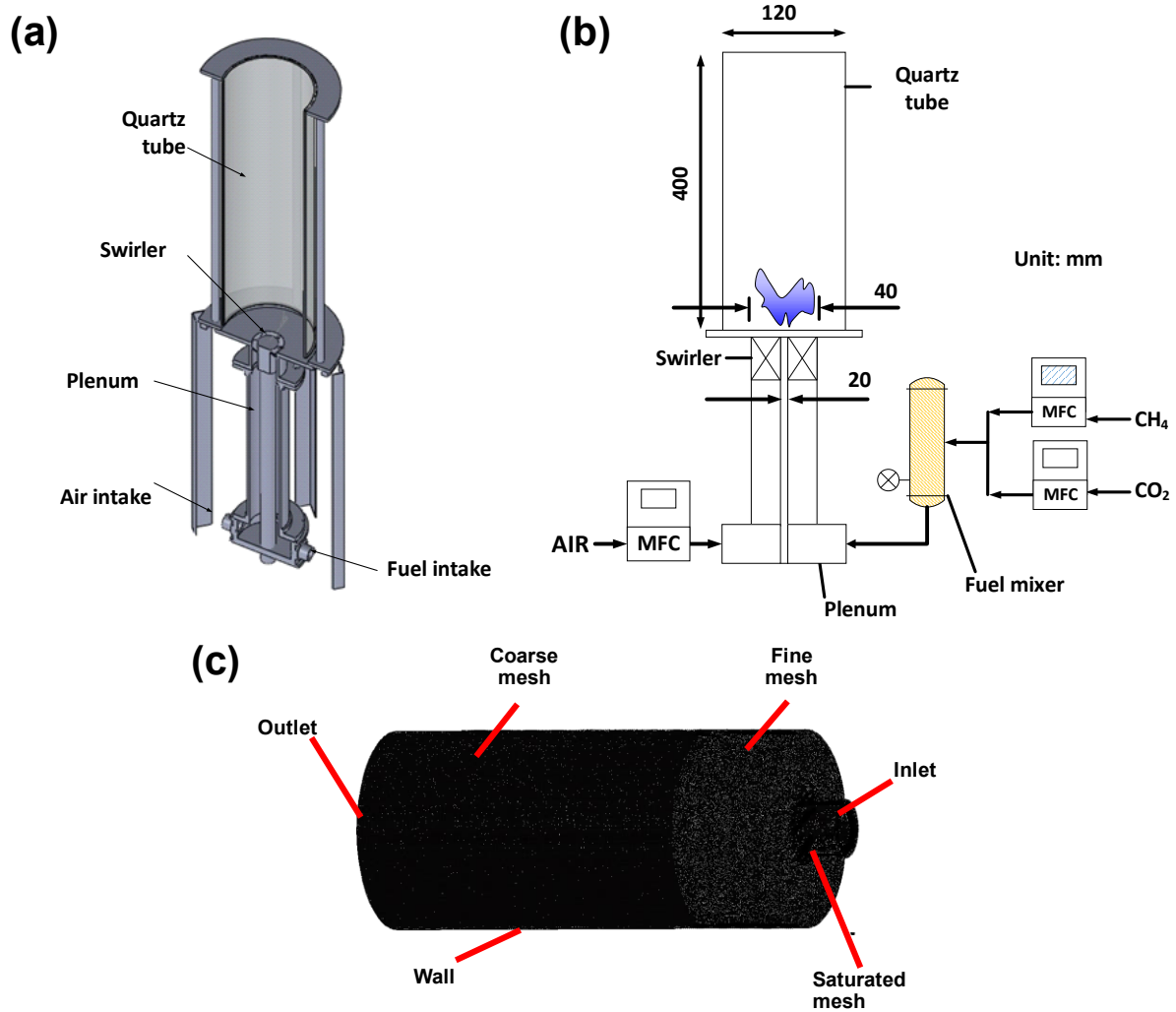


Figure 1 (a) Generic gas turbine swirl combustion system, (b) Experimental setup for data collection, (c) Grid setup for numerical study (Adapted from [25] and [26]).

2.2 Chemical kinetic modelling

Chemical kinetic analysis was performed using CHEMKIN. The gas turbine combustion network was modelled based on the previous studies [20,27] and is shown in Figure 2. The Okafor mechanism [28] was chosen for chemical kinetics and sensitivity analysis. The aim was to find the reactions that have the greatest impact on the formation of key species. The reaction zones are modelled using a separate perfectly stirred reactor (PSR). The recirculation strength was approximated from previous experimental works [20,27] and experimental data from section 2.1. A PSR is a zero-dimensional ideal reactor in which reactions occur within the

control volume uniformly without any spatial variation of parameters [29]. A steady flow of reactants and oxidiser are introduced through the inlet of the control volume. The equation for the global conservation of mass of various gaseous substances over time in the control volume is expressed as:

$$\rho V^{(j)} \frac{dY_k^{(j)}}{dt} = \sum_{i=1}^{N_{inlet(j)}} \dot{m}_i^{*(j)} (Y_{k,i}^* - Y_k) + \sum_{r=1}^{N_{PSR}} \dot{m}^{(r)} R_{rj} (Y_k^{(r)} - Y_k^{(j)}) - Y_k^{(j)} \sum_{m=1}^M A_m^{(j)} \sum_{k=1}^{K_g} \dot{S}_{k,m}^{(j)} W_k + (\dot{\omega}_k V)^{(j)} W_k + \sum_{m=1}^M A_m^{(j)} \dot{S}_{k,m}^{(j)} W_k \quad (1)$$

where, j represents the number of reactors, ρ denotes the mass density, V stands for the volume of the reactor, $\dot{m}_i^*$ represents the inlet mass flow rate, and $\dot{m}$ represents the outlet mass flow rate. $N_{inlet(j)}$ indicates the inlet quantity for each reactor j , while N_{PSR} represents the total number of reactor modules in the reactor network. R_{rj} represents the proportion of the effluent that is recirculated back to the reactor j from reactor r . Y_k represents the mass fraction of the k^{th} species, W_k denotes the molecular weight of the k^{th} species, and $\dot{\omega}_k$ refers to the molar generation rate of the k^{th} species produced by gas-phase chemical reactions per unit volume. The superscript $*$ is used to identify quantities associated with the inlet stream i . When deposition or etching of material occurs within the reactor, there is a difference between the outlet mass flow rate and the sum of the inlet and recirculation mass flow rates, which is represented by the last term on the right side of the equation. In this expression, A_m refers to the reactive area of the m^{th} material, and $\dot{S}_{k,m}$ represents the molar surface generation rate of the k^{th} species per unit surface area of the m^{th} material. The rate of reaction and species concentrations are governed by the chemical kinetics mechanism file.

Heat is generated during chemical reactions and is also dissipated to the surroundings.

The total internal energy equation for the entire reaction system is as follows:

$$\begin{aligned} \frac{dU_{sys}^{(j)}}{dt} = & \sum_{i=1}^{N_{inlet}^{(j)}} \dot{m}_i^{*(j)} \sum_{k=1}^{K_g} (Y_{k,i}^* h_{k,i}^*)^{(j)} + \sum_{r=1}^{N_{PSR}} \dot{m}^{(r)} R_{rj} \sum_{k=1}^{K_g} (Y_k h_k)^{(r)} - \left(\dot{m} \sum_{k=1}^{K_g} Y_k h_k \right)^{(j)} - Q_{loss}^{(j)} \\ & + Q_{source}^{(j)} - P^{(j)} \frac{dV^{(j)}}{dt} \end{aligned} \quad (2)$$

The total internal energy of the system U_{sys} includes the internal energies of the gas, surface phase, deposited or etched solid phase, and the reactor walls, h_k refers to the specific enthalpy of the k^{th} species, and P refers to the pressure. The net heat flux Q_{loss} refers to the heat lost from the reactor. This heat flux Q_{loss} can be specified directly by setting a constant, or by setting a constant heat transfer coefficient with the environmental temperature T_o . Carbon steel with a heat transfer coefficient of $80 \text{ J/m}^2 \cdot \text{K} \cdot \text{s}$ was chosen, while the environmental temperature was set at 298 K . Q_{source} refers to the energy deposited and generated in the reactor. The post-combustion zone was modelled as a one-dimensional Plug Flow Reactor (PFR) with a length of 40 cm .

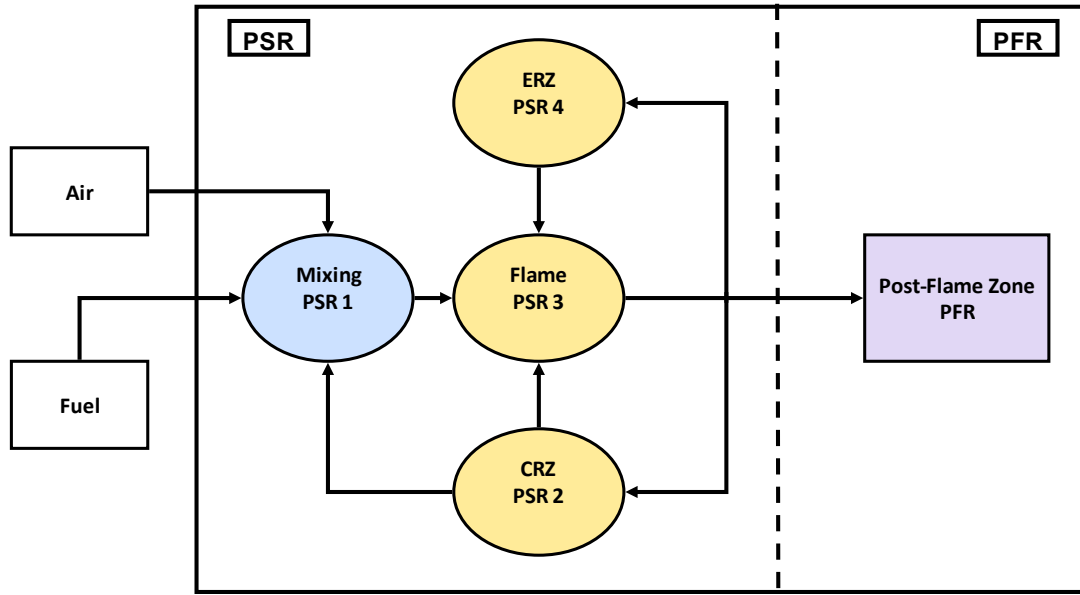


Figure 2 Gas turbine combustion network for chemical kinetic modelling [20,27]

2.3 Numerical modelling

ANSYS Fluent was used to model and simulate the reacting swirl flow. Okafor's mechanism [28] was chosen to model the species reactions in this research, as previous studies have shown that it has a good correlation with ammonia flames [30]. This mechanism is a simplified version of the Tian mechanism [31], which has been widely validated [32] and contains fewer species (27) and reactions (130), thus requiring less computational effort [30]. The Flamelet Generated Manifold (FGM) method with a comprehensive chemical reaction scheme that leverages the chemical data from a series of one-dimensional (1D) flame surface calculations was adopted for flame surface simulation in the present study. The 1D premixed flame surface was solved within the reaction progression space whereby the progression variable is defined as the normalised sum of the product species mass fractions among all species in the chemical process, given by:

$$c = \frac{[\sum_k \alpha_k (Y_k - Y_k^u)]}{[\sum_k \alpha_k (Y_k^{eq} - Y_k^u)]} = \frac{Y_c}{Y_c^{eq}} \quad (3)$$

where, u refers to the unburned reactant at the flame input, while eq signifies chemical equilibrium at the flame exit. To ensure that the reaction rate c of the flame increases monotonically, a coefficient α_k is introduced. For all species, $\alpha_k = 0$, except for $\alpha_{CO_2} = \alpha_{CO} = 1$ for hydrocarbon combustion and $\alpha_{H_2O} = 1$ for fuels containing no C element, such as H_2 . The adiabatic flamelet equations in one dimension can now be translated from physical space to reaction-progress space.

$$\rho \frac{\partial Y_k}{\partial t} + \rho \frac{\partial Y_k}{\partial c} \dot{w}_c = \rho \chi_c \frac{\partial^2 Y_k}{\partial c^2} + \dot{w}_k \quad (4)$$

$$\rho \frac{\partial T}{\partial t} + \rho \frac{\partial T}{\partial c} \dot{w}_c = \rho \chi_c \frac{\partial^2 T}{\partial c^2} - \frac{1}{c_p} \sum_k h_k \dot{w}_k + \frac{\rho \chi_c}{c_p} \left(\frac{\partial c_p}{\partial c} + \sum_k c_{p,k} \frac{\partial Y_k}{\partial c} \right) \frac{\partial T}{\partial c} \quad (5)$$

where, T is the temperature, t represents time, h stands for the total enthalpy and $c_{p,k}$ refers to the specific heat at constant pressure for species k^{th} . The scalar dissipation rate, denoted by χ_c is defined as follows:

$$\chi_c = \frac{\lambda}{\rho c_p} |\nabla c|^2 \quad (6)$$

where, λ represents heat conductivity. The variable c , along with the scalar dissipation χ_c , serves as an input to the equation set, with equation 2 (adiabatic flamelet equations) now given as:

$$\rho \frac{\partial Y_k}{\partial t} + \rho \frac{\partial Y_k}{\partial c} \dot{w}_c = \frac{\lambda}{c_p} |\nabla c|^2 \frac{\partial^2 Y_k}{\partial c^2} + \dot{w}_k \quad (7)$$

The maximum scalar dissipation, χ_{max} , of a premixed flamelet varies with different mixture fractions. The scalar dissipation $\chi_c(f, c)$ for any mixture fraction f is modelled as follows:

$$\chi_c(f, c) = \chi_{max}^{STO} \exp \left(-2 \left(\text{erfc}^{-1} \left(\frac{f}{f_{STO}} \right) \right)^2 \right) \exp \left(-2 \left(\text{erfc}^{-1}(2c) \right)^2 \right) \quad (8)$$

where STO and $erfc^{-1}$ are the stoichiometric proportion of the mixture and the inverse complementary error function, respectively. In ANSYS Fluent, scalar dissipation at the stoichiometric mixture fraction is an input for the premixed flamelet generator, denoted as χ_{max}^{STO} . The default value of $\chi_{max}^{STO} = 1000 \text{ s}^{-1}$ is generally applicable for strain-free fuel-rich, lean, and stoichiometric flamelets at standard temperature and pressure [26].

A SIMPLE computational method was used to calculate the pressure-velocity coupling [33,34]. A second-order upwind method was used to discretise the governing equations. For pressure, PRESTO! system was used due to its capability of accelerating the simulation convergence [33,34]. A high-quality mesh is essential in areas with high temperatures and gradients in species concentration. For this simulation study, primarily a structured hexahedral grid was chosen, as shown in Figure 1c. The aspect ratio and the orthogonal quality were used to calculate the mesh quality. A high-quality hexahedral grid has a minimum orthogonal quality of 0.15 and a maximum aspect ratio of 35 [35]. This study's lowest orthogonal quality was 0.19, and its greatest aspect ratio was 13.43, both being within the previously indicated range. The saturated and fine mesh was created at the swirler and the area immediately following its outflow; the grid became coarser as it approached the burner outlet. To estimate the flow in these areas, a refined mesh is needed especially at the swirler exit. Several compositions of NH_3 /biogas were examined in this study, denoted as C_xN_y , where x and y denote the mass fraction of CO_2 in the biogas and NH_3 , respectively (Table 1). At the inlet, a mass flow rate model setup was set using these compositions. The value of turbulence intensity was derived from [36]. The border of the combustor wall was configured to be non-slip. The flow output was configured to be the burner outlet.

Table 1 Biogas and NH₃ compositions in the premixed biogas/NH₃ mixture.

Abbreviation	Biogas components		NH ₃ mass fraction in the NH ₃ /biogas (wt.%)
	CH ₄ mass fraction in biogas (wt.%)	CO ₂ mass fraction in biogas (wt.%)	
C0N20	100	0	20
C0N30	100	0	30
C0N40	100	0	40
C0N60	100	0	60
C30N20	70	30	20
C30N30	70	30	30
C30N40	70	30	40
C30N60	70	30	60
C40N20	60	40	20
C40N30	60	40	30
C40N40	60	40	40
C40N60	60	40	60

The grid-independent test was performed where the NO emissions from biogas converged at 1.7 million elements as ϕ varied from 0.75 to 0.9. Thus, the 1.7 million grid elements were considered grid-independent because the NO emissions results were almost identical for the >1.7 million grid. According to Mayr et al. [33,34], when the residual for the species concentration < 0.001 , the simulation is regarded as converged. Furthermore, the residuals for continuity, velocity, and k-epsilon, should also be $< 10^{-3}$, and the mixture fraction variance and mean mixture fraction residuals should be reduced to $< 10^{-6}$ [33,34]. Apart from the residual, another measure of the simulation process's convergence is the number of iterations. After 5000 iterations, there are no discernible changes in the variations in NO emission. The NO mean value is considered to have converged when the NO value becomes less variable and approaches a steady state. Figure 3c shows the velocity flow field while Figure

3d depicts the flame temperature overlays with the flow field vector. The location of IRZ, high momentum flow region (HMFR), and outer recirculation zone (ORZ) are labelled. Figure 3a compares the CFD-generated NO emissions with those obtained via experimental in section 2.1, with φ varied from 0.7-0.9 at 7 kW input thermal power. A tendency towards agreement between the experimental results and the FGM-estimated NO concentration has been noted. The Root Mean Squared Error (RMSE) between experimental data and simulation results was found to be 2.05 ppm. In all, CFD-predicted results demonstrated good agreement with experimental data. Nevertheless, the NO concentration was overestimated when stoichiometry was approached. Figure 3b compares the simulation results with those obtained published by [11] using 60/40 NH_3/CH_4 at 44 kW input thermal power, with φ varied from 0.81-1.14. The RMSE between experimental data and simulation results was 124 ppm.

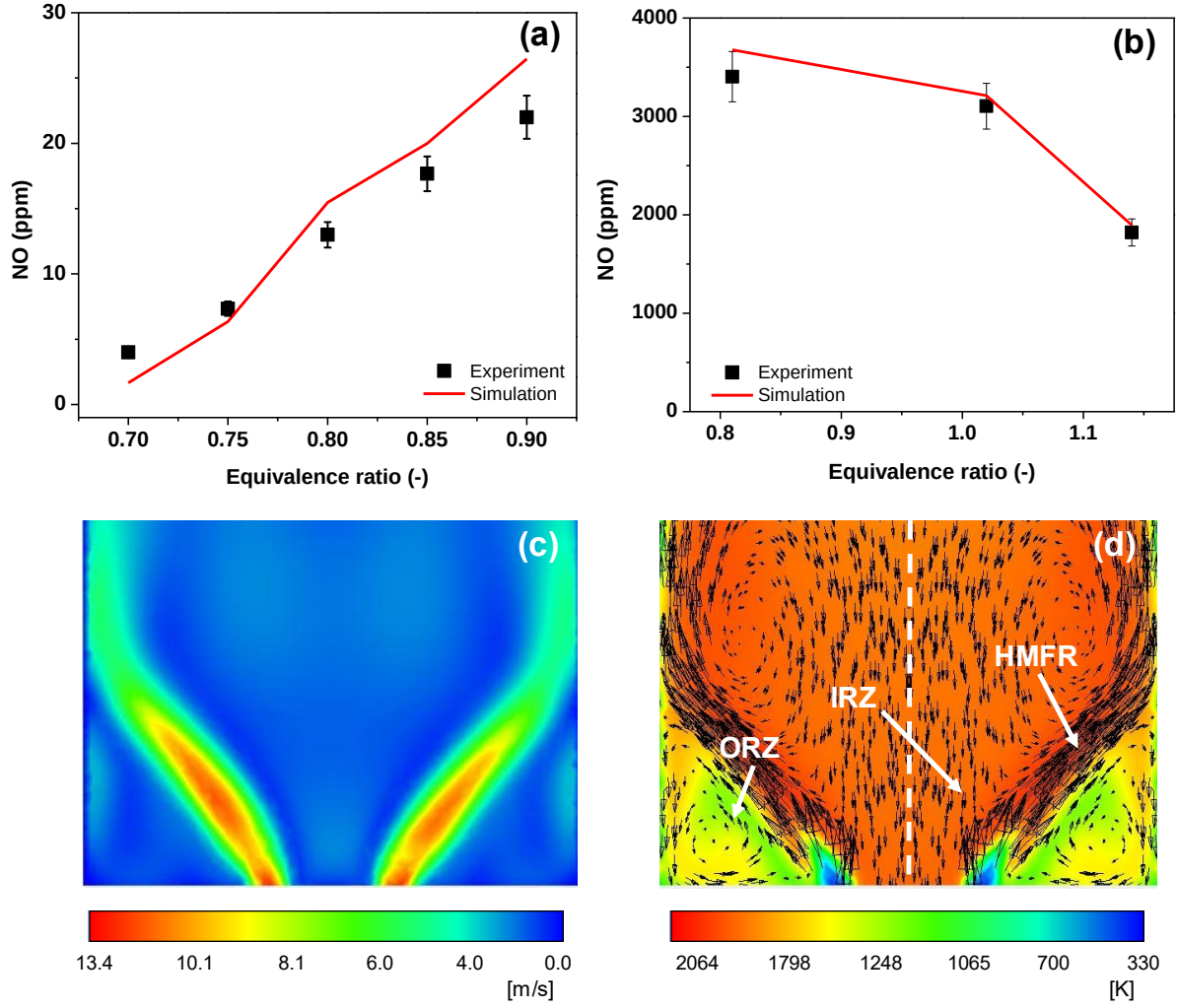


Figure 3 Simulation results comparison with (a) experimental biogas NO emissions data obtained in section 2.1 and (b) experimental NO emissions data of 60/40 NH_3/CH_4 published by [11]. (c) numerical velocity profile and (d) numerical flame temperature profile overlays with flow field vector for biogas swirl flame established at 7 kW input thermal power, $\varphi = 0.8$.

3.0 Result and Discussion

Figure 4 shows the normalised temperature profiles for the combustion of NH_3/CH_4 and $\text{NH}_3/\text{biogas}$. In the absence of CO_2 , fuel-lean operation at $\phi = 0.8$ increases the average reaction zone temperature (T_{avg}) by ~ 0.09 (Figure 4a & i) as the NH_3 mass fraction is raised from 20% to 60%. In the swirl-stabilised flame, the IRZ traps hot combustion gases due to the presence of central recirculating flow. Hence, higher temperature mixtures prevail within the IRZ. This aligns with flames characterised by the recirculation of burned gas documented by [37]. Increased NH_3 mass fraction lowers the mixture reactivity which slows down fuel oxidation, causing the heat to build up and give rise to the local temperature as seen in Figure 4i, despite the overall lower mixture reactivity. This effect is augmented when CO_2 is added to the fuel mixture (Figure 4b, f & j), where T_{avg} is elevated by a factor of averaging 1.22 when compared with the operation without CO_2 (Figure 4a, e & i). Furthermore, the disparities in T_{avg} between C40N20, C40N40, and C40N60 are only marginal (~ 0.03), signifying that CO_2 is an effective heat absorbent agent at $\phi = 0.8$ operation. Furthermore, higher CO_2 molecular weight than CH_4 and NH_3 is also expected to decelerate the flow. As shown in Figure 5, the normalised velocity for C0N20 is constantly higher than that of C40N20. Increased mixture residential time scale consequently raises heat retention effect. Furthermore, CO_2 addition also suppresses the primary chain branching reaction $\text{H} + \text{O}_2 \rightarrow \text{O} + \text{OH}$ [38]. A comparatively high O_2 concentration is, therefore, needed to advance the primary chain branching reaction $\text{H} + \text{O}_2 \rightarrow \text{O} + \text{OH}$, resulting in the peak T_{avg} for C40N20 to take place at a leaner operation than C0N20. It was reported that elevating the CO_2 fraction in the CH_4/air from 0% to 60% shifted its peak laminar flame speed (S_L) from $\phi = 1.1$ to $\phi = 1.0$ [39]. This denotes that a comparatively high O_2 concentration is essential in achieving the peak S_L for the reactant doped with CO_2 .

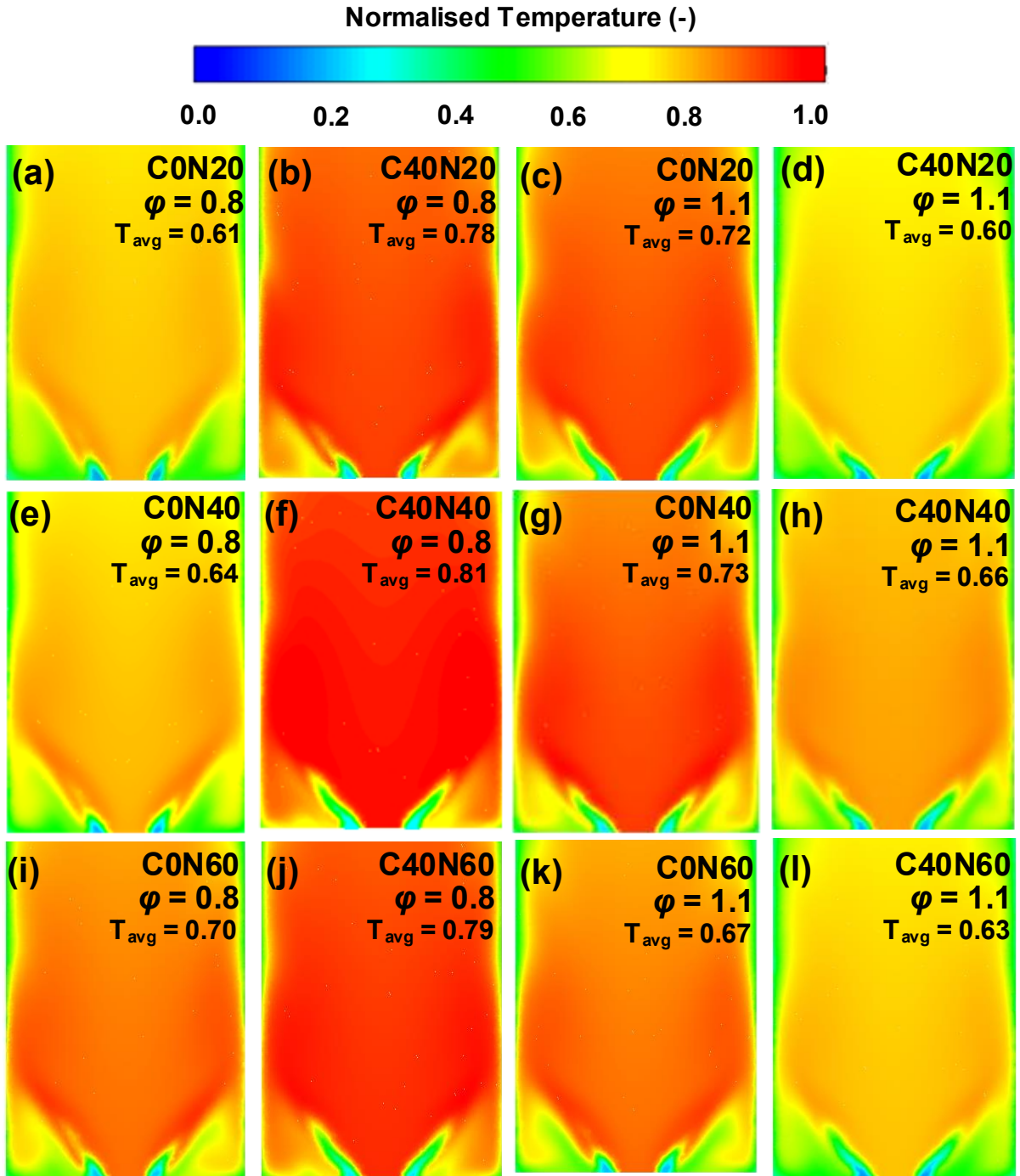


Figure 4 Normalised flame temperature for (a) C0N20 and (b) C40N20 at $\phi = 0.8$ combustions, (c) C0N20 and (d) C40N20 at $\phi = 1.1$ combustions, (e) C0N40 and (f) C40N40 at $\phi = 0.8$ combustions, (g) C0N40 and (h) C40N40 at $\phi = 1.1$ combustions, (i) C0N60 and (j) C40N60 at $\phi = 0.8$ combustions, (k) C0N60 and (l) C40N60 at $\phi = 1.1$ combustions.

Figure 4 also shows that at $\varphi = 1.1$ and in the absence of CO_2 , the T_{avg} for C0N20 and C0N40 (Figure 4c & g) are higher than their operation at $\varphi = 0.8$ by ~ 0.1 (Figure 4a & e). This is likely due to the peak S_L for neat methane taking place at about $\varphi = 1.1$ [28]. Excessive air supply at $\varphi = 0.8$ causes T_{avg} to decline by ~ 0.1 . In other studies, the maximum S_L for neat methane was found to be ~ 36 cm/s at $\varphi = 1.05$ and reduced by a factor of ~ 1.44 as φ lowered to 0.8 [28,40]. In contrast to C0N20 and C0N40, T_{avg} for C0N60 at $\varphi = 1.1$ is lower than that of $\varphi = 0.8$ by ~ 0.03 (Figure 4i & k). Unlike fuel-lean operation, air flow momentum is lowered at $\varphi = 1.1$. Weakened recirculating flow reduces the heat retention effect. This, along with the lowered mixture reactivity, results in the reduction of T_{avg} . For fuel mixture with CO_2 added (Figure 4d, h & l), the T_{avg} is reduced by averaging 0.16 as the combustion progresses from $\varphi = 0.8$ into $\varphi = 1.1$. This is partly due to the O_2 concentration in the air decreasing by a factor of ~ 1.38 from $\varphi = 0.8$ to 1.1, the presence of CO_2 intensifies the suppression of the primary chain branching reaction $\text{H} + \text{O}_2 \rightarrow \text{O} + \text{OH}$. In addition to suppressing the primary chain branching reaction $\text{H} + \text{O}_2 \rightarrow \text{O} + \text{OH}$, elevated CO_2 mass fraction also promotes the reaction $\text{H} + \text{O}_2 + \text{M} \rightarrow \text{HO}_2 + \text{M}$ that inhibits the formation of OH, O, and H radicals [41]. Together with the weakened heat retention at $\varphi = 1.1$, these lead to T_{avg} reduction by averaging 0.16. In a related study, it was shown that the disparities in S_L between syngas mixture with 0% and 34% CO_2 increased from 40 cm/s at $\varphi = 0.8$ to 60 cm/s at $\varphi = 1.1$ [38], denoting that the diluent effect of CO_2 is more pronounced at $\varphi = 1.1$ than $\varphi = 0.8$. Overall, increased NH_3 mass fraction at the $\varphi = 0.8$ NH_3/CH_4 combustion raises the T_{avg} , due to the heat retention. This effect is intensified with the addition of CO_2 . Furthermore, the higher CO_2 molecular weights, compared to CH_4 and NH_3 , also affect the molecular transport and residence time scale, elevating the T_{avg} in $\text{NH}_3/\text{biogas}$ combustion by a factor of averaging 1.2 as compared to NH_3/CH_4 . At $\varphi = 1.1$ combustion where the heat retention effect is reduced, increased NH_3 mass fraction in the

NH₃/CH₄ mixture results in a lower T_{avg} . In contrast to the $\varphi = 0.8$ operation, adding CO₂ at $\varphi = 1.1$ combustion does not elevate T_{avg} . The T_{avg} for NH₃/biogas is lowered by a factor of averaging 1.1 when compared with NH₃/CH₄. The reduction in O₂ concentration is another reason that contributes to the lower NH₃/biogas flame temperature at $\varphi = 1.1$ combustion.

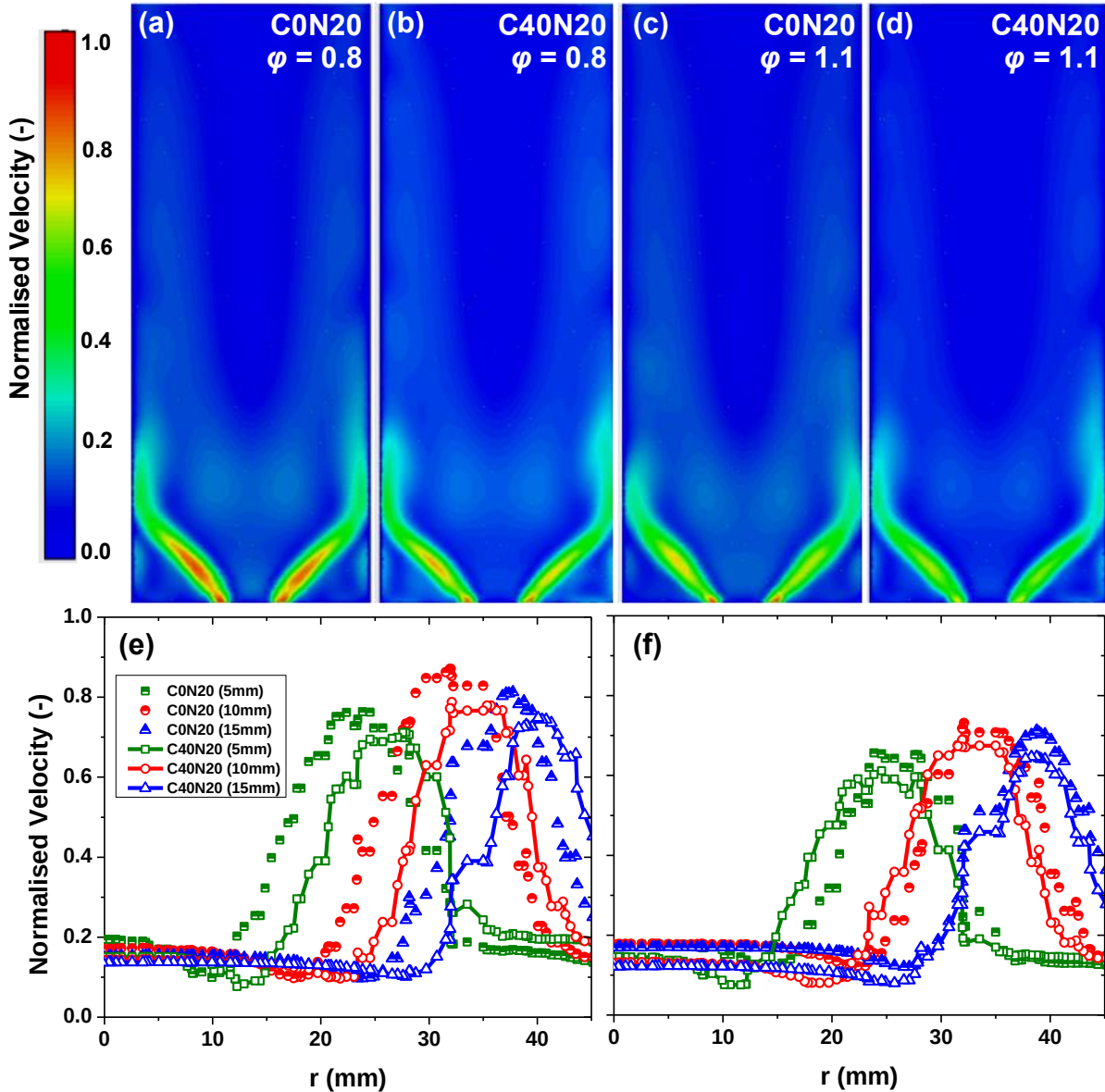


Figure 5 Normalised velocity for (a) C0N20, (b) C40N20 combustion at $\varphi = 0.8$, and (c) C0N20, (d) C40N20 combustion at $\varphi = 1.1$. Radial velocity profiles for C0N20 and C40N20 at (e) $\varphi = 0.8$ and (f) $\varphi = 1.1$ combustion.

Turbulence-flame interactions were characterised using the Damköhler number (Da) in this study. Figure 6 shows the Da at different streamwise locations at $h = 10$ mm, unveiling that in the fuel-lean operations of $\varphi = 0.8$, the IRZ peak Da for C0N20 (~ 35.35) is notably higher than those of C30N20 (~ 21.39) and C40N20 (~ 15.55). Nonetheless, as the global equivalence ratio progresses to 1.1, the disparities in IRZ peak Da among fuel mixtures are not illustrious. The peak Da for C30N20 increased from ~ 21.39 ($\varphi = 0.8$) to ~ 36 ($\varphi = 1.1$), and the peak Da for C40N20 increased from ~ 15.55 ($\varphi = 0.8$) to ~ 30 ($\varphi = 1.1$). Of which, the Da profiles for C0N20 and C30N20 practically overlap with one another. A similar trend is also seen in the HFMR, whereas in the fuel-lean combustion, the Da for C30N20 (Da ~ 3.1) and C40N20 (Da ~ 1.78) are lower than that of C0N20 (Da ~ 5.28). Conversely, the Da for all fuel mixtures in the fuel-rich combustion overlays in the HMFR, with an average Da of ~ 3.3 . The HMFR Da for C0N20 is reduced by ~ 1.98 while the HMFR Da for C40N20 is increased by ~ 1.52 when the combustion progresses from $\varphi = 0.8$ to 1.1.

The present study unveils that the variation in local Da is more sensitive to the increase in the global equivalence ratio when CO_2 is added to the NH_3/CH_4 mixture. The relatively large Da disparities between C0N20, C30N20, and C40N20 are practically diminished as the global equivalence ratio is raised from 0.8 to 1.1 (Figure 6). A similar trend is also observed for the mixture with 40 wt.% NH_3 . This is likely due to the increase in the length scale of the flame. The molecular weight of CO_2 is 2.74 and 2.58 times higher than those of CH_4 and NH_3 , respectively. A considerably higher CO_2 molecular weight causes it to diffuse slower as compared to CH_4 and NH_3 , especially at $\varphi = 1.1$ where the normalised flow velocity is reduced by ~ 0.15 as seen in Figure 5. Increased length scales of the flow are reflected in Figure 5, where the reacting flow field for the C40 mixture at $\varphi = 1.1$ shows visibly lower velocity in the HMFR and IRZ as compared to the C0 mixture at $\varphi = 1.1$. It was shown in a numerical study involving turbulent premixed combustion that the Da was elevated from 0.3 to 0.71 when the turbulent

Reynolds number was reduced by a factor of 2.5 from 208 to 82 (corresponding to a reduction in u'/S_L from 10 to 4) [42]. In another study, the Da was escalated from 0.27 to 2.63 as u'/S_L was reduced from 10 to 1 when the ratio between turbulent length scale and flame thickness was kept at 2.63 [43]. A similar trend was also observed when the ratio between the turbulent length scale and flame thickness was increased to 5.25, whereas the Da increased from 0.53 to 5.3 as u'/S_L reduced from 10 to 1 [43]. Overall, in the absence of CO₂, the changes in local Da are only marginal when the global equivalence ratio is increased from 0.8 to 1.1. Conversely, with the presence of CO₂, the increase in local Da is more prominent for the same variation in the global equivalence ratio, indicating the distinct impact of CO₂ on local flame-turbulence interactions at $\varphi = 1.1$.

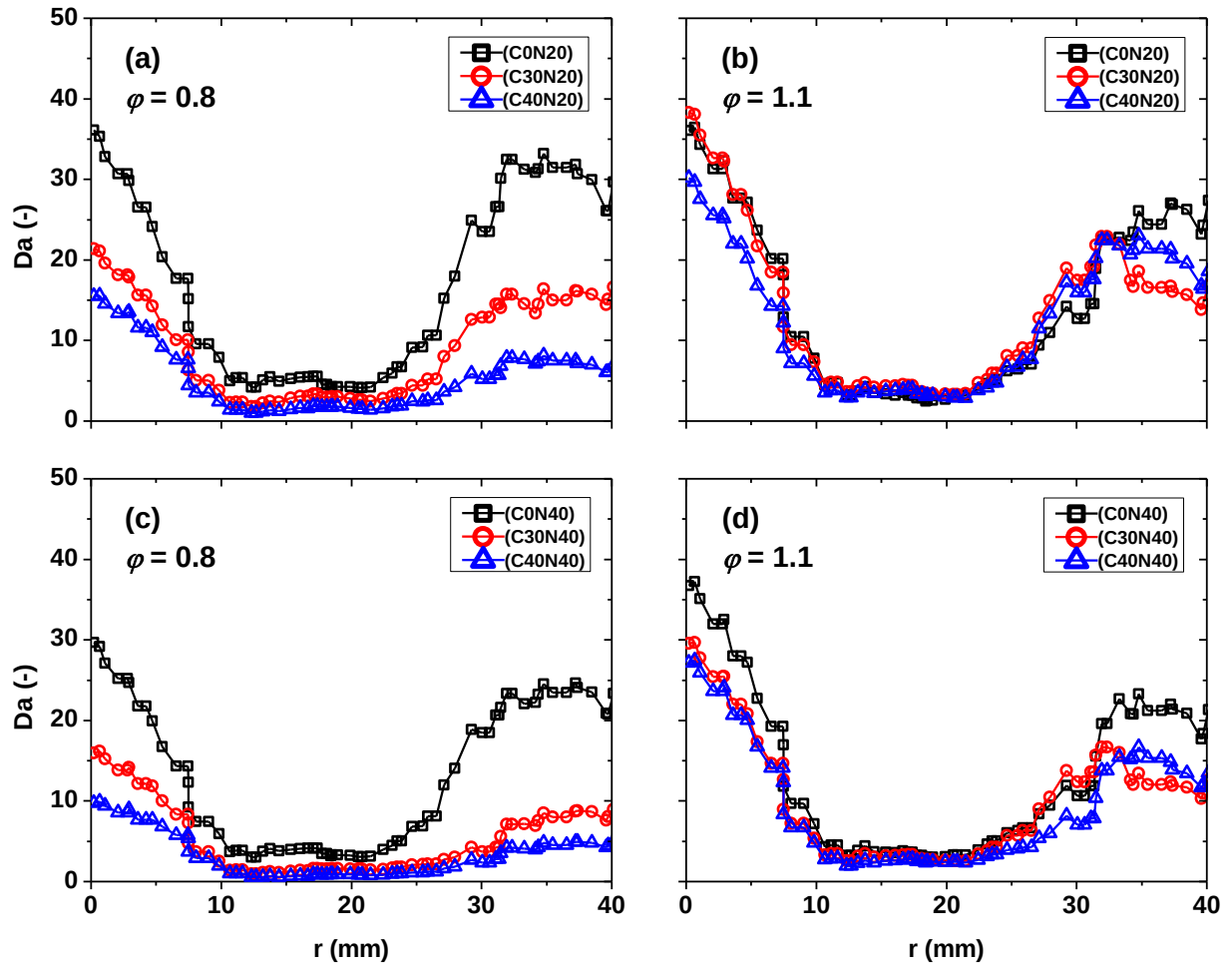


Figure 6 Variations of Da across streamwise location at $h = 10$ mm for (a) $\phi = 0.8$ (b) $\phi = 1.1$ for N20 fuel mixtures, and (c) $\phi = 0.8$ (d) $\phi = 1.1$ for N40 fuel mixtures.

Figure 7 shows that increased NH_3 mass fraction generally gives rise to the global NO emission index (EI_{NO}), whereas $\text{NH}_3/\text{biogas}$ typically results in notably higher EI_{NO} than NH_3/CH_4 from $\varphi = 0.9$ to 1.1. At $\varphi = 0.8$, however, EI_{NO} produced by $\text{NH}_3/\text{biogas}$ combustions are lower than that of NH_3/CH_4 by averaging 2.5 times (Figure 7b & c). As shown in Figure 8, $\text{N} + \text{OH} \rightarrow \text{NO} + \text{H}$ and $\text{H} + \text{HCNO} \rightarrow \text{CH}_2 + \text{NO}$ are two prominent reactions that lead to the NO formation, regardless of the variation in φ and fuel compositions. The $\text{N} + \text{OH} \rightarrow \text{NO} + \text{H}$ was also reported to be dominant, especially at near stoichiometric combustion by an early study [44]. The formation of nitrogen atoms at near stoichiometric conditions can be due to the dissociation of N_2 at high temperatures. Likewise, OH is produced at near stoichiometric via the thermal decomposition of water vapour (H_2O) and CO_2 through $\text{H} + \text{H}_2\text{O} \rightarrow \text{OH} + \text{H}_2$ and $\text{H} + \text{CO}_2 \rightarrow \text{CO} + \text{OH}$, respectively. HCNO (Isocyanic acid) is present due to the combustion of CH_4 and CO_2 in nitrogen-rich conditions that prompts the formation of HCN (Hydrogen Cyanide). HCN reacts with OH to form HCNO through the reaction $\text{HCN} + \text{OH} \rightarrow \text{HCNO} + \text{H}$. As depicted in Figure 8d, C40N40 exhibits a noticeable increase in $\text{N} + \text{OH} \rightarrow \text{NO} + \text{H}$ and $\text{H} + \text{HCNO} \rightarrow \text{CH}_2 + \text{NO}$ reactions when compared with C0N40, C40N20, and C0N20. A plausible reason is that increased CO_2 composition leads to a higher T_{avg} as illustrated in Figure 4f & h, thereby intensifying the $\text{N} + \text{OH} \rightarrow \text{NO} + \text{H}$ and $\text{H} + \text{HCNO} \rightarrow \text{CH}_2 + \text{NO}$ reactions.

When NH_3 mass fraction is increased to 60%, $\text{N} + \text{OH} \rightarrow \text{NO} + \text{H}$ and $\text{H} + \text{HCNO} \rightarrow \text{CH}_2 + \text{NO}$ remain the predominant pathways of producing NO. Other reaction pathways such as $\text{NH} + \text{O} \rightarrow \text{NO} + \text{H}$, and $\text{HNO} + \text{H} \rightarrow \text{NO} + \text{H}_2$ also emerge as important routes in producing the NO. Nonetheless, the NO formation via HNO (i.e. $\text{NH}_3 \rightarrow \text{NH}_2 \rightarrow \text{NH} \rightarrow \text{HNO} \rightarrow \text{NO}$) is not prevalent yet in $\varphi = 0.8\text{--}1.1$, it is expected to be more influential at a leaner operation such as $\varphi = 0.65$ as observed by [20]. As the global equivalence ratio marches into 1.1, the EI_{NO} for all fuel mixtures shows decreasing trends, primarily because of the reduction in the O_2 supply. Nevertheless, $\text{N} + \text{OH} \rightarrow \text{NO} + \text{H}$ and $\text{H} + \text{HCNO} \rightarrow \text{CH}_2 + \text{NO}$ remain the predominant

421 reactions that produce the NO, whereas $N + NO \rightarrow N_2 + O$ rests as the principal NO
 422 consumption route. Figure 7 also shows that the N_2O emission index (EI_{N_2O}) is generally
 423 increased as the mass fraction of NH_3 is raised from 20% to 60%. In low NH_3 combustion
 424 (Figure 7d), the disparities in EI_{N_2O} between NH_3 /biogas and NH_3/CH_4 are distinct. In the high
 425 NH_3 combustion (Figure 7f), however, the disparities in EI_{N_2O} between NH_3 /biogas and
 426 NH_3/CH_4 are not obvious. As shown in Figure 9, N_2O is mainly produced via NO consumption
 427 route $NH + NO \rightarrow N_2O + H$. When the NH_3 mass fraction is increased, a higher NO
 428 concentration promotes the production of N_2O . Overall, EI_{N_2O} decreases with the increase in
 429 the global equivalence ratio. The EI_{N_2O} for C40N20 is ~ 0.035 g/kg at $\phi = 0.8$ and reduced to
 430 ~ 0.025 g/kg at $\phi = 1.1$. A similar trend was also reported by Zhang et al. [45] where the N_2O
 431 emissions from the combustion NH_3/CH_4 with 30 vol.% CH_4 reduced by ~ 60 ppm as ϕ
 432 increased from 0.6 to 1.2 [45]. The N_2O is mostly consumed by $N_2O + H \rightarrow N_2 + OH$ and N_2O
 433 $+ H \rightarrow NNH + O$.

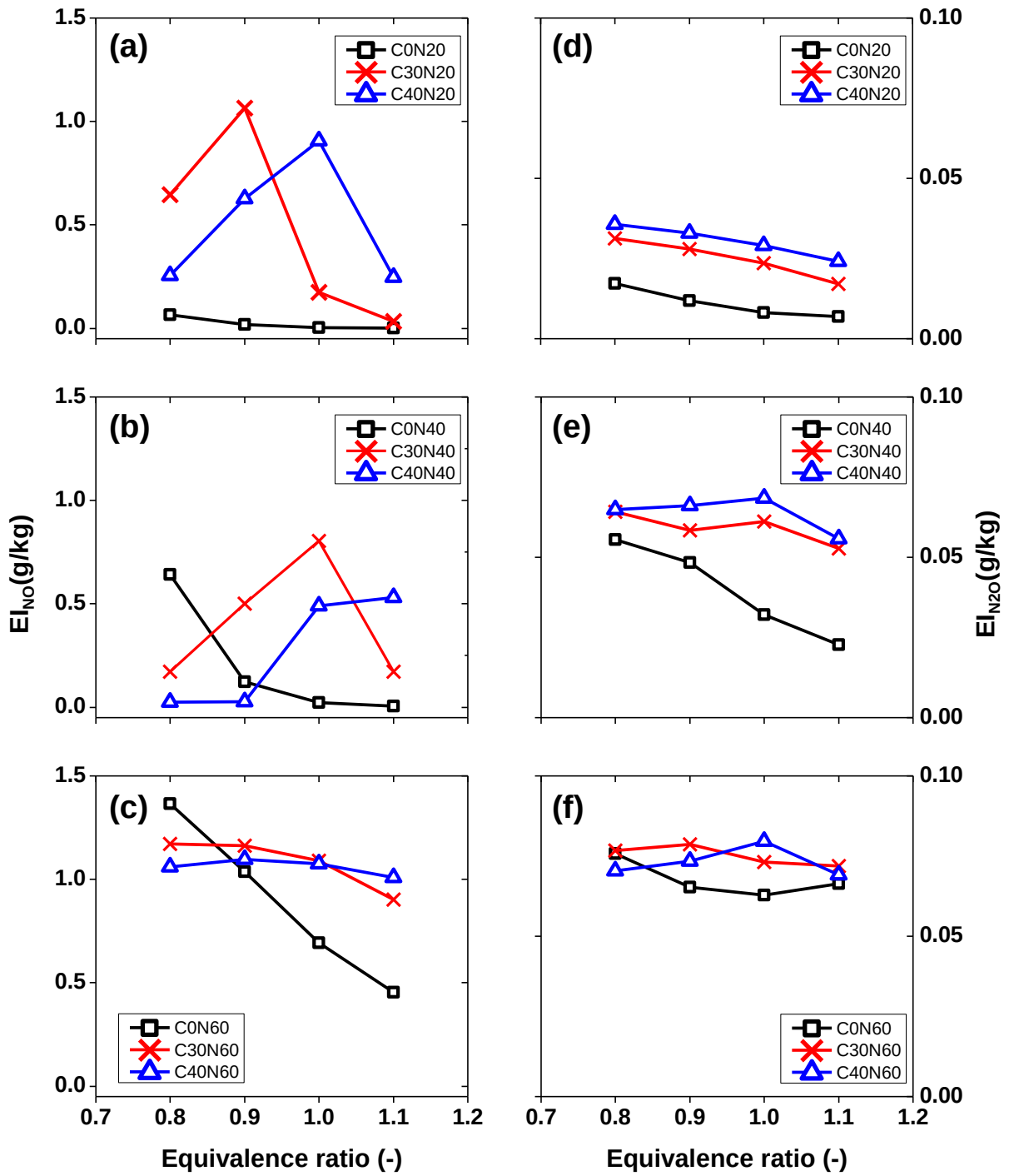


Figure 7 EI_{NO} for fuel mixtures with (a) 20 wt.% NH₃, (b) 40 wt.% NH₃, and (c) 60 wt.% NH₃ as global equivalence ratio varied from 0.8 – 1.1. EI_{N₂O} for fuel mixtures with (d) 20 wt.% NH₃, (e) 40 wt.% NH₃, and (f) 60 wt.% NH₃ as global equivalence ratio varied from 0.8 – 1.1.

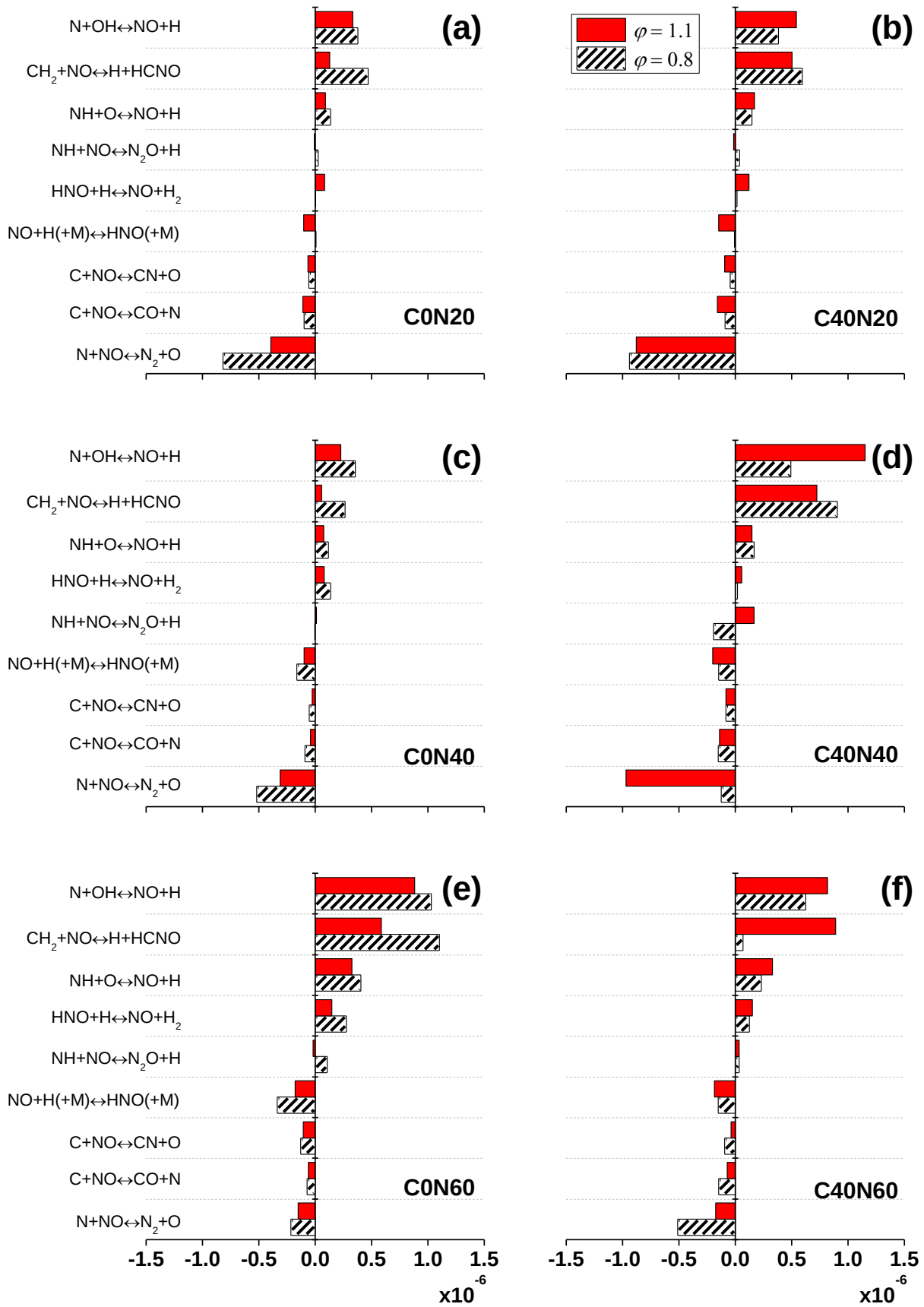


Figure 8 NO Rate of Production in the flame zone for (a) C0N20, (b) C40N20, (c) C0N40, (d) C40N40, (e) C0N60, (f) C40N60 at $\phi = 0.8$, and $\phi = 1.1$.

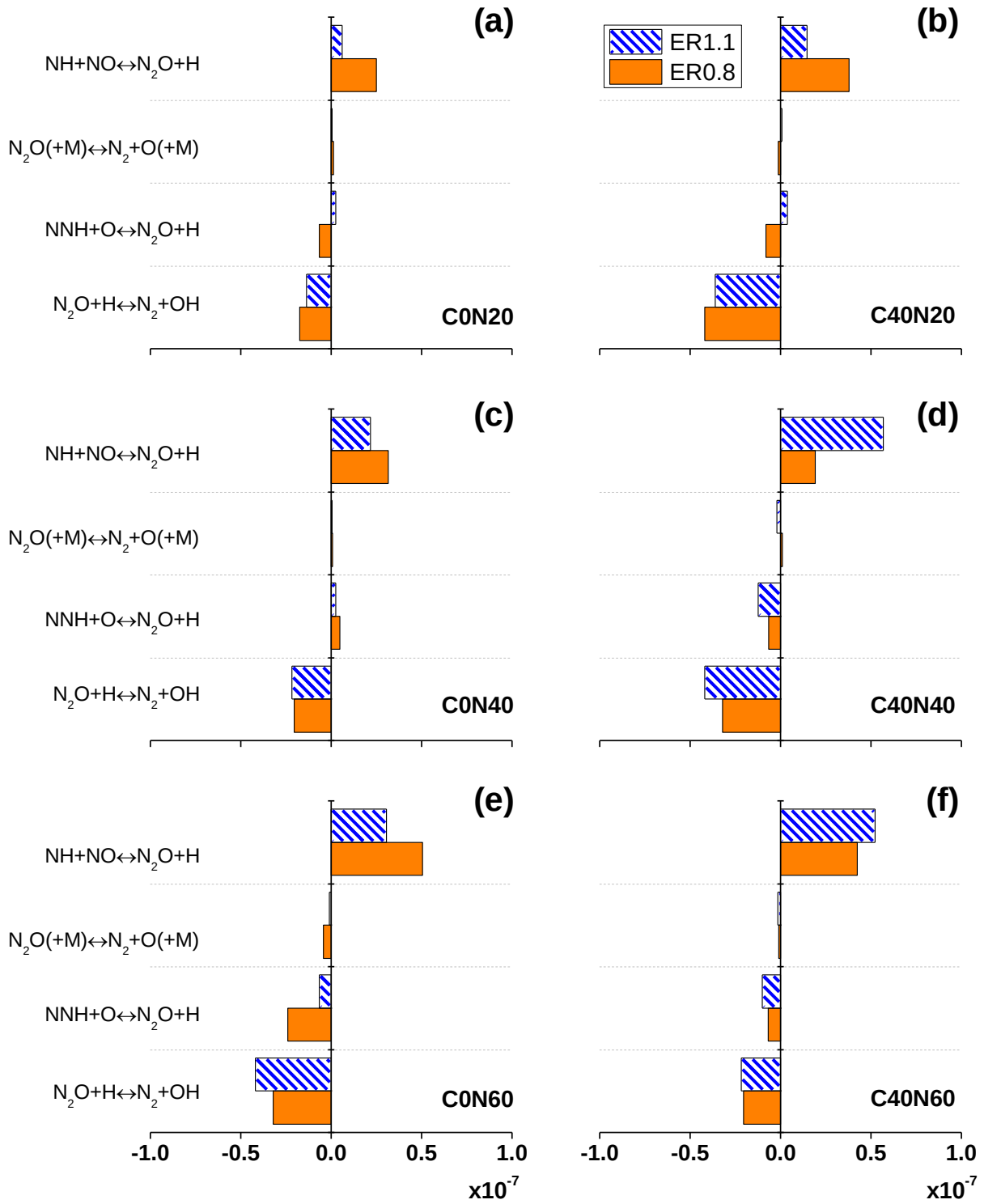


Figure 9 N₂O Rate of Production in the flame zone for (a) C0N20, (b) C40N20, (c) C0N40, (d) C40N40, (e) C0N60, (f) C40N60 at $\varphi = 0.8$, and $\varphi = 1.1$.

4.0 Conclusions

The swirl combustion of NH₃/biogas was examined at a global equivalence ratio of 0.8 – 1.1 via a numerical approach. Increasing NH₃ wt.% in NH₃/CH₄ combustion at $\varphi = 0.8$ elevated the T_{avg} because of the heat retention. It was augmented by CO₂ addition, raising the T_{avg} in NH₃/biogas combustion by a factor of averaging 1.2 as compared to NH₃/CH₄. At $\varphi = 1.1$, heat retention was weakened, and higher NH₃ mass fractions in NH₃/CH₄ turnout lower the T_{avg} . Unlike $\varphi = 0.8$, adding CO₂ at $\varphi = 1.1$ lowered T_{avg} in NH₃/biogas combustion by a factor of averaging 1.1 when compared with NH₃/CH₄. Furthermore, CO₂ also had a considerable influence on local flame-turbulence interactions at $\varphi = 1.1$, as evidenced by a notable rise in local Da for the same change in the global equivalence ratio. In the absence of CO₂, the changes in local Da were only minor when the global equivalence ratio was increased from 0.8 to 1.1. NO emission was mainly produced via $N + OH \rightarrow NO + H$ and $H + HCNO \rightarrow CH_2 + NO$. NH₃/biogas produced a higher EI_{NO} than NH₃/CH₄ from $\varphi = 0.9$ to 1.1, whereas escalated NH₃ wt.% generally prompted the NO formation. EI_{NO} decreased as φ approached 1.1, due to reduced O₂ supply. N₂O was mostly produced via $NH + NO \rightarrow N_2O + H$. The NH₃/biogas combustion produced noticeably more EI_{N_2O} than NH₃/CH₄ at low NH₃ operation, but the disparity was not distinct at high NH₃ combustion. The fuel-lean NH₃/biogas combustion at $\varphi = 0.8$ presents a viable approach to lowering EI_{NO} compared to NH₃/CH₄ combustion, where EI_{NO} was reduced by a factor of averaging 1.2 in the 60 wt.% NH₃ operation.

Acknowledgment

The authors gratefully acknowledge the funding support from UCSI University through the Research Excellence & Innovative Grant (REIG-FETBE-2024/007).

Reference

- [1] A. Valera-Medina, R. Banares-Alcantara, eds., *Techno-Economic Challenges of Green Ammonia as an Energy Vector*, Elsevier, 2021.
- [2] A. Valera-Medina, H. Xiao, M. Owen-Jones, W.I.F. David, P.J. Bowen, Ammonia for power, *Prog Energy Combust Sci* 69 (2018) 63–102. <https://doi.org/10.1016/j.pecs.2018.07.001>.
- [3] K.-H. Chung, Y.-K. Park, S.-J. Kim, S.-C. Kim, S.-C. Jung, Green hydrogen production from ammonia water by liquid–plasma cracking on solid acid catalysts, *Renew Energy* 216 (2023) 119052. <https://doi.org/https://doi.org/10.1016/j.renene.2023.119052>.
- [4] M.H. Khoshgoftar Manesh, S. Davadgaran, S.A. Mousavi Rabeti, New procedure for designing an innovative biomass-solar-wind polygeneration system for sustainable production of power, freshwater, and ammonia using 6E analyses, carbon footprint, water footprint, and multi-objective optimization, *Renew Energy* 230 (2024) 120802. <https://doi.org/https://doi.org/10.1016/j.renene.2024.120802>.
- [5] H. Driscoll, N. Salmon, R. Bañares-Alcántara, Exploiting the temporal characteristics of tidal stream power for green ammonia production, *Renew Energy* 226 (2024) 120377. <https://doi.org/https://doi.org/10.1016/j.renene.2024.120377>.
- [6] B. Farhang, H. Ghaebi, S. Naseri Gollo, N. Javani, Thermo-economic analysis of an innovative multi-generation system based on ammonia synthesis, *Renew Energy* 227 (2024) 120487. <https://doi.org/https://doi.org/10.1016/j.renene.2024.120487>.
- [7] R. Tu, C. Liu, Q. Shao, Q. Liao, R. Qiu, Y. Liang, Pipeline sharing: Optimal design of downstream green ammonia supply systems integrating with multi-product pipelines, *Renew Energy* 223 (2024) 120024. <https://doi.org/https://doi.org/10.1016/j.renene.2024.120024>.
- [8] J. Tian, L. Wang, Y. Xiong, Y. Wang, W. Yin, G. Tian, Z. Wang, Y. Cheng, S. Ji, Enhancing combustion efficiency and reducing nitrogen oxide emissions from ammonia combustion: A comprehensive review, *Process Safety and Environmental Protection* 183 (2024) 514–543. <https://doi.org/10.1016/j.psep.2024.01.020>.
- [9] G. Issayev, B.R. Giri, A.M. Elbaz, K.P. Shrestha, F. Mauss, W.L. Roberts, A. Farooq, Ignition delay time and laminar flame speed measurements of ammonia blended with dimethyl ether: A promising low carbon fuel blend, *Renew Energy* 181 (2022) 1353–1370. <https://doi.org/https://doi.org/10.1016/j.renene.2021.09.117>.
- [10] B. Luo, J. E, J. Chen, F. Zhang, J. Ding, Effect of NH₃/H₂/O₂ premixed combustion on energy conversion enhancement and NO_x emission reduction of the segmented nozzle micro-combustor in thermophotovoltaic system, *Renew Energy* 228 (2024) 120682. <https://doi.org/https://doi.org/10.1016/j.renene.2024.120682>.
- [11] A. Valera-Medina, R. Marsh, J. Runyon, D. Pugh, P. Beasley, T. Hughes, P. Bowen, Ammonia–methane combustion in tangential swirl burners for gas turbine power generation, *Appl Energy* 185 (2017) 1362–1371. <https://doi.org/10.1016/j.apenergy.2016.02.073>.
- [12] K.D.K.A. Somarathne, E.C. Okafor, D. Sugawara, A. Hayakawa, H. Kobayashi, Effects of OH concentration and temperature on NO emission characteristics of turbulent non-premixed CH₄/NH₃/air flames in a two-stage gas turbine like combustor at high pressure, *Proceedings of the Combustion Institute* 000 (2020) 1–8. <https://doi.org/10.1016/j.proci.2020.06.276>.

- [13] E.C. Okafor, K.D.K.A. Somarathne, A. Hayakawa, T. Kudo, O. Kurata, N. Iki, H. Kobayashi, Towards the development of an efficient low-NO_x ammonia combustor for a micro gas turbine, *Proceedings of the Combustion Institute* 37 (2019) 4597–4606. <https://doi.org/10.1016/j.proci.2018.07.083>.
- [14] Z. An, M. Zhang, W. Zhang, R. Mao, X. Wei, J. Wang, Z. Huang, H. Tan, Emission prediction and analysis on CH₄/NH₃/air swirl flames with LES-FGM method, *Fuel* 304 (2021) 121370. <https://doi.org/10.1016/j.fuel.2021.121370>.
- [15] M. Zhang, X. Wei, J. Wang, Z. Huang, H. Tan, The blow-off and transient characteristics of co-firing ammonia/methane fuels in a swirl combustor, *Proceedings of the Combustion Institute* 38 (2021) 5859–5868. <https://doi.org/10.1016/j.proci.2020.08.056>.
- [16] J. Zhang, C. Sui, B. Zhang, J. Li, Effects of swirl intensity on flame stability and NO emission in swirl-stabilized ammonia/methane combustion, *Applications in Energy and Combustion Science* 14 (2023). <https://doi.org/10.1016/j.jaecs.2023.100138>.
- [17] D. Füzesi, S. Wang, V. Józsa, C.T. Chong, Ammonia-methane combustion in a swirl burner: Experimental analysis and numerical modeling with Flamelet Generated Manifold model, *Fuel* 341 (2023). <https://doi.org/10.1016/j.fuel.2023.127403>.
- [18] D. Wei, H. Fang, L. Hu, Y. Rong, H. Zhou, Effect of acoustic excitation on the combustion and emission characteristics of methane-ammonia-air swirling flame, *Fuel* 352 (2023). <https://doi.org/10.1016/j.fuel.2023.129117>.
- [19] S. Mashruk, M.O. Viguera-Zuniga, M.E. Tejeda-del-Cueto, H. Xiao, C. Yu, U. Maas, A. Valera-Medina, Combustion features of CH₄/NH₃/H₂ ternary blends, *Int J Hydrogen Energy* 47 (2022) 30315–30327. <https://doi.org/10.1016/j.ijhydene.2022.03.254>.
- [20] S. Mashruk, E.C. Okafor, M. Kovaleva, A. Alnasif, D. Pugh, A. Hayakawa, A. Valera-Medina, Evolution of N₂O production at lean combustion condition in NH₃/H₂/air premixed swirling flames, *Combust Flame* 244 (2022). <https://doi.org/10.1016/j.combustflame.2022.112299>.
- [21] S. Wang, C.T. Chong, T. Xie, V. Józsa, J.H. Ng, Ammonia/methane dual-fuel injection and Co-firing strategy in a swirl flame combustor for pollutant emissions control, *Energy* 281 (2023). <https://doi.org/10.1016/j.energy.2023.128221>.
- [22] G. Wang, T.F. Guiberti, S. Cardona, C.A. Jimenez, W.L. Roberts, Effects of residence time on the NO_x emissions of premixed ammonia-methane-air swirling flames at elevated pressure, *Proceedings of the Combustion Institute* 39 (2023) 4277–4288. <https://doi.org/10.1016/j.proci.2022.07.141>.
- [23] N. Jusoh, Y.F. Yeong, S.S.M. Lock, L.S. Lai, M.S. Suleman, Biomethane generation from biogas upgrading by means of thin-film composite membrane comprising Linde T and fluorinated polyimide: Optimization of fabrication parameters, *RSC Adv* 10 (2020) 3493–3510. <https://doi.org/10.1039/c9ra06358g>.
- [24] C.W.M. Ch'ng, Y.F. Yeong, N. Jusoh, N.H. Suhaimi, L.S. Lai, High performance membranes containing zeolitic imidazolate framework-8 and polysulfone for CO₂ removal from CH₄, *Journal of Chemical Technology and Biotechnology* 97 (2022) 995–1005. <https://doi.org/10.1002/jctb.6990>.

- [25] G. Ren, M. Chiong, C. Tung, J. Ng, S. Mashruk, Fuel-lean ammonia / biogas combustion characteristics under the reacting swirl flow conditions, *Fuel* 331 (2023) 125983. <https://doi.org/10.1016/j.fuel.2022.125983>.
- [26] N. Afzanizam, C. Tung, J. Ng, M. Tran, H. Chyuan, A. Valera-medina, Experimental and numerical studies on the premixed syngas swirl flames in a model combustor, *Int J Hydrogen Energy* 44 (2019) 24126–24139. <https://doi.org/10.1016/j.ijhydene.2019.07.158>.
- [27] A. Valera-Medina, D.G. Pugh, P. Marsh, G. Bulat, P. Bowen, Preliminary study on lean premixed combustion of ammonia-hydrogen for swirling gas turbine combustors, *Int J Hydrogen Energy* 42 (2017) 24495–24503. <https://doi.org/10.1016/j.ijhydene.2017.08.028>.
- [28] E.C. Okafor, Y. Naito, S. Colson, A. Ichikawa, T. Kudo, A. Hayakawa, H. Kobayashi, Experimental and numerical study of the laminar burning velocity of CH₄–NH₃–air premixed flames, *Combust Flame* 187 (2018) 185–198. <https://doi.org/10.1016/j.combustflame.2017.09.002>.
- [29] S. Mashruk, M. Kovaleva, A. Alnasif, C.T. Chong, A. Hayakawa, E.C. Okafor, A. Valera-Medina, Nitrogen oxide emissions analyses in ammonia/hydrogen/air premixed swirling flames, *Energy* 260 (2022). <https://doi.org/10.1016/j.energy.2022.125183>.
- [30] S. Mashruk, H. Xiao, D. Pugh, M. Chiong, J. Runyon, B. Goktepe, A. Giles, A. Valera-medina, S. Mashruk, H. Xiao, D. Pugh, M. Chiong, Numerical Analysis on the Evolution of NH₂ in Ammonia / hydrogen Swirling Flames and Detailed Sensitivity Analysis under Elevated Conditions hydrogen Swirling Flames and Detailed Sensitivity Analysis, *Combustion Science and Technology* 00 (2021) 1–28. <https://doi.org/10.1080/00102202.2021.1990897>.
- [31] Z. Tian, Y. Li, L. Zhang, P. Glarborg, F. Qi, An experimental and kinetic modeling study of premixed NH₃/CH₄/O₂/Ar flames at low pressure, *Combust Flame* 156 (2009) 1413–1426. <https://doi.org/https://doi.org/10.1016/j.combustflame.2009.03.005>.
- [32] O. Elishav, B. Mosevitzky Lis, E.M. Miller, D.J. Arent, A. Valera-Medina, A. Grinberg Dana, G.E. Shter, G.S. Grader, Progress and Prospective of Nitrogen-Based Alternative Fuels, *Chem Rev* 120 (2020) 5352–5436. <https://doi.org/10.1021/acs.chemrev.9b00538>.
- [33] B. Mayr, R. Prieler, M. Demuth, C. Hochenauer, The usability and limits of the steady flamelet approach in oxy-fuel combustions, *90* (2015) 1478–1489. <https://doi.org/10.1016/j.energy.2015.06.103>.
- [34] B. Mayr, R. Prieler, M. Demuth, M. Potesser, C. Hochenauer, CFD and experimental analysis of a 115 kW natural gas fired lab-scale furnace under oxy-fuel and air – fuel conditions, *Fuel* 159 (2015) 864–875. <https://doi.org/10.1016/j.fuel.2015.07.051>.
- [35] Z. Turkeli-ramadan, R.N. Sharma, R.R. Raine, Two-dimensional simulation of premixed laminar flame at microscale, *Chem Eng Sci* 138 (2015) 414–431. <https://doi.org/10.1016/j.ces.2015.08.026>.
- [36] G.C. Krieger, A.P. V Campos, M.D.B. Takehara, F. Alfaia, C.A.G. Veras, Numerical simulation of oxy-fuel combustion for gas turbine applications, *Appl Therm Eng* 78 (2015) 471–481. <https://doi.org/10.1016/j.applthermaleng.2015.01.001>.

- [37] W. Meier, X.R. Duan, P. Weigand, Investigations of swirl flames in a gas turbine model combustor: II. Turbulence-chemistry interactions, *Combust Flame* 144 (2006) 225–236. <https://doi.org/10.1016/j.combustflame.2005.07.009>.
- [38] F. Pignatelli, S. Derafshzan, D. Sanned, N. Papafilippou, R.Z. Szasz, M.A. Chishty, P. Petersson, X.S. Bai, R. Gebart, A. Ehn, M. Richter, D. Lörstad, A.A. Subash, Effect of CO₂ dilution on structures of premixed syngas/air flames in a gas turbine model combustor, *Combust Flame* 255 (2023). <https://doi.org/10.1016/j.combustflame.2023.112912>.
- [39] Z. Wang, S.C. Yelishala, G. Yu, H. Metghalchi, Y.A. Levendis, Effects of Carbon Dioxide on Laminar Burning Speed and Flame Instability of Methane/Air and Propane/Air Mixtures: A Literature Review, *Energy and Fuels* 33 (2019) 9403–9418. <https://doi.org/10.1021/acs.energyfuels.9b02346>.
- [40] E.C. Okafor, Y. Naito, S. Colson, A. Ichikawa, T. Kudo, A. Hayakawa, H. Kobayashi, Measurement and modelling of the laminar burning velocity of methane-ammonia-air flames at high pressures using a reduced reaction mechanism, *Combust Flame* 204 (2019) 162–175. <https://doi.org/10.1016/j.combustflame.2019.03.008>.
- [41] S. Li, X. Zhang, D. Zhong, F. Weng, S. Li, M. Zhu, Effects of inert dilution on the lean blowout characteristics of syngas flames, *Int J Hydrogen Energy* 41 (2016) 9075–9086. <https://doi.org/10.1016/j.ijhydene.2016.02.099>.
- [42] I. Han, K.Y. Huh, Roles of displacement speed on evolution of flame surface density for different turbulent intensities and Lewis numbers in turbulent premixed combustion, *Combust Flame* 152 (2008) 194–205. <https://doi.org/10.1016/j.combustflame.2007.10.003>.
- [43] A.R. Varma, U. Ahmed, M. Klein, N. Chakraborty, Effects of turbulent length scale on the bending effect of turbulent burning velocity in premixed turbulent combustion, *Combust Flame* 233 (2021). <https://doi.org/10.1016/j.combustflame.2021.111569>.
- [44] G.A. Lavoie, J.B. Heywood, J.C. Keck, Experimental and Theoretical Study of Nitric Oxide Formation in Internal Combustion Engines, *Combustion Science and Technology* 1 (1970) 313–326.
- [45] M. Zhang, Z. An, L. Wang, X. Wei, B. Jianayihan, J. Wang, Z. Huang, H. Tan, The regulation effect of methane and hydrogen on the emission characteristics of ammonia/air combustion in a model combustor, *Int J Hydrogen Energy* 46 (2021) 21013–21025. <https://doi.org/10.1016/j.ijhydene.2021.03.210>.