Reproduction and Adaptation of Literature-Derived Modeling: Numerical Simulation of Methane/Hydrogen Non-Premixed Combustion

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It is crucial to reduce CO_2 (Carbon dioxide) emissions to mitigate climate impacts. A viable strategy for this reduction is to wholly or partially replace the use of natural gas with hydrogen, a carbon-free molecule, in the combustion processes of the industrial and residential sectors. In this context, the objective of this study is to investigate the combustion of methane/hydrogen binary mixtures using Computational Fluid Dynamics (CFD). Combustion will be simulated in the vertical non-premixed burner of the Senai CIMATEC Laboratory. To optimize computation time, a 2D axisymmetric model was developed. Fundamental aspects of combustion, including flow velocity, temperature, species formation, fuel consumption, and pollutant emissions, will be analyzed to evaluate the impact of partial methane substitution with hydrogen.

Keywords: Combustion. Hydrogen. Methane. Computational Fluid Dynamics.

By the early 2030s, an annual investment of USD 4.5 trillion will be needed to accelerate the deployment of clean energy technologies and infrastructure, up from USD 1.8 trillion in 2023 [1]. A strong dependence on natural gas characterizes the industry. Even in the paper, pulp, and printing industry, where renewables, biofuels, and electricity are more significant, natural gas still represents around one-quarter to one-third of final energy consumption in various sectors [2]. Blending hydrogen into natural gas is a cost-efficient alternative for transitioning to cleaner combustibles, enabling the use of existing pipelines and machinery for industrial and domestic purposes, such as burners and gas turbines.

This study provides a numerical approach to predict the effect of a hydrogen-enriched methane diffusion flame. Small additions of hydrogen were chosen to precisely understand and quantify the impact of incremental hydrogen concentrations on the combustion process. Previous works using flamelet models have achieved low error results when simulating non-premixed combustion blends of methane and hydrogen, showing good agreement with experimental data [3]. Kubilay Bayramoğlu and colleagues (2023) [3], Lotfi Ziani and colleagues (2012) [4], and Ravikanti (2009) [5] used GRI 3.0 mechanism to predict NOX formulation in a turbulent flame of blended methane and hydrogen. Their studies demonstrated excellent agreement with experimental data for temperature and major species.

Lotfi Ziani and colleagues (2012) [4] conducted a numerical study comparing the influence of changing modeling parameters. They achieved good results using the turbulence k- model for methane and hydrogen mixtures, with the approximation of experimental data becoming more accurate as the coefficient C1ε was increased. These numerical approaches reduce project budgets and process time while ensuring high accuracy in predicting combustion properties such as temperature, velocity, and species concentration.

Due to the differences in the properties of these two fuels, the flames exhibit distinct characteristics, necessitating technological adaptations in systems subjected to new conditions to minimize the impact on processes. Combustion behavior involves complex processes, including fluid flow, heat transfer, chemical reactions, and radiative heat

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transfer, all of which require detailed models for accurate numerical predictions. The complexity of fluids and combustion dynamics, coupled with varying fuel compositions, properties, and geometry, makes this a non-trivial task. By refining and applying these models, we aim to further enhance our understanding and control of hydrogen-enriched methane combustion systems for industrial applications.

Materials and Methods

A Computational Fluid Dynamics (CFD) approach, utilizing the Ansys Fluent software, has been chosen for this study of methane/hydrogen blend combustion. The 2D axisymmetric model presented here is a pressure-based steady model governed by two major equations [6]:

The continuity equation:

$$\nabla . \rho\vec{v} = 0 \tag{1}$$

Whith ρ (in kg/m^3), the density of the fluid and $\vec{v}$ the velocity (in m/s).

And the momentum equation:

$$\nabla . (\rho\vec{v}\vec{v}) = -\nabla p + \nabla . \tau + \rho g \tag{2}$$

With ρ the static pressure, ρg the gravitational body force, and τ the stress tensor, which is defined as:

$$\bar{\bar{\tau}} = \mu\left[(\nabla\vec{v} + \nabla\vec{v}^T) - \frac{2}{3}\nabla\vec{v}I\right] \tag{3}$$

Where μ is the molecular viscosity, and I is the unit tensor.

The turbulence treatment in this numerical study was performed using the RANS approach (Reynolds-Averaged Navier-Stokes equations) with the k-ε model. Various studies have shown that the precision of the k-ε model can be augmented by modifying the C1ε coefficient up to 1.6. [4,7]. For the simulations presented in this study, a C1ε of 1.5 has been chosen due to better accuracy in the results. The model has also been simplified to an adiabatic process, without considering radiation.

The different simulations have been conducted with a non-premixed model, a model particularly suited for diffusion flames. In this model, the thermochemical state of the fluid is represented by a conserved scalar quantity, the mixture fraction, noted f. It varies between 0 (pure oxidizer) and 1 (pure fuel), and can be written as:

$$f = \frac{X_i - X_{i,ox}}{X_{i,fuel} - X_{i,ox}} \tag{4}$$

Where $X\_\imath$ represents the elemental mass fraction for element i. The subscript "ox" is used to define the value at the oxidizer stream inlet, and the subscript "fuel" is used to define the value at the fuel stream inlet.

In addition to the non-premixed model, a steady laminar flamelet approach is used to represent the detailed chemistry and thermodynamics of a flame in a simplified manner. It assumes that the flame is composed of a series of thin, locally one-dimensional flame structures, known as flamelets. These flamelets are calculated using a chemical mechanism. The mechanism used in this study is the GRI Mechanism 3.0, a widely recognized and detailed chemical model consisting of 53 species and 325 reactions. It has already demonstrated accurate results in methane-hydrogen combustions [8,9].

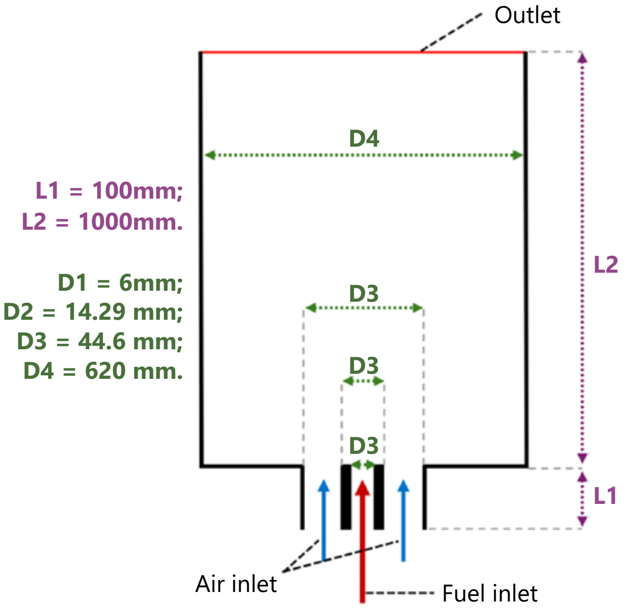
This adiabatic model, using the flamelet method, calculates energy based on pre-generated flamelet tables. These tables are generated by solving detailed chemistry for a range of mixture fractions and scalar dissipation rates, using the chemical mechanism thermodynamic data imported. Based on the local mixture fraction and dissipation rate, interpolations from these tables are then made to calculate temperature. This method captures the effects of detailed chemical kinetics and turbulence-chemistry interactions, allowing efficient and accurate determination of thermal properties without directly solving energy equations. A laminar opposed-flow diffusion flamelet is then calculated and embedded in a turbulent flame using the statistical Probability Density Function (PDF) method. The pressure-velocity coupling is achieved using the Simple algorithm, with the

Green-Gauss Gradient Schemes. At the same time, the equations of momentum, pressure, turbulent kinetic energy, turbulent dissipation rate, and species are discretized using a second-order scheme.

The model described earlier has been used to simulate the Sandia flame D [9-11]. Figure 1 illustrates that the numerical and experimental results are in close agreement, validating the model. The average of the error between numerical and experimental data is about 10.6 %, with a slight overprediction of the temperature from x/d = 25 to the exit of the combustion chamber. Before x/d = 25, the numerical model provides a temperature lower than the experimental data due to the flame starting further away (with d = 7.2 mm, the fuel inlet diameter of the system used for the Sandia Flame D experimental data acquisition).

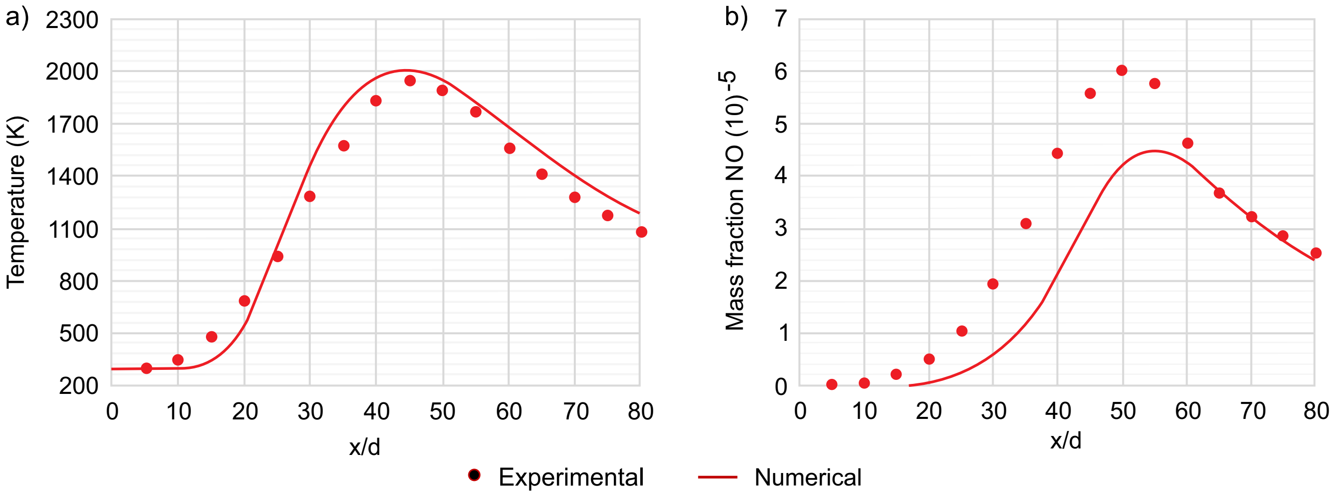
The circular shape of the vertical coaxial non-premixed burner used in this article for the simulations enables the creation of a numerical 2D axisymmetric model, as shown in Figure 2. A mesh of 65,700 cells was used for simulations. Significant refinement was applied along the axial direction and at the beginning of the combustion chamber to provide a more detailed mesh in the combustion zone, where the flame occurs. A total of 5 simulations were conducted in this study.

Figure 2. Burner geometry.



Each simulation was performed with a constant fuel inlet velocity of 12 m/s. The fuel mixtures used consisted of methane with varying concentrations of hydrogen, ranging from 0% to 20% (vol.). To maintain an equivalence ratio of 1 for each simulation, the air inlet velocity was adjusted accordingly, varying from 0.712 m/s for the 80% methane – 20% hydrogen fuel to 2.3 m/s for the 100% methane fuel. The walls are considered adiabatic, and the pressure outlet is fixed at 101,325 Pa.

Figure 1. Experimental and numerical data comparison of Sandi Flame D.



Results and Discussion

By adjusting the air velocity according to the hydrogen concentration in the fuel, five different simulations were conducted. The temperature contour of the five flames is presented in Figure 3.

It shows that increasing the hydrogen concentration in the fuel up to 20% reduces the length of the flame and increases the temperature slightly. Indeed, the maximum temperature calculated for the methane flame is 1,819 K. In contrast, the maximum temperature of the methane flame with 20 % hydrogen reaches 1,854 K. This increase in temperature can be attributed to the higher calorific value (PCI) of hydrogen compared to methane. Hydrogen has a higher energy content per unit mass, resulting in greater heat release during combustion. Additionally, hydrogen's higher flame speed enhances the combustion process, contributing to higher peak temperatures

The axial temperature profiles of the five flames, presented in Figure 4(a), allow us to observe that the maximum temperatures in the axial direction are reached between a length of 426 mm (for the methane fuel with 20% hydrogen) and 467 mm (for the 100% methane flame) along the centerline of the combustion chamber. The addition of hydrogen to the fuel accelerates the temperature rise, resulting in a steeper initial increase in temperature. This indicates that hydrogen enhances the combustion process, leading to quicker and higher peak temperatures. After reaching the peak temperature, the fuel with higher hydrogen content shows a faster reduction in temperature. This indicates that while hydrogen accelerates the heating process, it also leads to a faster cooling post-combustion phase compared to pure methane. This faster reduction in temperature can be attributed to several factors. Enriching methane with hydrogen accelerates the combustion process, promoting rapid heat release and energy transfer within the combustion chamber. This efficient combustion results in a more complete utilization of fuel energy, reducing

Figure 3. Temperature contours.

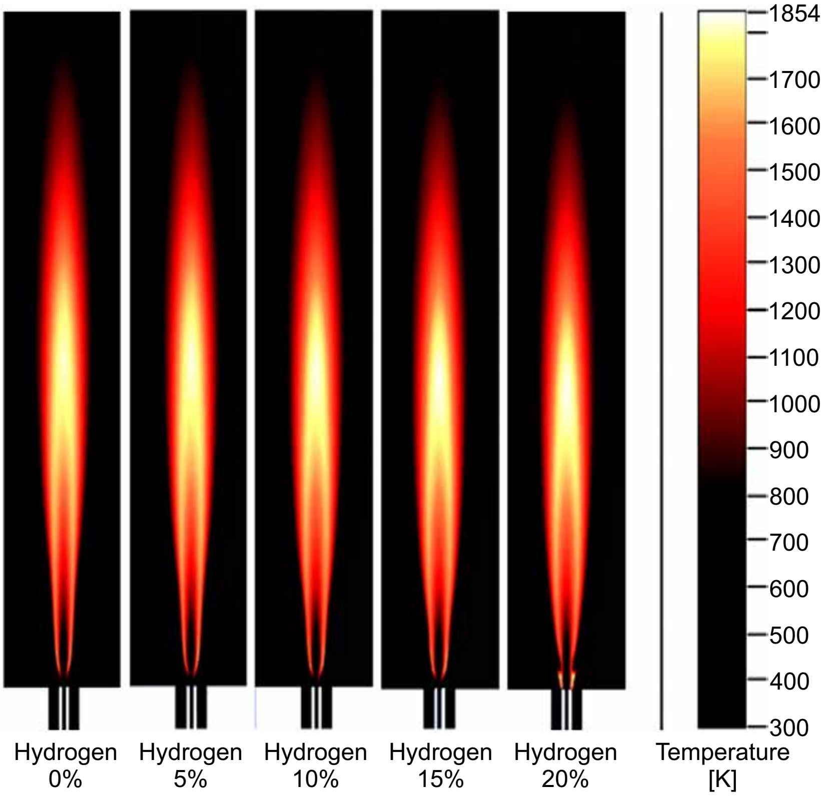
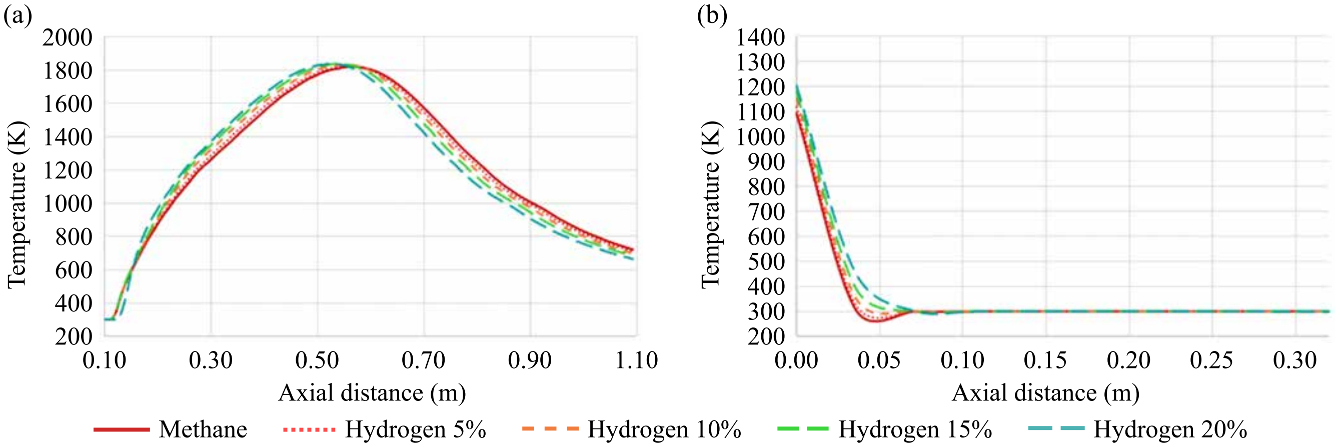


Figure 4. Temperatures along the central axial direction (a) and radial temperatures at x = 0.25 m (b).



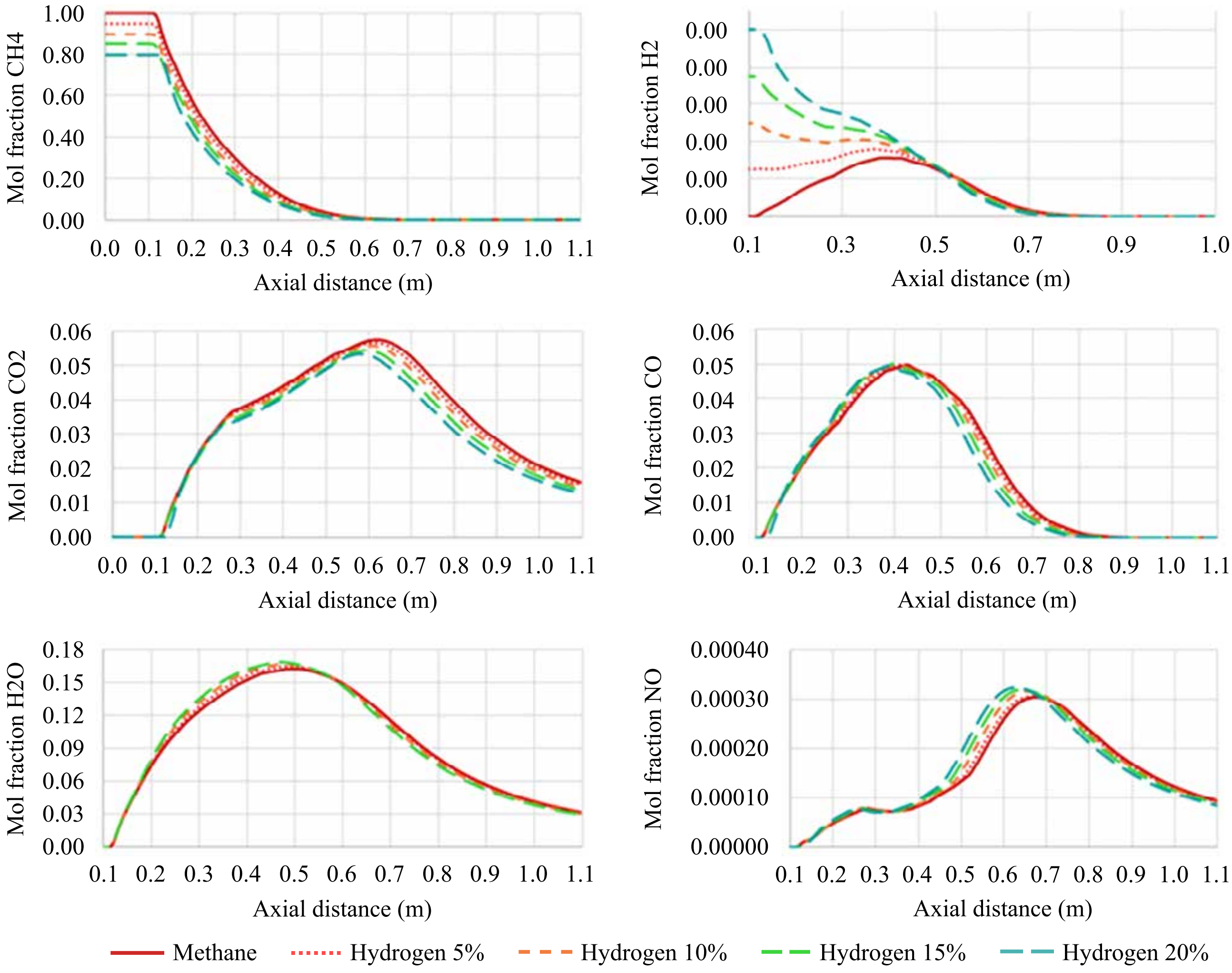
the residual heat in the combustion zone after peak temperature is reached. Moreover, the specific heat capacity of hydrogen is lower compared to methane, which means that it requires less energy to raise the temperatures of hydrogen-enriched flames, but also cools down faster once combustion is made. These dynamics show the hydrogen addition effect in combustion efficiency and post-combustion thermal dynamics. Figure 4(b) also shows the radial temperature profiles of the five flames at x = 0.25 m. It is observable that increasing the hydrogen concentration in the fuel results in a broader flame, due to higher temperatures from y = 0 to y = 0.075 m. For flames with lower hydrogen content, a slight temperature depression is observable around y = 0.4 m, indicating a less intense combustion process compared to hydrogen-enriched flames. This trend highlights that even small additions of hydrogen can significantly impact the flame structure and combustion characteristics.

Figure 5 shows the mol fraction of species along the combustion chamber. The addition of hydrogen to methane significantly alters flame behavior, accelerating the overall combustion process. The mole fraction of methane decreases rapidly along the flame axis, indicating efficient combustion of methane. Concurrently, the mole fractions of CO_2 and H_2O increase, reflecting the oxidation of methane. As hydrogen is introduced into methane, the mole fractions of the chemical species along the flame axis undergo notable changes. For a mixture with 5% hydrogen, methane still decreases rapidly; however, the presence of H_2 influences the product distribution.

For mixtures containing 15% and 20% hydrogen, the H_2 mole fraction decreases rapidly, attributed to the faster formation of H_2O for these mixtures, indicating a higher combustion rate of hydrogen compared to methane. With hydrogen addition, the H_2O fraction increases due to the additional contribution of hydrogen to water formation. All H_2 mole fractions decrease at approximately 36% of the axial distance of the combustion chamber. At this point, the CO fraction begins to increase slightly, indicating changes in oxidation pathways. Similar results are reported by Lotfi Ziani and colleagues (2012) [4].

The CO appears as an intermediate product of incomplete oxidation. In all mixtures, CO shows a noticeable increase in mole fractions, suggesting that the presence of hydrogen favors the formation of intermediate combustion products. The CO_2 fraction reaches its maximum at approximately x = 0.6 m of the combustion chamber, with a difference in mole fraction of 0.418% for the 20% hydrogen mixture compared to pure methane. The presence of hydrogen also tends to raise the flame temperature, which can explain the increase in CO mole fraction, a byproduct of incomplete combustion. It also increases the NO mole fraction. The variance of CO, CO_2, and NO

Figure 5. Species mole fraction along the central axial direction.



becomes significant by 27% of the axial distance of the combustion chamber. The rapid combustion rate of hydrogen also contributes to an increase in flame temperature. Hydrogen's higher diffusivity compared to methane allows it to spread more quickly and evenly in the fuel mixture, improving the air-fuel mixture and resulting in more efficient and complete combustion. As the hydrogen content in the mixture increases, the amount of carbon available for CO_2 formation decreases, leading to a significant reduction in CO_2 emissions. While hydrogen oxidation mainly produces water, combining with methane can lead to greater formation of CO and other intermediate products due to changes in chemical reactions and temperature distribution.

Previous studies have shown a substantial reduction in CO_2 emissions with increased hydrogen content in the mixture, attributed to hydrogen's carbon-free nature. Additionally, it has been observed that hydrogen addition enhances combustion efficiency due to the higher flame speed and superior diffusivity of hydrogen. This effect is consistent with observations in the combustion of hydrogen and ammonia mixtures, where increasing the hydrogen rate significantly enhances the maximum flame temperature and the surface area of the maximum temperature zone [4]. The results of this study also demonstrate that adding hydrogen leads to slightly higher temperature distributions in the central region of the flame. This increase in temperature can lead to higher NOx emissions.

Conclusion

The numerical model used in this study allowed for the investigation of the effect of hydrogen enrichment on methane fuel combustion within a coaxial non-premixed burner. The various simulations have demonstrated that adding a small hydrogen fraction (ranging from 0% to 20%) to methane fuel has a significant impact on global combustion.

Increasing the hydrogen amount in the fuel affects the flame structure, reducing its length and increasing its width. A slight temperature depression on the side of the flame, observable for methane combustion, disappears when hydrogen is added to the fuel. Moreover, it has been demonstrated that the maximum temperature of hydrogen-enriched fuels is higher. These two phenomena, observed at varying temperatures, affect the global flame behavior and have a significant impact on the species created during and after combustion.

Hence, the addition of hydrogen to methane also alters the distribution of chemical species. Higher hydrogen content results in a faster decrease in H_2, increased H_2O formation, and slightly higher CO due to changes in oxidation pathways. The flame temperature rises with the addition of hydrogen, which increases NOx emissions, as thermal NOx production is directly related to the flame temperature. The consistency of these results with previous studies reinforces the conclusion that adding hydrogen to fuel mixtures can improve combustion efficiency while reducing CO_2 emissions; however, it may also increase NOx emissions, presenting new challenges in emissions control.

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References

1. International Energy Agency. Scaling up of innovative clean energy technologies needed to achieve net zero emissions targets globally [Internet]. Available from: https://www.iea.org/news/scaling-up-of-innovative-clean-energy-technologies-needed-to-achieve-net-zero-emissions-targets-globally.
2. Eurostat. Industry relied mostly on natural gas & electricity [Internet]. Available from: https://ec.europa.eu/eurostat/web/products-eurostat-news/w/ddn-20230512-1.
3. Bayramoğlu K, Bahlekeh A, Masera K. Numerical investigation of the hydrogen, ammonia and methane fuel blends on the combustion emissions and performance. Int J Hydrogen Energy. 2023;48(99):39586-98. doi:10.1016/j.ijhydene.2023.06.079.
4. Ziani L, Chaker A, Chetehouna K, Malek A, Mahmah B. Numerical simulations of non-premixed turbulent combustion of CH4–H2 mixtures using the PDF approach. Int J Hydrogen Energy. 2013;38(20):8597-603. doi:10.1016/j.ijhydene.2012.11.104.
5. Ravikanti M, Hossain M, Malalasekera W. Laminar flamelet model prediction of NOx formation in a turbulent bluff-body combustor. J Power Energy. 2009.
6. Versteeg HK, Malalasekera W. Computational fluid dynamics: the finite volume method. 2nd ed. Harlow (UK): Pearson Education; 2007.
7. Sayadzadeh ME, Samani MR, Toghraie D, Emami S, Eftekhari SA. Numerical study on pollutant emissions characteristics and chemical and physical exergy analysis in mild combustion. Energy. 2023;278(Pt B).
8. Xiao J, Liu Q, He S, Wang S, Zhang Z. Numerical simulation on combustion characteristics of methane/hydrogen blended fuel for non-premixed conical bluff body burner. Int J Hydrogen Energy. 2024;65:50-60. doi:10.1016/j.ijhydene.2024.03.377.9.
9. Barlow RS, Frank JH. Proc Combust Inst. 1998;27:1087-95.
10. Barlow RS, Frank JH, Karpetis AN, Chen JY. Piloted methane/air jet flames: scalar structure and transport effects. Combust Flame. 2005;143:433-49.
11. Schneider C, Dreizler A, Janicka J. Flow field measurements of stable and locally extinguishing hydrocarbon-fuelled jet flames. Combust Flame. 2003;135:185-90.