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Simulation of Sustainability and Energy Efficiency of NH3/CH4 Co-firing Flames in Swirl Combustors

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Abstract

Ammonia has emerged as a promising candidate due to its carbon-free and renewable nature. As a green energy carrier, ammonia can significantly reduce greenhouse gas emissions, but its utilization as a fuel faces challenges, including lower laminar flame speed, lower adiabatic flame temperature, higher ignition energy, narrower flammability limits, and increased nitrogen oxide emissions. To investigate their sustainability and energy efficiency, the study aims to simulate NH_3/CH_4 co-firing flames in a swirl combustor. The research focuses on premixed NH_3/CH_4/air reactants with varying methane fractions (0%, 25%, 50%, 75%, and 100%) at standard atmospheric pressure. The study simulates the steady flow field using ANSYS Fluent and the RNG k-ε model and uses the results for unsteady simulations. Through the simulation, it indicates a trade-off between CO_2 and NO_x emissions. High CO_2 emissions correspond to the complete combustion of methane, while low CO_2 emissions indicate incomplete combustion, resulting in unburned methane. From the simulation results, 25% of methane fraction, with its highest energy efficiency and temperature, emerges as the most sustainable despite producing unwanted NO_x emissions. Overall, 25% of methane fraction results are identified as the optimal mixture for energy production, highlighting the need for balancing efficiency and emission controls in sustainable combustion processes.

1. Introduction

The imperative to mitigate CO_2 emissions and address global warming has propelled the exploration of carbon-free fuels as a key strategy. Midst the various alternatives, ammonia (NH_3) has emerged as a promising candidate due to its carbon-free and renewable nature. As a result, ammonia has gained attention as a green energy carrier with the potential to significantly contribute to the reduction of greenhouse gas emissions. However, the utilization of ammonia as a fuel faces challenges that limit its widespread adoption. Ammonia exhibits distinctive characteristics compared to conventional hydrocarbon fuels, including a substantially lower laminar flame speed, lower adiabatic flame temperature, higher minimum ignition energy, narrower flammability limits, and increased nitrogen oxide, NOx emissions when compared to conventional hydrocarbon fuels [1-4]. These characteristics pose obstacles to its seamless integration into existing combustion systems. Lean premixed combustion (LPM) stands out as an effective approach for achieving low *Nox* emissions in gas turbines. Nevertheless, LPM combustion, when fueled with ammonia, introduces complexities such as blow-off, flashback, and thermoacoustic oscillation [5,6]. Of particular concern is the propensity for blow-off, a phenomenon where combustion extinguishes due to insufficient fuel-air mixture.

However, there is a challenge of using ammonia as a fuel. Ammonia has a slower rate of chemical reaction compared to hydrocarbon fuels. It is because ammonia has high nitrogen content compared to hydrocarbon fuels [7,8], and ammonia is toxic and dangerous. The poor combustion properties will limit its utilization as a direct substitute for standard fuels in internal combustion engines [9-11]. During the combustion process, the formation and the emissions of NOx will be affected at the same time. According to De Joannon et. al [12], the swirl burner designs configurations will contribute to enhance the flame stability by shaping the flame structure and preventing the flame from blowout or instability during ammonia combustion process. The optimal configurations of the swirl burner shows that it will produce a better air-fuel mixing [13,14]. This will lead to less local peak temperatures and lower the formation of NOx during the combustion process.

The research that has shown some developments in the understanding of these systems are limited and the results showed a series of challenges when using this fuel. The stabilization of premixed flame in lean premixed swirl burner is challenging due to the complex interaction between the dynamic fluid flow and fuel combustion chemistry [15-18]. Hydrogen and ammonia fuel combustion also produce amounts of NOx emission that leads to environmental pollution. Additionally, the Fukushima Renewable Energy Institute (FREA) has created new platforms for burning kerosene and liquid ammonia produced by solar and wind energy in a 50 kW micro-gas turbine [19]. It has been shown that ammonia-kerosene blends at various concentrations can be used to operate the equipment. Nevertheless, there is little evidence of ammonia/hydrogen mixtures being used in gas turbines to generate power [20]. Because this mix emits no CO_2, a sufficient understanding of it will lay the groundwork for moving forward with more sophisticated blends that contain ammonia and hydrogen.

In a gas turbine, combustion is a complicated process that combines heat transmission, reaction, and turbulence. Ammonia is a relatively new fuel, so there are a lot of challenges in simulating it. Some of these challenges include the necessity for high resolution meshes for complicated geometries, the need to describe turbulence/reaction interactions and the chemical kinetic mechanism for ammonia combustion [21-25]. Among these, thorough consideration of the chemical kinetic mechanisms is necessary to produce high-quality CFD analyses for suitable simulations of ammonia combustion that are reflective of experimental tests and suitable for industrial designs [26-28]. As a result, it is necessary to simplify the intricate ammonia combustion mechanisms and test them in a gas turbine combustor environment. Despite the paucity of research in the sector, it is obvious that there is a lot of potential for the development of novel processes, CFD models, experimental configurations, and industrial designs.

While extensive experimental research has explored blow-off characteristics of compact flames, there remains a notable gap in understanding when it comes to numerical simulations focused on ammonia/methane NH_3/CH_4 co-firing flames in swirl combustors. Hence, this research focuses on numerical simulations to study blow-off characteristics and stretch rates of NH_3/CH_4 co-firing flames in swirl combustors. To investigate a sustainability, energy efficiency, and optimal methane fractions, this research will utilize a premixed swirl burner with varying methane ratios (0%, 25%, 50%, 75%, 100%) under standard atmospheric conditions through the simulation work. The simulation employs the RNG k-ε model for steady flow simulations, transitioning to unsteady simulations based on initial calculation results. This approach seeks to deepen insights into the dynamics of co-firing combustion, contributing to advancements in combustion science through CFD analysis.

2. Methodology

This investigation simulates gaseous fuel flow in a swirl combustor using SolidWorks for 3D modelling, which is then imported into ANSYS Fluent for CFD analysis. ANSYS Fluent models fluid flow, heat transfer, and chemical reactions. The study focuses on gaseous flow and combustion analysis, providing insights into combustion patterns, flame velocity, temperature, and stretch rate. CFD involves three stages: pre-processing (geometry modeling), solver, and post-processing, each interconnected to optimize the design and performance of the swirl combustor and combustion chamber.

2.1 Configuration Model of Swirl Combustor

The simulated combustion process of ammonia-hydrogen combustion in a swirl burner is based on the actual experimental setup from previous study by Dániel Füzesi et. al [29]. The computational domain of the swirl burner, as well as the related components and boundary condition locations, are shown in Fig. 1. The swirler in the combustor body setup comprises 8 blades with startup angle 45° while the height 25mm are shown in Fig. 2. The pin of the combustor has 25mm and 13mm diameter respectively of its head and its tail. The total length of the pin is 45mm. The external angle of the head to its tail are 135°. For combustion chambers are in a cylindrical geometry with diameter of 60mm and height of 62mm. It's also had a circular slot for easy for mating during assembly afterwards. The slot has depth of 2mm and diameter of 35mm which same with the diameter of the body.

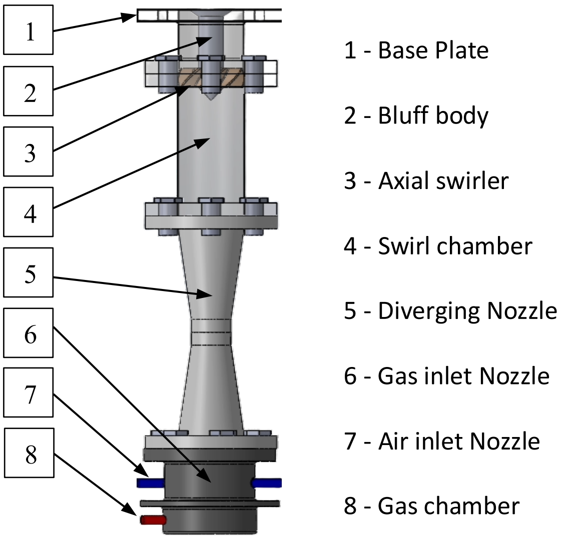


Fig. 1 *Swirl combustor configuration model*

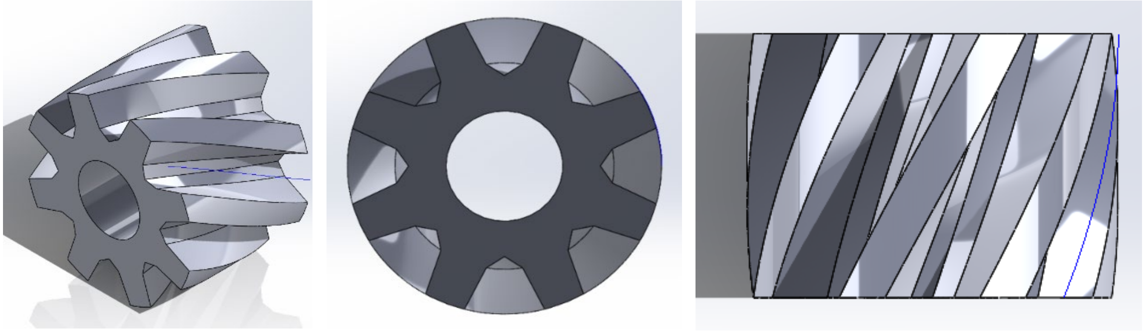


Fig. 2 *Drawing of swirler in different views*

The body of the model are a long cylinder which have height of 67mm and diameter of 35 mm. The pin and the swirler are located 2mm below to make the combustor separate with the combustion chamber. It also has 4 inlets attached from 7mm away from the center of the inlets to the bottom the cylinder. The diameter of the inlet is 7mm. The assembly is done after applying well mating with every parts. Firstly, the pin and the swirler were mate together into the right position and the rotate motion are available for the swirler. The body are then mate concentric to the pin and width 2mm below the upper surface of the body. The combustion chamber are last parts to be assemble on top of the body. The function of cavity for the pin and swirler are then added to the assemble to create the require model geometry. The assembly of the swirl combustor shown in Fig. 3, with the solid model and in term of wireframe to shows the swirler component inside the model.

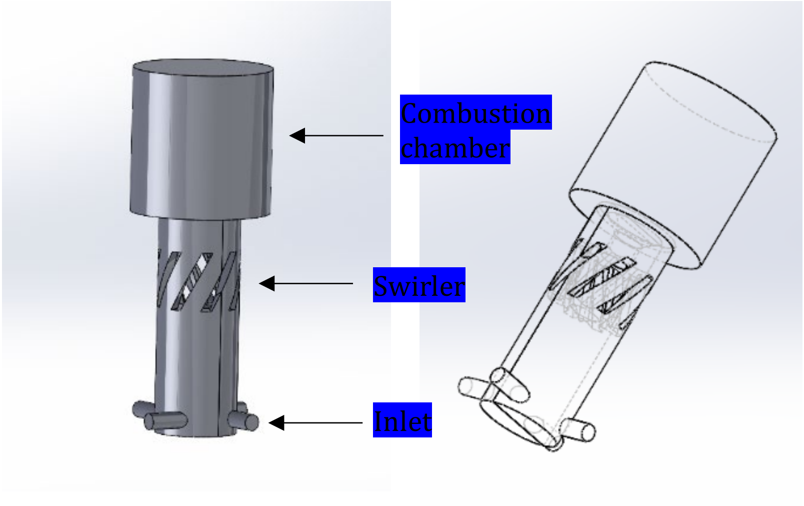
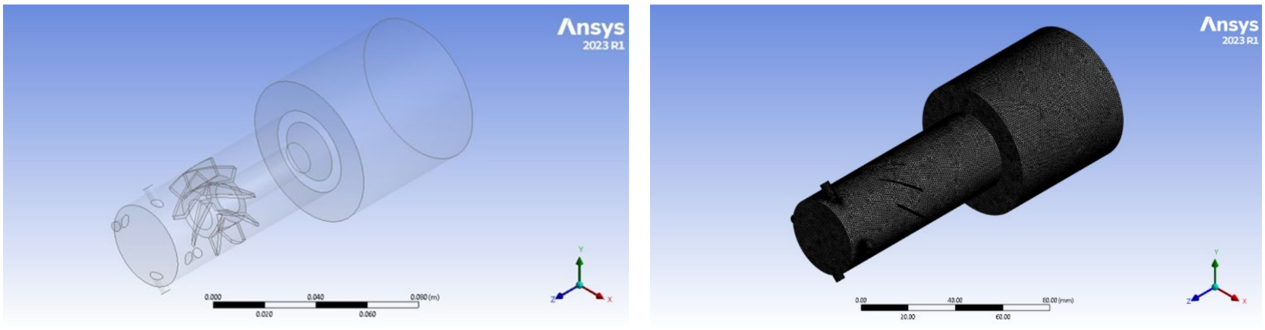


Fig. 3 *Simulation model for the swirl combustor*

2.2 Simulation Model and Meshing

The swirl burner geometry model consists of bluff body and axial swirler. The shape of the geometry model is three-dimensional. The swirl combustor has 4 inlets with the same diameter which the gases were injected with some amount of velocity. The length of the chamber is 90 mm, and the outlet dimension is 60 mm x 60 mm. Fig. 4(a) shows the geometry of combustor designed by Ansys design modeler. To use a high-quality mesh, a structured system containing about 800,000 cells was generated for the simulation of the combustor, as shown in Fig. 4(b). The mesh was refined in the middle section to better capture turbulence and reactions across the flame. The simulation was performed for 5 different ratios of mol percentage and species fuel of ammonia and hydrogen. Specific boundary conditions for this study are listed in Table 1 below.



(a) **(b)**

Fig. 4 *Simulation model and meshing (a) Geometry of the simulation model; (b) Meshing of the simulation model*

Table 1 *Boundary conditions for the simulation of swirl combustor*

Operating pressure	1 atm	
Air inlet velocity	30 m/s	
Fuel inlet velocity	30 m/s	
Oxidiser (Mol %)	O_2	21%
	N_2	79%
Fuel (Mol %) - Baseline	NH_3	50%
	H_2	50%
Ambient temperature	300 K	

In ANSYS Fluent, the setup, solution, and results are all put under a single section. In this section, accommodates a large number of variables and parameters, which can be flexibly manipulated to obtain different results. The physical parameters of the study, including the ratio of gas mixture and the fluid velocity at the inlet, are the main part of the setup.

ANSYS Fluent simulations focusing on the optimal methane-ammonia gas mixture for combustion and sustainability. Various ratios (1:0, 0.75:0.25, 0.5:0.5, 0.25:0.75, 0:1) are analyzed to identify the most efficient and eco-friendly combination. The ratios of each cases simulated summarised in Table 2 below, while the chemical equation of combustion of CH_4/NH_3 and NO_x formation are as in Table 3. Key factors like velocity, temperature, and pollutant mass fractions (NOx, CO_2) will be captured through the simulation work. The findings, visualized through contour maps, aim to enhance understanding of combustion processes and support sustainable energy solutions. Sub-chapters will compare and discuss results for each variable.

Table 2 *Ratio represent by the case*

Cases	Methane/Ammonia composition
Case 1	75% methane 25% ammonia
Case 2	50% methane 50% ammonia
Case 3	25% methane 75% ammonia
Case 4	100% ammonia

Table 3 *Chemical equation used for the fluid properties of CH4/NH3*

$$CH_4 + 2O_2 \rightarrow CO_2 + 2H_2O$$

$$CH_4 + 2O_2 \rightarrow CO_2 + 2H_2O$$

$$4NH_3 + 3O_2 \rightarrow 2N_2 + 6H_2O$$

Through a programme devoted to developing gas turbine combustors using ammonia mixes for power production, numerical results were compared and correlated with experimental data collected in prior campaigns. The NO emission obtained by the Large Eddy Simulation (LES) compared with experimental work by A. Valera-Medina et. al [30] and the comparison shows in Fig. 5. As can be shown, the model accurately anticipated that, generally speaking, the trend of NO emission varied with equivalency ratio. Further comparisons were made possible by the results' confidence, despite the expectation for more thorough validation work.

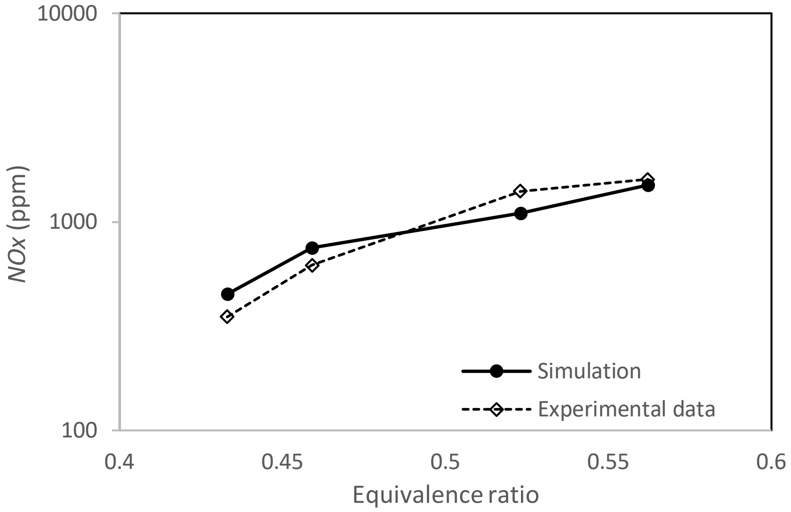


Fig. 5 *NOx emission results compared to simulation*

3. Results and Discussion

The focus for results is on determining which ratio of methane and ammonia gas mixture yields optimal combustion and sustainability. Through a series of detailed analyses and simulations, we will explore various gas mixture ratios to identify the most efficient and environmentally friendly combination. The factors of velocity, temperature, mass fraction of pollutant *Nox*, CO_2 and CH_4 will be discussed. This investigation is crucial for advancing an understanding of combustion processes and developing more sustainable energy solutions. The methane and ammonia gas ratios are represented as 1:0, 0.75:0.25, 0.5:0.5, 0.25:0.75, and 0:1, corresponding to case 1, case 2, case 3, case 4, and case 5 respectively.

3.1 Velocity and Temperature Distribution

Fig. 6 shows the results for temperature distribution for all cases simulated. The temperature patterns exhibit a similar flow style, spreading to both sides once entering the combustion chamber. Notably, case 4, with a ratio of 0.25:0.75, achieves the highest temperature of 650 K and also has the largest area where temperatures rise from green to red, indicating a range of 475 K to 650 K. Case 3 records the second highest temperature at 545 K, though the area of temperature increase is smaller compared to case 4. Cases 1, 2, and 5 exhibit a greenish-yellow tone at their highest temperatures, around 480 K. The temperature growth and the area of temperature increase can be observed from the figures showing that the static temperature rises from case 1 to case 4, then drops to the lowest in case 5, which disperses more and has the smallest area of temperature increase.

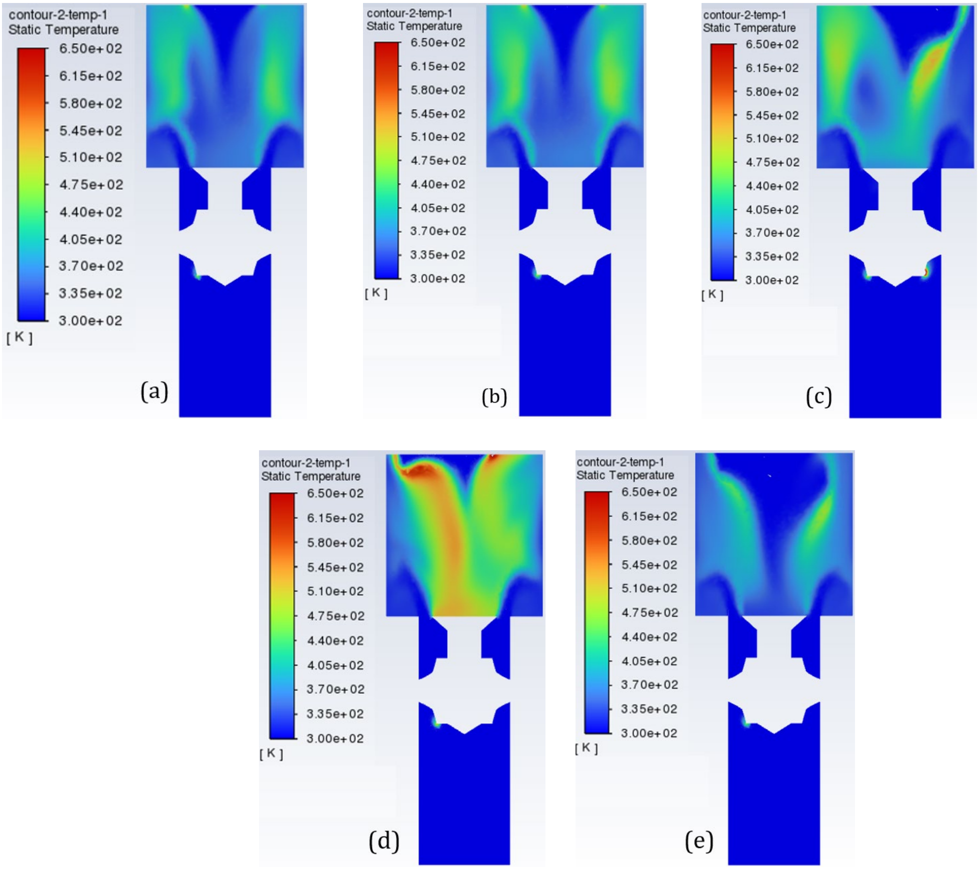


Fig. 6 *Temperature profile (a) case 1; (b) case 2; (c) case 3; (d) case 4; (e) case 5*

For the velocity, as shown in Fig. 7, its all exhibit a similar, almost identical pattern and velocity magnitude distribution throughout all parts of the model. The Initial inlet air velocity is set as 4 ms^{-1}. The result in Fig. 7 showed for the highest velocity magnitude are 24.4 ms^{-1}.

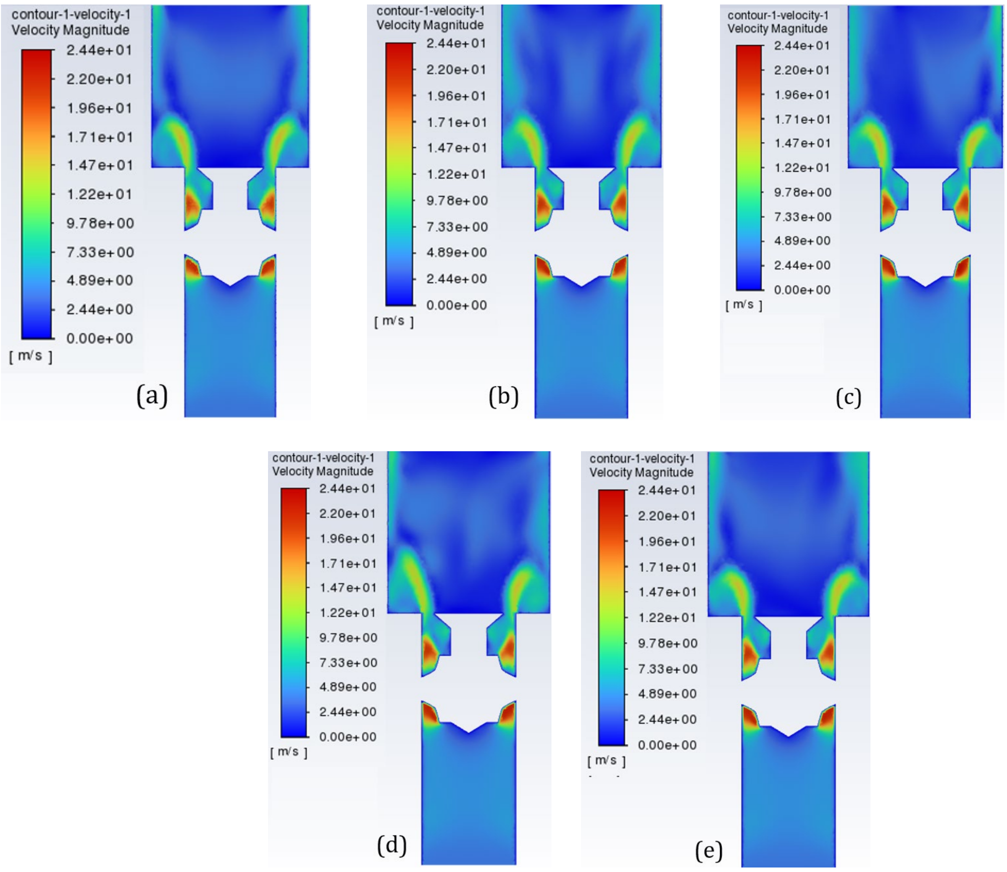
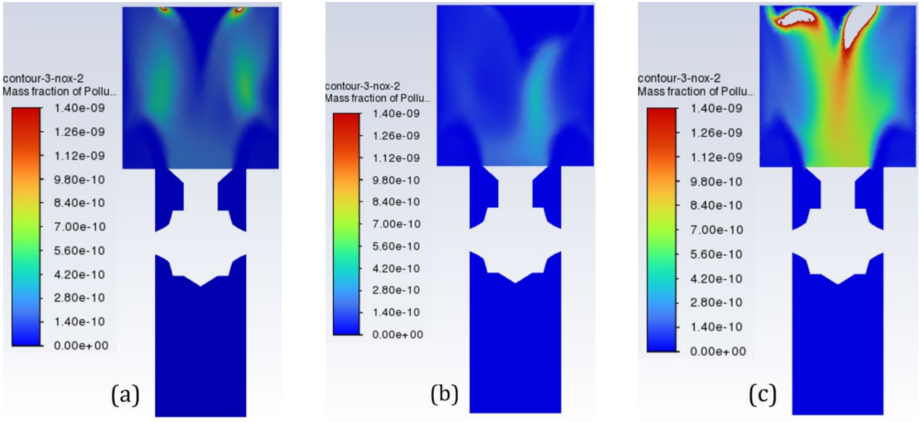


Fig. 7 *Velocity profile (a) case 1; (b) case 2; (c) case 3; (d) case 4; (e) case 5*

3.2 Mass Fraction of Pollutant *NOx*

Evaluate the mass fraction of pollutant *NOx* is important because nitrogen oxides contribute significantly to air quality issues and the formation of acid rain. Monitoring *NOx* levels is essential for assessing the environmental impact of the combustion process.

In terms of the mass fraction of pollutant *NOx*, we only consider cases 2, 3, 4, and 5. This is because, during the case 1 simulation, NH_3 does not participate in the combustion process. Notably, case 4 shows radical changes in tone; since I set the highest range display to 1.4e-9, the highest mass fraction of pollutant *NOx* in case 4 is not shown. This was done to ensure we could observe the gradient tones in the other cases. In case 5, which involves 100% ammonia gas, no pollutant *NOx* is produced, followed by case 3, which has the second lowest *NOx* production. Surprisingly, case 2 shows a higher and wider gradient color than case 3, indicating more *NOx* production. Fig. 8(e) shows the maximum mass fraction of *NOx* of case 4 fall on 2.0e-8.



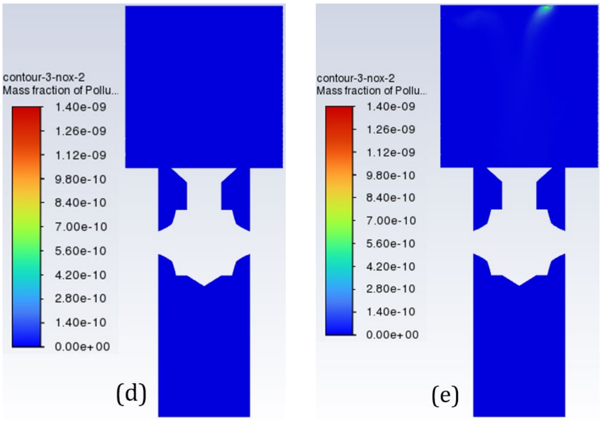


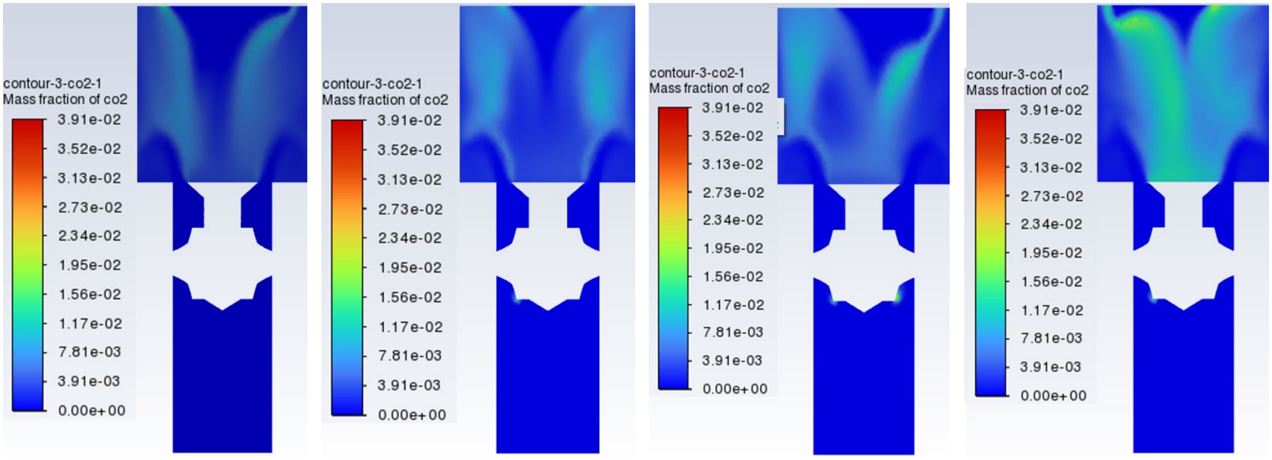
Fig. 8 *Mass fraction of NOx (a) case 1; (b) case 2; (c) case 3; (d) case 4; (e) case 5*

3.3 Mass Fraction of CO_2 and CH_4

Conversely, case 5 is not involved in these factors as NH_3 does not contain any carbon particles. The mass fraction of CO_2 clearly increases from case 1 to case 4, with case 4 having the highest value at approximately 2.10e-2. Cases 1, 2, and 3 have their highest values in the green tone, around 1.95e-2. The volume and tone become denser moving from case 1 to case 4, indicating a progressive increase in CO_2 production. All the results were clearly shown in Fig. 9(a) to 9(d) for cases.

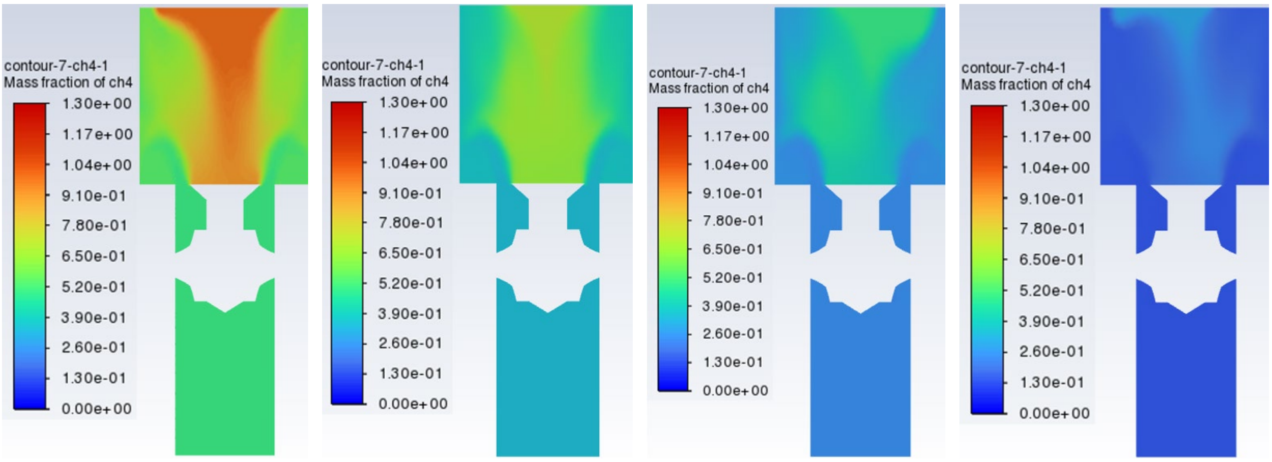
By evaluate the factors of the mass fraction of CH_4 as it helps to investigate the amount of un-burned methane. The presence of un-burned methane indicates incomplete combustion, which affects both the energy output and the emission characteristics of the fuel mixture. By analyzing the mass fraction of CH_4, we can determine how effectively each methane-ammonia ratio burns. From the Fig. 10(a), it is clear that case 1 has the highest and widest spread of CH_4, with a peak value of 1.04. The overall tone of case 1 appears as green, averaging around 0.65. For case 2, as shown in Fig. 10(b), the highest value is greenish-yellow at 0.71, with the overall tone being turquoise, around 0.45. Case 3 has a light blue overall tone, close to 0.26, while case 4's tone is blue, nearly approaching 0, as in Fig. 10(c) and 10(d) respectively. This indicates a decrease in the mass fraction of CH_4 from case 1 to case 4.

From the simulation results obtained, it has shown that the high carbon dioxide emissions correlate with low unburned methane and vice versa. It is because the emission of indicating the complete or incomplete combustion of methane. The lowest the emission of carbon dioxide the highest the unburned methane during the combustion. Whereas the pollutant, nitrogen oxide as the side product of combustion of ammonia which is unwanted. Since it will cause acid rain and other environmental issues.



(a) **(b)** **(c)** **(d)**

Fig. 9 *Mass fraction of CO2 (a) case 1; (b) case 2; (c) case 3; (d) case 4*



(a) **(b)** **(c)** **(d)**

Fig. 10 *Mass fraction of CH4 (a) case 1; (b) case 2; (c) case 3; (d) case 4*

4. Conclusion

In conclusion, velocity's uniformity of all cases indicates that the changes in the methane and ammonia ratios do not significantly impact the overall flow characteristics within the combustion chamber. Each case exhibits a consistent velocity profile, suggesting that other factors, such as temperature distribution and chemical reactions, may play a more critical role in determining the optimal fuel mixture for better combustion and sustainability.

Overall, case 4 emerges as the most sustainable among all five cases. It boasts the highest energy efficiency, facilitated by attaining the highest temperature during the combustion process, which is favorable for energy production. Despite exhibiting the highest level of CO_2 emissions, it virtually eliminates CH_4 emissions, indicating complete combustion of methane and minimal methane escape into the atmosphere, which is crucial for mitigating climate change. While Case 4 also shows the highest level of *NOx* emissions among the five cases, with maximum levels at 2.0e-8, these emissions are lesser than other fuel combustion and can be reduced through additional filtration or processing. To summarize, case 4, ratio of 0.25 methane: 0.75 ammonia stands out as the most sustainable option due to its high energy efficiency and potential for controlled emissions.

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Conflict of Interest

Authors declare that there is no conflict of interests regarding the publication of the paper.

Author Contribution

The authors confirm contribution to the paper as follows: ***study conception and design:*** *Mithun Mondal, Bukhari Manshoor, Kamarul-Azhar Kamarudin;* ***data collection:*** *Izzuddin Zaman, Reazul Haq Abdul Haq, Mohammad Fahmi Abdul Ghafir;* ***analysis and interpretation of results:*** *Djamal Hissein Didane, Mohd Fairusham Ghazali;* ***draft manuscript preparation:*** *Mithun Mondal, Nurhayati Baharudin, Sudher Kumar. All authors reviewed the results and approved the final version of the manuscript.*

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