



Hydrogen-Enriched Natural Gas Swirling Flame Characteristics: A Numerical Analysis

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ABSTRACT

Increasing the amount of hydrogen (H₂) in natural gas mixtures contributes to gas turbine (GT) decarbonisation initiatives. Hence, the swirling flame characteristics of natural gas mixtures with H₂ are investigated in the current work using a numerical assessment of a single swirl burner, which is extensively employed in GT combustors. The baseline numerical and experimental cases pertained to natural gas compositions largely consisting of methane (CH₄). The results show that the numerical model adequately describes the swirling component of the flame observed in the experiment. Altogether, the findings show that hydroxyl (OH) radical levels increase in H₂-enriched CH₄ flames, implying that greater OH pools are responsible for the change in flame structure caused by considerable H₂ addition. The addition of 10 % H₂ is predicted to raise the peak flame temperature by 4 % compared to the baseline CH₄ flame. Therefore, adding 10 % H₂ into a GT combustor without any flowrate tuning raises the risk of turbine material deterioration and increased thermal NO_x emission. Due to the lower volumetric Lower Heating Value (LHV) of H₂, which needs a higher volumetric fuel flow rate than burning natural gas/CH₄ at the same thermal output, the addition of 2 % H₂ is predicted to reduce the peak flame temperature by 4 % compared to the baseline CH₄ flame. Hence, if 2 % H₂ is fed into a GT combustor without any flowrate tuning, the required load may not be obtained. When compared to the baseline CH₄ case, the addition of 5 % H₂ is predicted to provide almost identical peak flame temperature, which can be postulated that the addition of 5 % H₂ can produce roughly the same peak flame temperature as the pure CH₄ flame because the Wobbe Index is comparable. Therefore, it reveals that incorporating 5 % H₂ in the natural gas-fired GT combustor with nearly no modification is viable. More research, however, is required to fully capture the flame structure and strain for assessing transient-related phenomena such as flashback and blow off by raising the H₂ proportion and utilising a higher precision turbulence model.

1. Introduction

Malaysia's energy sector is the main source of greenhouse gas (GHG) emissions [1-2]. Thus, in order to minimise GHG emissions, Malaysia's National Determined Contribution by 2030 [3] is to cut its carbon intensity against Gross Domestic Product (GDP) by 45 % compared to 2005 levels.

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Malaysia's Green Technology Master Plan (2017-2030) [4] comprises policies and action plans aimed at achieving a low-carbon, resource-efficient economy as part of the National Green Technology that relates to Energy, Environment, Economy, and Social.

Among these are improvements in power generation efficiency. Nonetheless, the Malaysian government has yet to adopt emerging technology such as using hydrogen in power plants due to the expensive cost. Efforts to reduce carbon dioxide (CO₂) emissions, such as hydrogen co-firing, have gained pace, and its potential as part of power plant development is being investigated further. Malaysia Renewable Energy Roadmap (MyRER) [5] emphasises decarbonisation of Malaysia's electricity sector by 2025, with a focus on bioenergy exploration such as biomass and biogas co-firing due to its renewable resources [6]. Hydrogen is yet to be emphasised. Nonetheless, hydrogen has received attention since the Eight Malaysia Plan (2001-2005) through funding for hydrogen fuel cell research and development [7]. Currently, Malaysia's Ministry of Science, Technology and Innovation (MOSTI) [8] initiatives led by Nano Malaysia, in collaboration with Malaysia Green Technology Corporation, Academy Science Malaysia, local institutions, and Nano Verify, are doing research to develop Malaysia's Hydrogen Road Map, which is expected to be finished in 2022. The Asia Energy Transition Initiatives (AETI) in Japan [9] have identified prospective technologies to support the energy transition agenda, including conversion to gas technologies (coal to gas, diesel to gas) and co-firing or full combustion of ammonia-hydrogen.

Due to the lack of commercial deployment of hydrogen co-firing or full firing at Malaysian power plants, this paper investigates the potential of employing hydrogen at specific percentages within natural gas mixtures (primarily methane) to support decarbonisation initiatives using Computational Fluid Dynamics (CFD) modelling from a single swirl burner. The use of a single swirl burner is intended to mimic the swirler features seen in a typical gas turbine combustor. Despite the fact that the gas turbine (GT) is a relatively adaptable technology in terms of accepting variations in the quality of the gaseous fuel that it uses [10], a GT built and calibrated to run on a specific fuel quality range will always prefer to operate within the tolerance limits in exchange for reliability and the highest possible operational efficiency [10]. However, depending on the GT design and the setup of the hardware and controls, GTs can only sustain modest variations in fuel composition and must be tuned for a specific fuel composition range [11]. Hence, the current study's hydrogen co-firing insights are valuable in providing fundamental information on the essential combustion properties to be exploited in tuning the hydrogen-natural gas firing in the actual GT combustor.

CFD simulations employing validated flow and combustion models are one way for establishing cold flow and combustion characterisation in a burner/combustor model [6, 12-16]. The Large Eddy Simulation (LES) approach provides a far deeper and more accurate insight into the physics of combustion than the Reynolds Averaged Navier–Stokes (RANS) approach [17]. The LES enables the analysis of exceedingly complex combustion phenomena such as transient ignition behaviour and local extinctions, to name a few [17]. In these situations, the LES with advanced combustion models and complex reaction pathways offers excellent agreement with the experimental results [17]. The major hurdle to LES applications, however, is their high computing costs [17, 18]. Even for small-scale combustor models, the LES demands computational meshes with tens of millions of nodes and simulation periods of many weeks [17]. LES formulations are at least 100 times more computationally intensive than typical RANS formulations [6]. Tylic *et al.*, [17] employed a model GT combustor and discovered that the LES solutions did not depart from the experimental findings any more than the steady state values obtained using the RANS model. They also discovered that the chemical kinetics had a higher influence than the turbulence model. Therefore, the RANS formulation with a detailed chemistry mechanism is more appropriate for combustion analysis in a model burner under diverse hydrogen co-firing conditions.

Hence, the current numerical analysis employs the RANS formulation and a detailed chemistry mechanism to investigate the effect of hydrogen proportions in natural gas on combustion characteristics in a swirl combustor. Validations are performed using actual experiment data. The numerically anticipated hydroxyl (OH) radical and flame temperature, as well as the portrayal of a flame front, were used as indicators to analyse the essential combustion properties.

2. Experimental Setup

To create a premixed gaseous swirl flame under steady state conditions, a single annulus, axial swirl gas turbine type burner was used. Figure 1 depicts the swirl flame burner setup schematic. A circular quartz tube with a diameter of 100 mm and a length of 180 mm was used to replicate a combustor wall at the burner outlet. To generate powerful swirl flow, an axial swirler with eight straight guide vanes was positioned concentrically at the burner outlet. The guide vanes are angled at 45° from the centreline axis. The thickness of the vane is 1.5 mm. The swirler hub (D_h) and swirler (D_s) diameters are 19.2 and 38.4 mm, respectively, resulting in a blockage ratio of 0.45. The geometric swirl number of the axial swirler is calculated to be S_N 0.78, and the swirling flow generated is powerful enough to aid in flame stability, as demonstrated in prior research using the same swirl burner [11].

The supplies of natural gas mixture (Methane (CH_4) = 94 %, Ethane (C_2H_6) = 2.5 %, Nitrogen (N_2) = 1.5%, and CO_2 = 2%) were regulated by mass flow controllers (Sierra; accuracy $\pm 1\%$ full scale). These gases were pre-mixed in a gas mixing chamber to ensure thorough mixing. A mass flow controller (Sierra; accuracy $\pm 1\%$ full scale) regulated the main dry air flow supplied by a compressor. Two in-line air heaters (600 W/heater) were used to raise the temperature of the primary airflow. The air was premixed with the natural gas at the burner plenum to generate a flammable mixture. To maintain the premixed mixtures at elevated temperature, two rope heaters (500 W/rope) were employed to heat the burner plenum and body. The burner was insulated with high temperature, heat resistant ceramic wool to decrease heat loss. To measure the temperature of the preheated main air flow, a 3 mm thermocouple is positioned 10 mm upstream of the burner. The thermocouple signal serves as a feedback signal to the temperature controller, allowing it to control the temperature of the mixture.

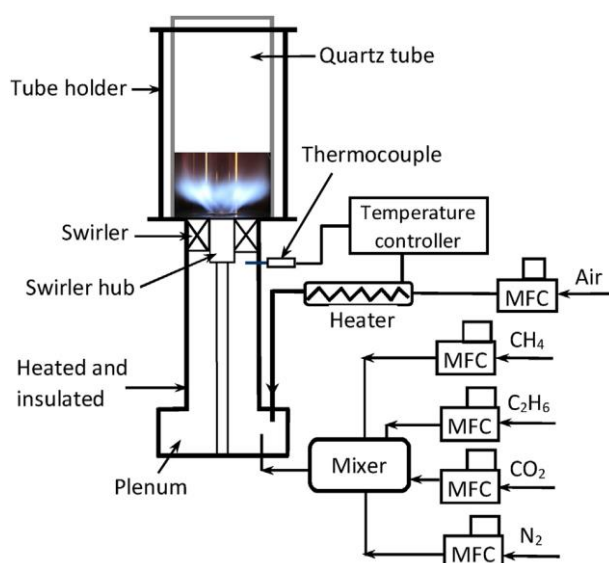


Fig. 1. Schematic of the burner and flow supply system, MFC stands for mass flow controller

3. Physical Setup

This study used as-built dimensions from the swirl burner to develop the three-dimensional (3D) geometry of the burner. The burner geometry was simplified to capture important features, while non-critical components were left out to reduce computational expenses. The computational domain of the burner, as well as the related boundary condition locations, are shown in Figure 2.

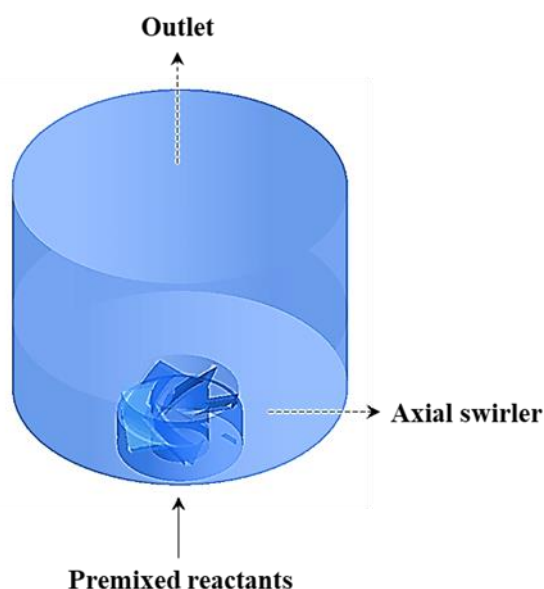


Fig. 2. Computational domain of the swirl burner

4. Numerical Setup

The governing equations (steady state and compressible) are translated into discrete forms using the finite volume technique utilising a commercial CFD software package, ANSYS Fluent V.19 R1. ANSYS Fluent V.19 R1 is used for all setups and numerical processing. The pressure-based solver is used to solve the governing equations. To solve the pressure-velocity coupling, the Semi-Implicit Method for Pressure Linked Equations (SIMPLE) technique was used. The study of Ferziger *et al.*, [19] contains detailed information on the constants and formulations used in the SIMPLE algorithm. To address the radiative heat transfer from the reacting flow, the Discrete Ordinates (DO) model was used.

Previous studies have shown that the probability density function (PDF) and flamelet formulations are adequate for describing the complex turbulence-chemistry interaction within the combustor [10, 20]. As a result, the current study employed the non-adiabatic steady flamelet model with a detailed chemistry mechanism (GRI Mech 3.0), which computes temperature and species composition through the use of a variable known as the mixture fraction, which reflects the local fuel/oxidizer ratio [17]. The convection-diffusion transport equation [17] governs the mixture fraction, which is a conserved quantity. A turbulent flame brush is described by the steady flamelet method as a collection of discrete, steady laminar flamelets known as diffusion flamelets. The diffusion flamelets are then implanted in a turbulent flame using statistical PDF methods, allowing realistic chemical kinetic effects to be incorporated into turbulent flames. The pre-processed and tabulated chemistry saves a significant amount of calculation time. References [10, 20] provide more information on the constants and formulations used in the flamelet technique.

Table 1 shows the case studies for investigating the effect of hydrogen (H₂) co-firing on combustion parameters in the burner model. A pure CH₄/air mixture (case B) is used as the baseline scenario. In comparison to the experiment, the natural gas mixture for the baseline case of CFD simulation is different, where a number of species accounted for the natural gas, yet pure CH₄ is implemented for baseline CFD simulation. This is done to reduce computational complexity by lowering the number of reactants used in the kinetics calculation. Furthermore, more than 90 % of the natural gas analysed in the swirl burner experiment contains CH₄. Hence, the use of pure CH₄ in the baseline CFD case can be considered suitable for direct validation with the swirl burner experiment, which used natural gas mixtures.

Table 1
Boundary conditions for each case studies

Case	B	H2-2%	H2-5%	H2-10%
CH ₄ (%)	100	98	95	90
H ₂ (%)	0	2	5	10
Flowrate (LPM)	200	200	200	200
Equivalence ratio	1.0	1.0	1.0	1.0

Referring to Table 1, the mass flow rates were determined from experimental measurements. Prior to the execution of parametric studies, grid-convergence analysis and validation studies were undertaken. All of these findings are described in greater detail in the next section.

5. Grid-Convergence Analysis and Model Validation Studies

5.1 Grid Independent Test and Validation I: Cold Flow

To get a good spatial convergence accuracy, the grid independent test is run. Meshes (elements) are built with orthogonal quality and skewness in mind to reflect mesh quality, because mesh quality affects the extent of spatial discretisation error [21]. To guarantee that appropriate mesh qualities can be constructed, the orthogonal and skewness characteristics of all generated meshes evaluated in the grid independent test were controlled. When the mesh number at the burner model is increased from 1.73 million to 1.92 million, the velocity and temperature profiles almost no longer vary, with a variation of less than 1 %. As a result, 1.92 million meshes are selected for the burner model.

Following that, the flow models used in the swirl burner computational domain were cold flow validated by comparing them to experimental data from the Sydney Swirl burner [22], as shown in Figure 3. The cold flow velocity profile from the Sydney Swirl burner experiment and numerical work were recorded at a height-above-burner (HAB) of 6.8 mm.

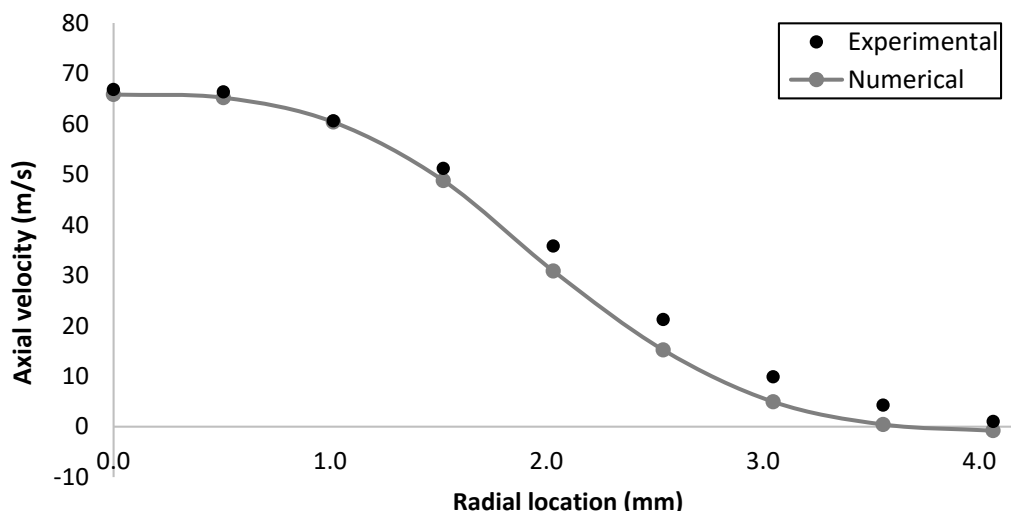


Fig. 3. Cold flow velocity profile

Referring to Figure 3, the flow models were successfully mirrored the actual velocity profile acquired from the Sydney Swirl burner with good accuracy. As a result, it demonstrates that the flow models used are capable of capturing the swirling flow with reasonable fidelity.

5.2 Validation II: Flame Front Qualitative Comparison

The flame front was reconstructed in the current study utilising information from the pre-processed flamelet library and the iso-surface technique. At various temperatures, OH is a radical species that dominates chain propagation, chain branching, and chain termination events in a combustion process [10, 23]. The OH is produced in a zone where extremely exothermic chemical reactions are occurring. As a result, using the chemical kinetics of OH in a combustion event, researchers can reconstruct the flame front [10, 24]. Our previous work [10] contains more details on the method. Figure 4 shows the OH and temperature profiles computed using the flamelet library.

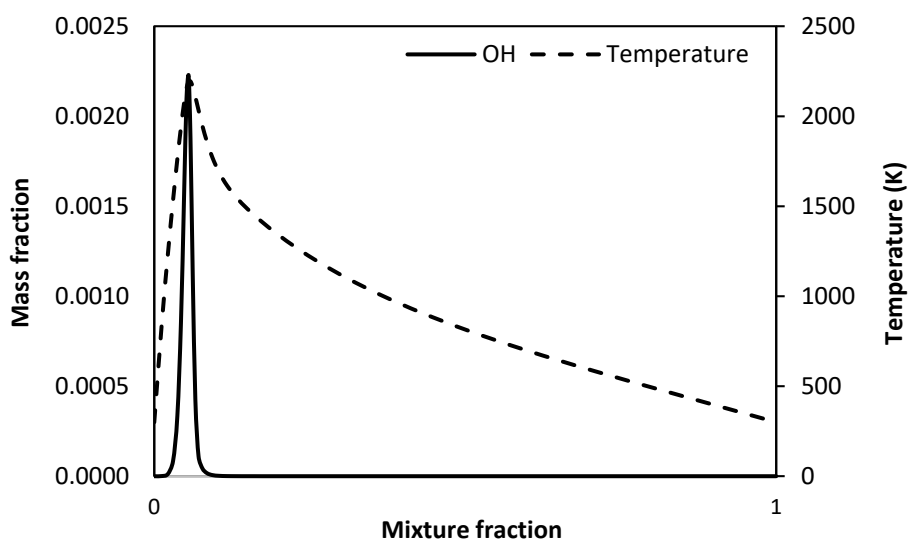


Fig. 4. Computed values from the flamelet library of OH and temperature profiles

Figure 4 depicts the peak of OH generation at the maximum temperature, as shown in the flamelet file. As a result, the peak mass fraction of OH, 0.0022, is used to plot the iso-surface representing the flame front, as shown in Figure 5. The temperature contour was drawn across the iso-surface to show the temperature distribution on the created surfaces. Figure 5 compares the predicted flame front for case B to the actual natural gas flame captured during the experiment.

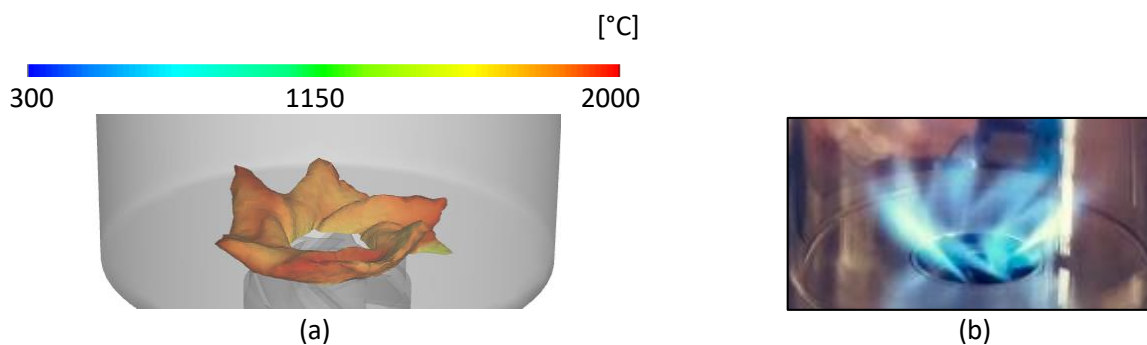


Fig. 5. Comparison of flame fronts between (a) numerical studies and (b) the actual experiment

As seen in Figure 5, the whirling aspect of the flame can be captured appropriately by the CFD model. The employment of a swirler allows the flame fronts to be stabilised at the angle of the swirl flow exit [10]. A bluish flame was produced as seen in the experiment data. The bluish flame appears in the heat reaction zone, which is where natural gas chemically reacts with air. The complete reaction of fuel and oxidizer molecules produces water (H_2O) and CO_2 , while the flame reaction zone is typically bluish [11]. This type of flame is desirable and has been used in low-emission GT combustor technology, specifically lean-premixing GT technology [11].

6. Results and Discussion

Following validation, the simulations for the H_2 co-firing cases were done. The comparison of OH radical species and temperature from baseline and H_2 co-firing simulations is shown in Figures 6 and 7. Table 2 shows the OH generation in terms of mass fraction and flame temperature at three HAB locations of 2, 4, and 6 mm. The HAB has a datum just after the burner inlet (above swirler).

Figure 6 shows that the flame with H_2 addition exhibits higher OH concentrations. Furthermore, the OH distributions are more continuous, as shown in HABs 2 mm and 4 mm, where the OH levels are higher along the periphery of the swirling flame. These findings show that OH levels improve in a H_2 -enriched flame, hinting that enlarged radical pools of OH are responsible for a change in flame structure with H_2 addition. The OH level is negligible in the centre of the toroidal swirling flame, indicating that there is no flame due to the fuel-air stream that travels throughout the swirler. At HAB 6 mm, a slightly higher OH concentration near the inner wall of the swirl burner domain was predicted in the H_2 co-firing cases, especially in the case H_2 -10%. Fluctuations in OH levels show the movement of the swirling flame in response to local flow turbulence.

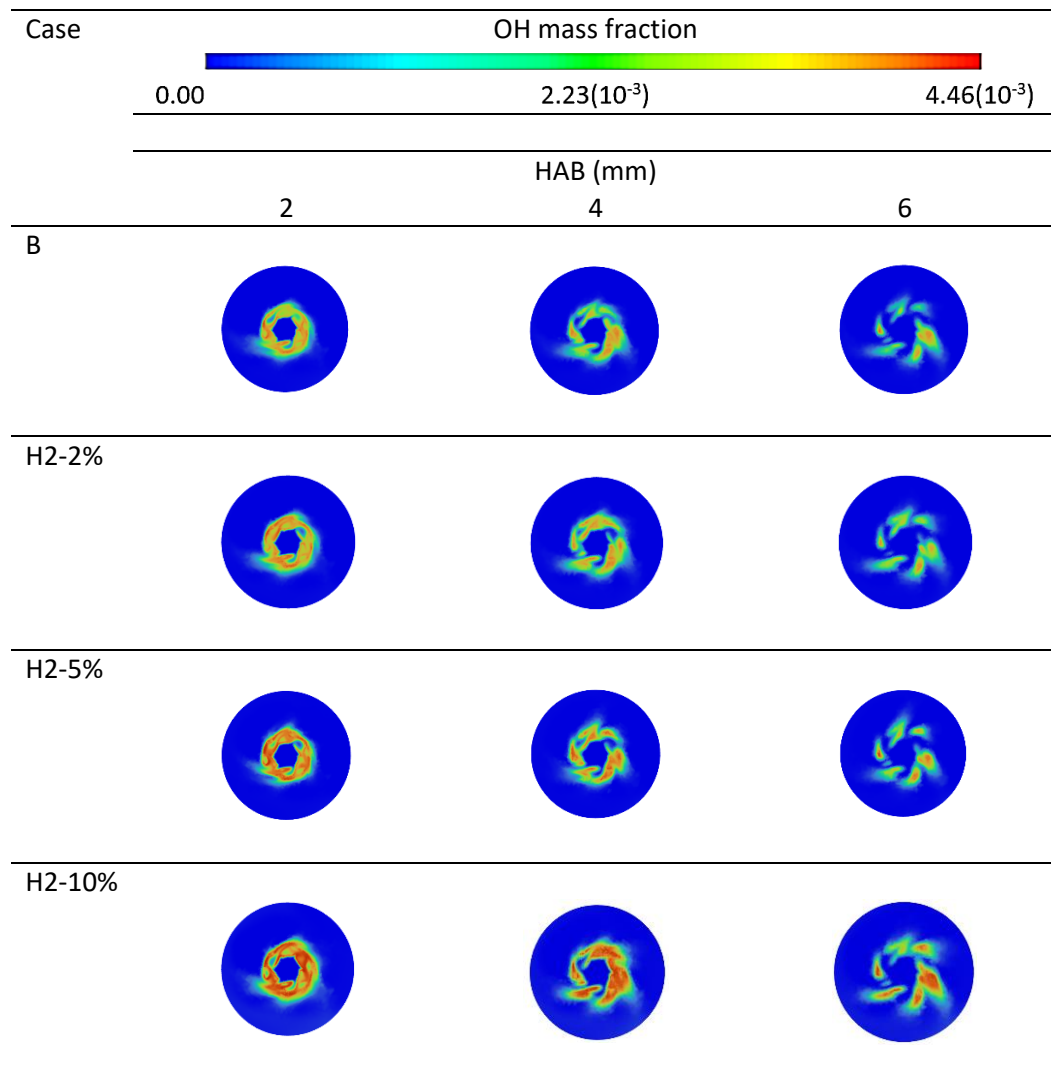


Fig. 6. OH radical behaviour in baseline and H₂ co-firing cases

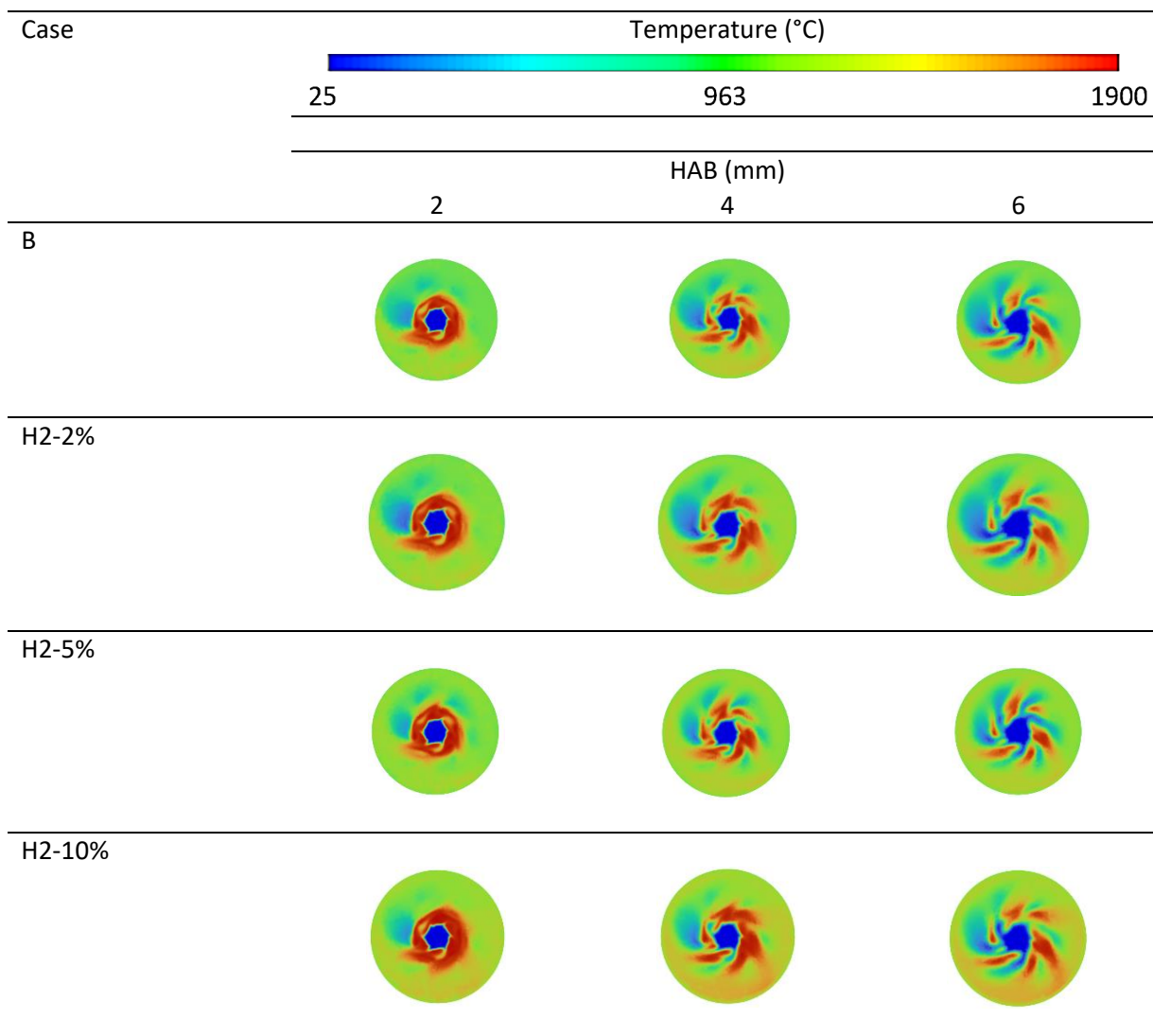


Fig. 7. Temperature behaviour in baseline and H₂ co-firing cases

The H₂-2% and H₂-5% cases created flames that were nearly comparable to those produced by the baseline CH₄ flame. However, as the H₂ addition increased further, the flame structure began to change substantially, as seen in the H₂-10% cases. High levels of H₂ enrichment, according to the CFD prediction, resulted in an increase in OH radical concentrations. Higher OH radical concentrations, which increase numerous key reaction rates [25], are assumed to be responsible for the slightly improved flame temperature exhibited in Figure 7. Table 2 provides a more in-depth comprehension of the peak flame temperature as the amount of H₂ is varied.

Table 2

Peak temperatures (HAB 4 mm) for all cases

Case	B	H2-2%	H2-5%	H2-10%
Peak temperature (°C)	1287.81	1235.72	1270.57	1344.61
Percentage difference (%)	Baseline	- 4.04	- 1.34	+ 4.41

Table 2 shows that increasing the H₂ proportion to 10 % with a constant flowrate of 200 LPM results in a roughly 4 % increase in peak temperature. Hence, current results show that simply injecting 10 % H₂ without tuning the flowrate greatly raises the flame temperature. This is a significant finding for H₂ utilisation in the actual GT combustor. In the actual GT combustor

application, the combustor outlet temperature (also known as the turbine inlet temperature) must be kept at the desired temperature to preserve the load and the hazard at bay [26]. When the temperature exceeds the specified temperature for the specific GT, it has the potential to damage the turbine material because it was built to accommodate for the specific turbine inlet temperature [27, 28]. As a result of the current findings, flowrate tuning is required to include more than 10 % H₂ in the GT combustor in order to reduce the flame temperature to its baseline/requisite temperature. Furthermore, the predicted increase in local flame temperature of H₂-10% case may result in greater thermal nitrogen oxides (NO_x) at the combustor exit if no extra measures are implemented [29].

The peak flame temperature in the case H₂-2% is about 4 % lower than in the baseline CH₄ flame. Burning H₂ requires a higher volumetric fuel flow rate than burning natural gas or pure CH₄ at the same thermal output because of its lower volumetric Lower Heating Value (LHV) [10]. Furthermore, H₂ has a lower Wobbe Index (WI), which is the most widely used criterion for specifying the acceptability of a gaseous fuel in a combustion system [10]. The Wobbe Index is significant because two gases with different compositions but the same Wobbe Index will offer the same energy input to the combustion system for a given fuel supply and combustor parameters (temperature and pressure) and a certain control valve position [10]. As a result, the higher the variation in the Wobbe Index, the greater the flexibility required of the combustion systems and related control.

It can be seen that injecting 5 % H₂ has generated a nearly comparable in flame temperature when compared to the baseline CH₄ case. The comparison of the OH structure and the generated flame temperature shows that with a constant flowrate, the influence of 5 % H₂ addition in the pure CH₄ stream is small. It can be postulated that the addition of 5 % H₂ can produce nearly the same peak flame temperature as the pure CH₄ flame because the Wobbe Index is about the same. As a result, it demonstrates that the incorporation of 5 % H₂ in the natural gas-fired GT combustor with almost minimal adjustment is feasible.

7. Conclusions

We have demonstrated how the effects of H₂ addition in a natural gas/CH₄ swirling flame, with the whirling component of the flame and the swirling flow velocity profile exhibited in the experiment, can be reproduced with reasonable accuracy by the numerical model. The validated numerical model yielded the following insights from all of the compositions that were examined:

- i. Overall, the results reveal that OH radical levels improve in a H₂-enriched CH₄ flame, especially when 10 % H₂ is added, implying that increased OH radical pools are responsible for a change in flame structure with substantial H₂ addition.
- ii. The addition of 10 % H₂ indicated the risk of elevated temperature if no flowrate tuning was undertaken. The addition of 10 % H₂ is expected to increase the peak flame temperature by 4 % over the baseline CH₄ flame. As a result, incorporating 10 % H₂ into a GT combustor without any flowrate tuning increases the potential threat to turbine material deterioration and increased thermal NO_x emission.
- iii. The addition of 2 % H₂ suggested a risk of inadequate temperature if no flowrate tuning was undertaken. The inclusion of 2 % H₂ is expected to reduce the peak flame temperature by 4 % compared to the baseline CH₄ flame. Because of its lower volumetric LHV, burning H₂ requires a larger volumetric fuel flow rate than burning natural gas or pure CH₄ at the same thermal output. As a result, if 2 % H₂ is introduced in a GT combustor without any flowrate tuning, there is a risk of not obtaining the required load.

- iv. When compared to the baseline CH₄ case, the addition of 5 % H₂ is predicted to give almost equivalent in peak flame temperature. It can be postulated that the addition of 5 % H₂ can create about the same peak flame temperature as the pure CH₄ flame because the Wobbe Index is comparable. As a result, it reveals that incorporating 5 % H₂ in the natural gas-fired GT combustor with nearly no modification is viable.

8. Recommendations

To provide more comprehensive insights into the impact of H₂ addition on the natural gas flame, a number of H₂ co-firing cases with increasing H₂ proportions are required. Furthermore, transient phenomena including flashback and blow off should be investigated further in future studies utilising the Large Eddy Simulation (LES) model rather than the RANS model used in this study. This is done to ensure that the majority of the time and length scales are resolved, allowing the flame structure and strain to be accurately captured.

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