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CFD Letters

Journal homepage:
https://semarakilmu.com.my/journals/index.php/CFD_Letters/index
ISSN: 2180-1363

Large Eddy Simulation of Hydrogen/Natural Gas/Air Premixed Swirling Flames and CIVB Flashback Risks

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ARTICLE INFO

Article history:
Received 15 June 2023
Received in revised form 12 July 2023
Accepted 14 August 2023
Available online 1 December 2023

Keywords:
Large Eddy Simulation (LES); Gas Turbine; Hydrogen; Combustion; Natural Gas; Flame

ABSTRACT

The desire to develop gas turbines (GTs) that can utilise natural gas (NG) blended with hydrogen (H_2) often encounters operability challenges related to combustion-induced vortex breakdown (CIVB) flashback issues. Hence, a detailed Large Eddy Simulation (LES) was employed in this study to examine the impact of H_2-NG co-firing on central recirculation zones (CRZs), combustion properties, and the risk of CIVB flashback in a pilot-scale swirl burner facility. The LES model successfully replicated the swirling component of the flame observed in the experiment with reasonable accuracy. The findings revealed that the introduction of H_2 into the burner increased the velocity and temperature of the burned gases. The higher reactivity of H_2 resulted in faster burning rates and a shift in the reaction zone, indicating that NG-H_2 firing burns more rapidly than pure NG firing. Additionally, H_2 was found to enhance the velocity gradient, pushing the CRZ upstream. Changes in the location of the CRZ can disrupt density and velocity gradients, affecting the generation of vorticity by the baroclinic torque and potentially increasing negative axial velocity, thereby increasing the risk of CIVB flashback. Further research is necessary to comprehensively assess the CIVB flashback risk, particularly when the proportion of H_2 exceeds 30 %.

1. Introduction

According to the International Energy Agency (1), as of 2021, gas turbine (GT) power plants predominately produce electricity in the majority of the world's regions, including Japan, the US, and the European region [1]. In light of this, the hydrogen (H_2) co-firing approach in the GT power plants is undeniably practical and desirable [2,3]. This is due to the fact that co-firing maximises the use of already-existing infrastructure in the numerous GT power plants, reducing resource waste and financial loss due to the early retirement of power plants [4-6]. Additionally, merely lowering the amount of carbon in the fuel stream could contribute to a rapid reduction in carbon dioxide (CO_2) emissions [7]. Furthermore, despite the global energy crisis, GT power plants have become more popular than traditional coal-fired plants as a means of producing electricity [1]. In many developed nations, the transition from conventional coal-fired plants to GT power plants has become a common occurrence [8]. This transition is primarily caused by coal's distinctive exhaust fumes, which have a

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https://doi.org/10.37934/cfdl.15.12.154165

higher potential to pollute the environment throughout the fuel's life cycle [8-10]. Furthermore, modern GT combined cycle power plants exhibit a thermal efficiency of at least 60 %, as opposed to conventional coal-fired plants with a thermal efficiency of only about 40 % [8]. Every 1 % increase in thermal efficiency is estimated to save 50 kilo tonnes of CO_2 per year [8].

As a result, designers of GT are focusing on improvements in thermal efficiency while limiting emissions [11]. Because efficiency and emission are controlled in diametrically opposed ways, there are constraints that make it difficult to strike a balance between them [11]. Thus, it is necessary to design and develop these systems in order to adhere to numerous fundamental design principles. A well-designed GT combustors will satisfy the stringent demands of a wide range of GT applications in terms of efficiency, reliability, fuel flexibility, and environmental compatibility [11]. Lean premixing (LPM) is a useful technique that has been applied to GTs in order to lower nitrogen oxides (NO_x) emissions and boost power outputs [11]. However, more research is still needed on this technique to prevent instabilities like extinction, flashback, blowoff, autoignition, and thermoacoustics, particularly when using environmentally sustainable fuels like H_2 [11]. Therefore, there are still a few key issues that are preventing the GT combustion systems from improving [11]. As a result, the desire to create GTs that can run on a variety of fuels, from natural gas (NG) to NG blended with H_2, frequently runs into operability problems in the form of the aforementioned instabilities [12-15].

Due to the high flame speed of H_2 and the rapid chemical reaction rates, flashback and autoignition represent high-risk occurrences for fuel mixtures containing H_2. Flashback happens when the flame stretches upstream from the GT combustor into the premixing section [3, 12] as the flame may stabilise upstream of the reaction zone, and may cause significant damage to the combustion system with an increase in pollutant levels [11]. Flashback may occur through a variety of mechanisms that are susceptible to turbulence and swirling flows, including turbulent flame propagation in the core flow, autoignition-induced flashback, combustion instabilities that cause flashback, a flashback in the boundary layers (BLF), and combustion induced by vortex breakdown (CIVB) [11]. It was suggested that a flashback could be triggered by several mechanisms at once [11].

The CIVB flashback mechanisms, however, are given special consideration because they frequently occur in swirl combustors. Due to their ability to stabilise the flame over a wide range of equivalence ratios, swirl combustors represent the most significant improvements to the GT combustion system [11]. Utilising coherent structures like the central recirculation zone (CRZ), which anchor the flame and circulate hot products and active chemical species while also lengthening their residence times, swirling flow technologies have demonstrated to provide high flame stability [16]. This enables the use of low equivalence ratios, resulting in lower flame temperatures and NO_x emissions. Additionally, combining LPM with swirling dynamics is already an established technology to lessen the NO_x [16]. However, when swirling flows were applied, the flashback instability had dissimilar propagation mechanisms, that frequently created the aforementioned BLF and CIVB flashback mechanisms [12]. Furthermore, LPM combustion is not flawless as such fuel and air mix well before entering the GT combustor, resulting in a significant level of heterogeneity. These produce intricate instabilities, which feed back into the mixing-reaction combustion dynamics [16]. Moreover, GTs must fulfil emissions regulations, which frequently necessitate running very close to lean blowoff [16]. As a result, blowoff remains a challenging phenomenon to foresee across combustor types and fuel compositions [16]. Therefore, undertaking combustion tuning on lean-premixed swirl burners and meeting the demands of efficient GT combustion systems while co-firing with an alternative green fuel like H_2 is much more challenging. This difficulty is exacerbated by the significant properties differences between NG and H_2 fuels [16] in addition to the numerous combustion concerns like extinction, instabilities, and mixing issues.

The creation of a CRZ, which stretches blowoff limits by recycling heat and reactive chemical species to the flame's root in the burner exit, is a critical element of stabilising lean premixed swirling flames. The CRZ is one of the mechanisms for stabilising flames since it creates a spot where the flow velocity and local flame speed are equal through an aerodynamically decelerating region [16]. This is especially important in preventing flashback, and it is common knowledge that in order to avoid flashback, the local premixed flow speed should match the flame speed [12]. Overall, the formation of a CRZ in the lean premixed swirling flame has a significant impact on both the flashback mechanisms.

When it comes to the CRZ, it has been shown that variations in design and fuel type can significantly alter the CRZ's shape and strength [16]. A number of studies have found that adding small amounts of H_2 improves the mixture's resistance to blowoff or extinction. For instance, fundamental studies show that adding 10 % H_2 doubles the extinction strain rate of methane (CH_4) flames [16]. Several studies have also shown that using up to 50 % CH_4 and H_2 blends causes fewer problems with flame stability and flashback than using pure H_2 [16]. However, numerical correlations of various stability phenomena and fuel blends in GTs are still in high demand, especially as we strive to meet our NZE goals by transitioning to H_2 GTs. Furthermore, the details of the interrelationship between the generated CRZs and their subsequent impact on H_2-NG premixed swirling flames in terms of flame stability, particularly in terms of the risk of CIVB flashback, remain hazy.

Computational fluid dynamics (CFD) has the ability to be a feasible method for providing informative assessments of the generated CRZs in relation to the combustion properties of H_2- NG premixed swirling flames. As a result, it can help with combustion tuning for actual H_2-NG co-firing in power plants. CFD has been used extensively to investigate flow dynamics, heat transmission, and combustion qualities [17-21]. As a result, a detailed Large Eddy Simulation (LES) was used in this study to investigate the effects of H_2-NG co-firing on CRZs, combustion properties, and CIVB flashback risks in a pilot-scale swirl burner facility. The CFD approach's prediction accuracy was first evaluated by comparing it with actual experimental data from the aforementioned gas-fired burner facility.

2. Methodology

2.1 Numerical Setup

The simulated combustion process of NG firing and NG-H_2 co-firing is based on the actual experimental setup from our previous study [14]. The computational domain of the burner, as well as the related boundary condition locations, are shown in Figure 1. The software ANSYS FLUENT 19.0 was employed. The numerical model utilised the reacting and compressible Navier-Stokes (NS) equations. To resolve the governing equations, the pressure-based solver was employed. The LES model was used to resolve turbulence. The LES governing and transport equations are created by filtering the time-dependent NS equations in coordinate space [22]. The filtering procedure effectively eliminates eddies whose scales are smaller than the filter width used in the computations. The dependent variables are decomposed into resolved and unresolved, or subgrid, components using spatial filtering of length. Rajpara *et al.,* [23] provides further detailed information on the formulations utilised in the NS equations and LES model for NG-H_2 combustion. The unclosed sub-grid stress tensor that appears in the filtered system has been closed using a dynamic Smagorinsky-Lilly model with a time step of 1e-4 s. The numerical method had second-order accuracy in space and time. For convective terms estimation and other spatial derivatives, the linear-upwind interpolation scheme (the second-order upwind scheme) and linear interpolation (second-order central differences) were used, respectively.

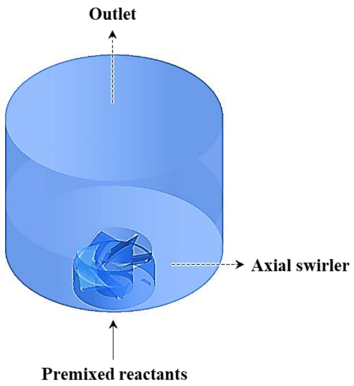

Fig. 1. Computational domain of the swirl burner

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 [13, 14-15, 24]. 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 [25]. The convection-diffusion transport equation [25] 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 [13, 24]. The pre-processed and tabulated chemistry saves a significant amount of calculation time.

The discrete ordinate (DO) approach was used to predict radiation, with an angular discretisation of 5 divisions and 3 pixels in both the polar and azimuthal orientations. The gas emissivity was calculated using the weighted-sum-of-gray-gases model (WSGGM) [26]. A post-processing method was used to simulate NO_x production. To begin, combustion simulations were used to derive temperature, major gas composition, and velocity distributions. The reactions of NH_3, hydrogen cyanide (HCN), thermal NO_x, and NO_x reduction by char were then incorporated based on the combustion computation. Only NO_x-related species such as NO, NH_3, HCN, O, hydroxide (OH), and N were computed, but flow, turbulence, other major gas compositions such as oxygen, CO_2, carbon monoxide (CO), and H_2, energy, as well as radiation equations were not solved.

The case studies for investigating the effect of H_2 co-firing on combustion parameters in the burner model are shown in Table 1. The baseline scenario is a pure CH_4/air mixture (case B). In contrast to the experiment, the natural gas mixture for the baseline case of CFD simulation is different, with a number of species accounting for the natural gas, but pure CH_4 is implemented for the baseline case. The number of reactants used in the kinetics calculation has been lowered to reduce computational complexity. Furthermore, CH_4 was found in more than 90 % of the natural gas tested in the swirl burner experiment. As a result, the baseline CFD case using pure CH_4 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	H2-5%	H2-10%	H2-15%	H2-20%	H2-30%
CH_4 (%)	100	95	90	85	80	70
H_2 (%)	0	5	10	15	20	30
Flowrate (kg/s)	0.0022	0.0022	0.0022	0.0022	0.0022	0.0022
Equivalence ratio	1.0	1.0	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.

3. Results

3.1 Grid-Convergence Analysis and Model Validation Studies

The grid independent test is used to obtain good spatial convergence accuracy. Since mesh quality impacts the level of spatial discretisation error, meshes (elements) were created with orthogonal quality and skewness in mind to represent mesh quality [27]. The orthogonal and skewness features of all generated meshes assessed in the grid independent test were controlled to ensure that adequate mesh qualities could be constructed. The velocity and temperature profiles nearly no longer vary when the mesh number at the burner model is increased from 2.49 million to 3.15 million, with a difference of less than 1 %. As a result, the burner model is made up of 2.49 million meshes, as seen in Figure 2 (blue arrow – inlet, red arrow – outlet).

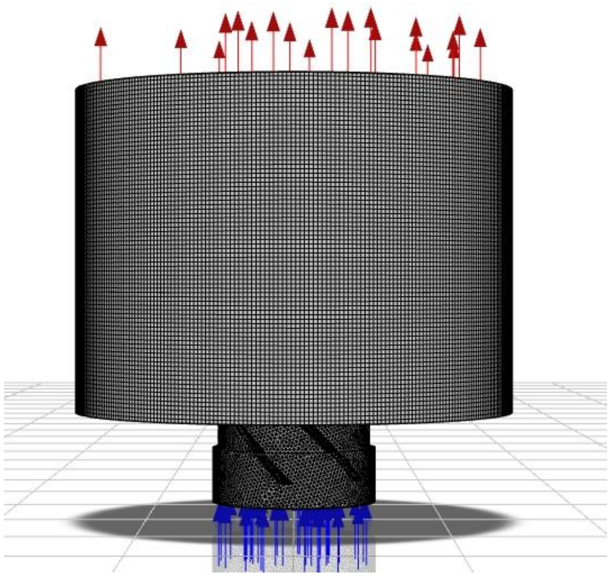

Fig. 2. Mesh model of the swirl burner

The iso-surface technique is used to recreate the flame front using an active radical generated during the chemical reaction, which is CO. The release of active radicals occurs at the flame front, which is typically a small zone few micrometres thick [28]. As a result, researchers can rebuild the flame front using the chemical kinetics of CO in a combustion event. The predicted flame front for case B is compared to the real natural gas flame captured during the experiment in Figure 3.

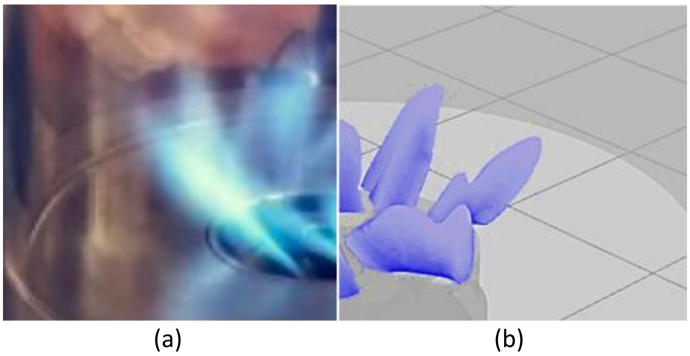

Fig. 3. Flame fronts between the (a) actual experiment and (b) numerical studies

The swirling feature of the flame, as shown in Figure 3, can be adequately captured by the CFD model. The use of a swirler stabilises the flame fronts at the angle of the swirl flow exit [13]. According to the experiment data, a bluish flame was produced. In the heat reaction zone, where natural gas chemically reacts with air, the bluish flame appears. Water (H_2O) and CO_2 are generated by the complete reaction of fuel and oxidizer molecules, and the flame reaction zone is typically bluish [29]. This type of flame is preferable and has been used in the development of low-emission GT combustor technology, particularly lean-premixing GT technology [29].

3.2 Temperature and Velocity Profiles

Following validation, the simulations for the H_2 co-firing cases were completed. To demonstrate the effects of H_2 addition on temperature and velocity variations, computational outcomes obtained for pure CH_4 combustion (Case B) are compared with several H_2 addition cases, as shown in Table 1. Figures 4 and 5 show a comparison of temperature and velocity contours plotted along the central plane of the swirl burner model. These findings demonstrate that the supply of H_2 in the burner increases the velocity and temperature of the burned gases. For H_2-enriched flame cases, combustion characteristics such as velocity and temperature are improved. This is primarily due to H_2's higher combustibility and diffusivity than CH_4 (H_2 is lighter than CH_4), which results in a large amount of heat energy released during combustion and thus increases flow velocity and temperature.

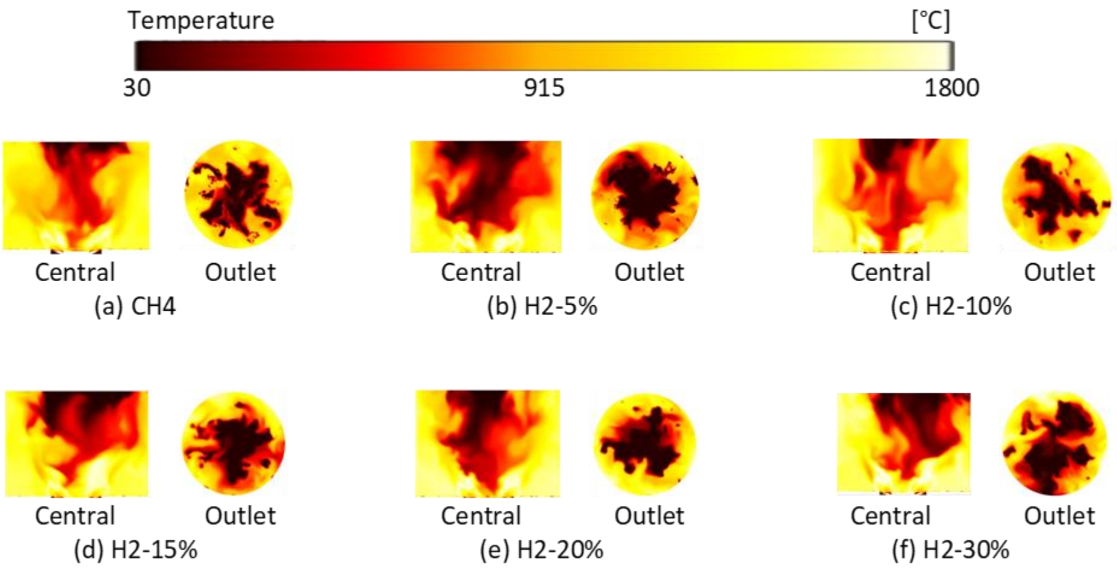

Fig. 4. Predicted temperature contours

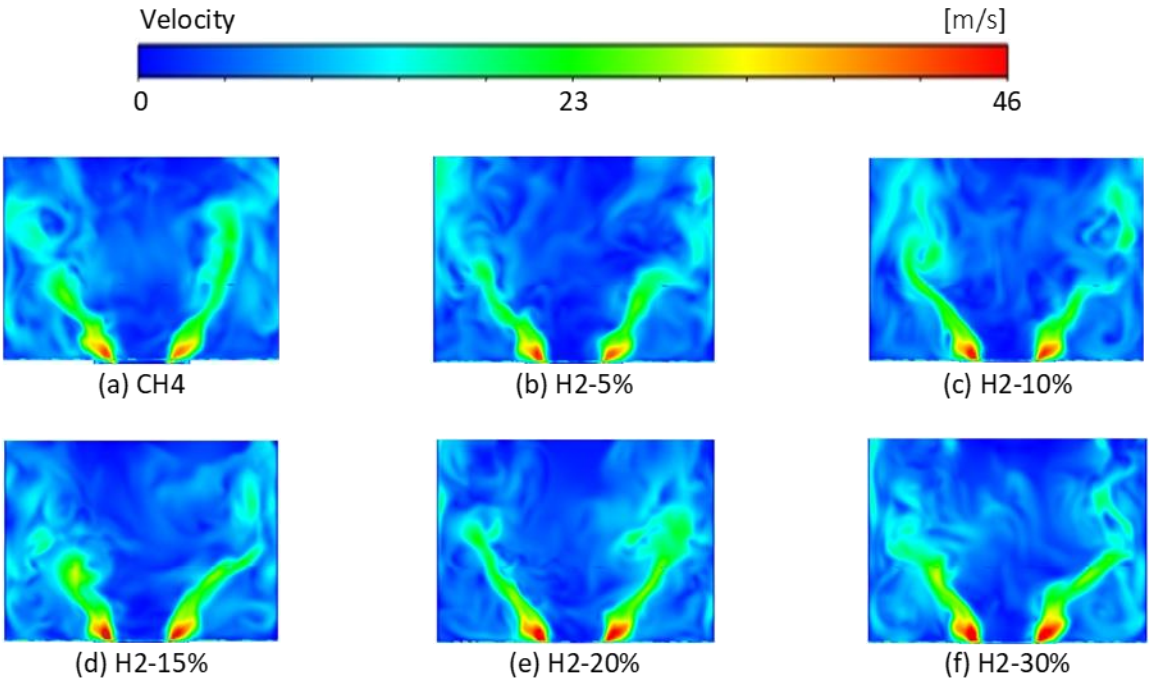

Fig. 5. Predicted velocity magnitude contours

Furthermore, LES results from CH_4-air combustion show that the combustion gases produced travel near the burner centreline and burner wall. However, as the proportion of H_2 increases, particularly when it reaches 30 %, a wider high temperature gas is produced, which expands further to the burner wall. Due to the high reactivity of H_2, wider high temperature gas at higher H_2 concentration is associated with increased hydroxyl (OH) radical concentration in flame, which increases the burning rates and shifts the reaction zone [14], as seen in Figure 6.

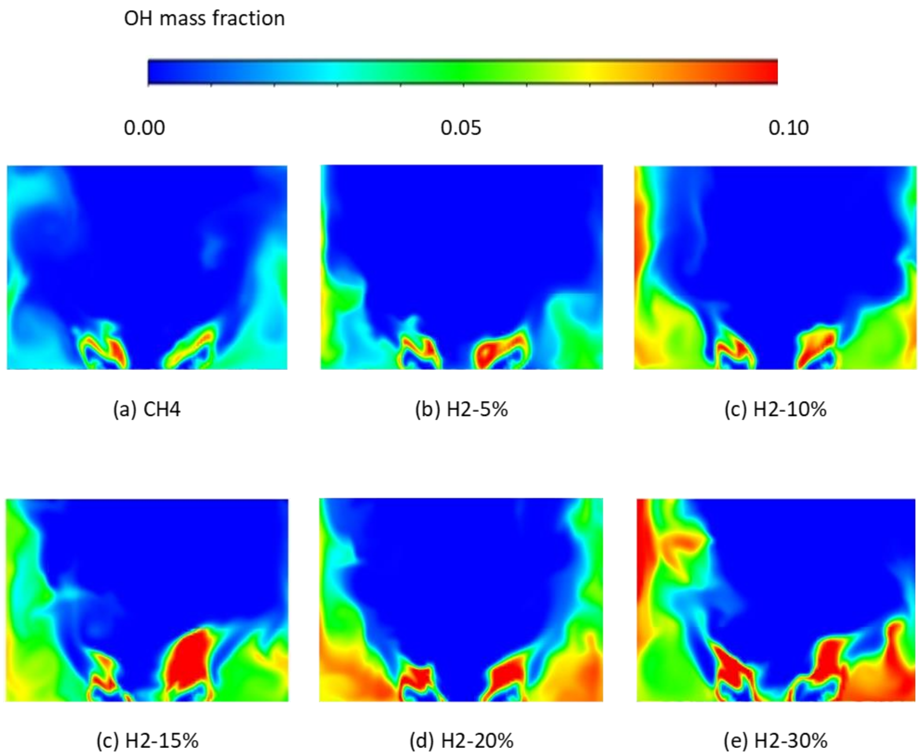

Fig. 6. Predicted OH contours

Temperature contours on the exit plane of the burner (outlet) also show displacement of high temperature gas with greater H_2 fractions. At 30 % H_2, the high temperature area decreases and shifts towards the burner inlet region, while expanding near the burner wall. The highest temperature obtained from H_2 co-firing cases is greater than that obtained from pure CH_4 combustion. Normally, the temperature of an adiabatic flame rises as the H_2 fraction increases. The increased reactivity of H_2 creates such a high temperature, demonstrating the existence of a comparatively shorter reaction zone near the burner inlet. A substantially shorter and wider high temperature burned gas at 30 % H_2 percentage suggests more rapid combustion.

While the geometry structure of the simulated swirl burner is symmetrical, the flame behaviour has asymmetrical characteristics. Flow instabilities in swirl burners can result in asymmetrical flow structures. The coupling between the combustion process and fluid dynamics causes these instabilities. The presence of these instabilities can cause changes in the shape and temperature distribution of the flame, resulting in the observed asymmetry. Combustion is a complex process with many interacting factors, including fuel-air mixing, flame propagation, and heat release. Small differences in reactant mixing or local conditions within the burner can cause differences in combustion behaviour, leading to the observed asymmetry in the flame structure and temperature distribution.

3.3 CIVB Flashback Risk

To assess the risk of CIVB flashback, two types of contours from the LES results were examined: the flame front contours and the streamline contours. Previous research has discovered that the position of the flame front relative to the tip of the CRZ is one of the key mechanisms that causes flashback [30].

In swirling flames, both the CRZ and baroclinic torque are important features, yet they stand for different aspects of the flow field. When the azimuthal velocity exceeds the axial velocity, the vortex breaks up and a CRZ forms [30]. The CRZ is a sudden alteration in vortex structure that results in the development of a stagnation point and recirculation region downstream [30]. The baroclinic torque, on the other hand, implies to the vorticity production caused by the interaction of the density gradient and the velocity shear in a swirling flow [31]. It is caused by the emergence of a baroclinic zone with radial density and tangential velocity gradients [31]. The baroclinic torque alters the flow pattern and helps to form and intensify the CRZ [31]. It improves flame stability and heat transfer by increasing vorticity and mixing within the CRZ [30,31].

A previous study, however, discovered the development of a closed bubble at the tip of the CRZ [30]. Positive vorticity caused by volumetric expansion moves the bubble downstream and stabilises the flame [30]. However, the baroclinic torque generates negative vorticity, which increases the negative axial velocity and causes the bubble to propagate upstream [30]. As a result of the flame volume expansion that compensates for an increase in baroclinic torque, the flame front tip located upstream of the tip of CRZ (where the bubble is located) will not provide a favourable condition for the generation of reverse flow caused by baroclinic torque [30].

Hence, leveraging this occurrence, a quantitative assessment of the risk of CIVB flashback via flame front and streamline contours from CFD simulations can be performed. As seen in Figure 7, all cases produced flame fronts upstream of the CRZ tip (shown in Figure 8). However, increasing the H_2 fraction has been shown to push the CRZ tip further downstream. Since H_2 has a higher laminar flame speed, increasing the percentage of H_2 in a swirling flame changes the flame properties [3]. As a result, it will have an effect on the CRZ by raising the velocity gradient and potentially changing the zone's extent and position. The altered CRZ has an effect on the baroclinic torque. Changes in the

CRZ could disturb the delicate balance between density and velocity gradients, impacting the formation of vorticity by the baroclinic torque and potentially increasing the negative axial velocity, which can cause the flame to propagate upstream. As a result, when a higher H_2 proportion is used, the flame front tip could end up situated downstream of the CRZ tip.

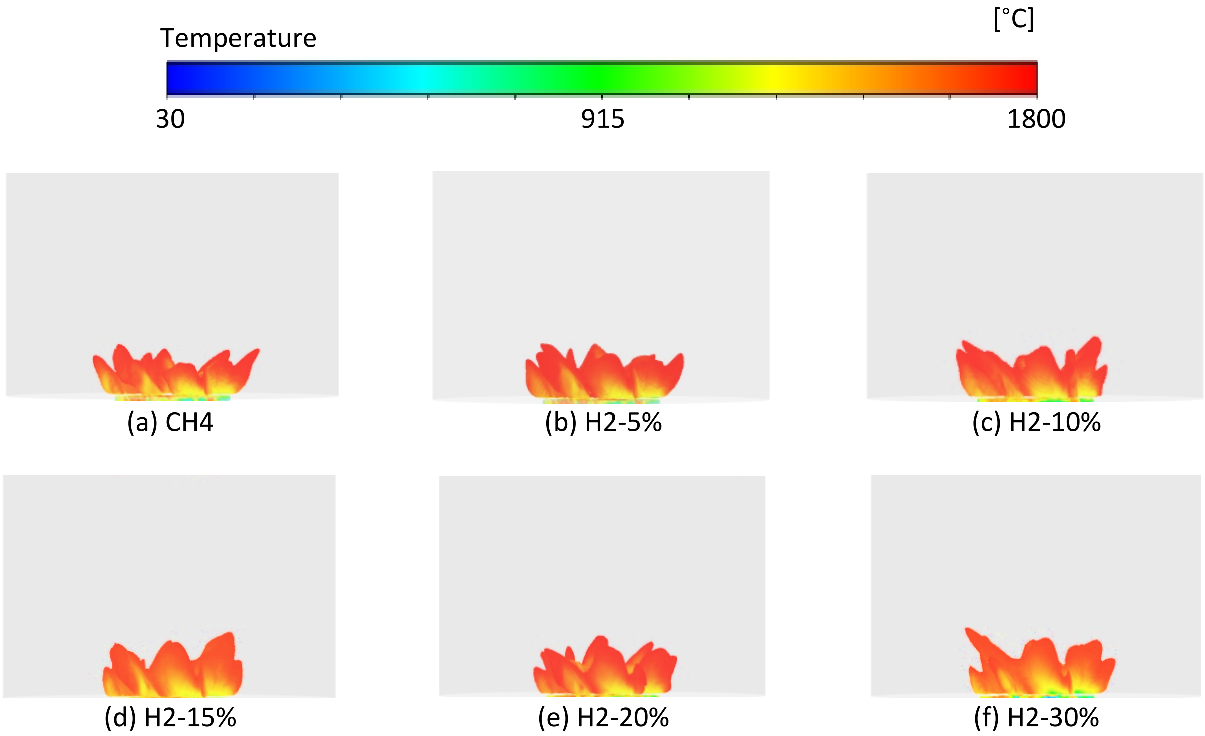

Fig. 7. Predicted flame front contours

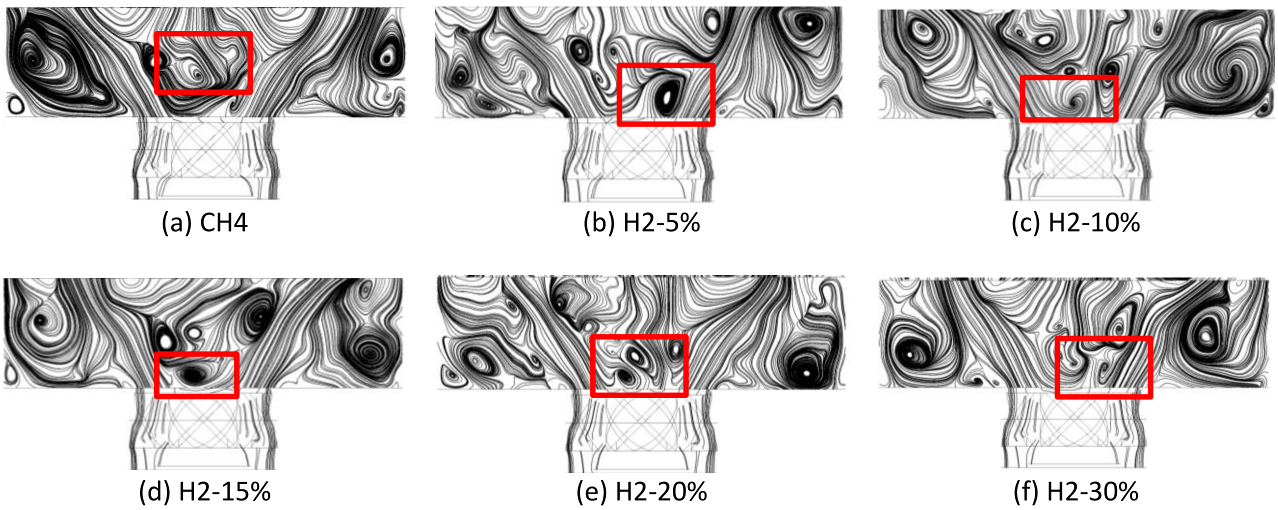

Fig. 8. Predicted flow streamlines

4. Conclusions

The impact of H2-NG co-firing on CRZs, combustion properties, and CIVB flashback risks in a swirling flame were demonstrated using LES techniques in this study. The numerical model is capable of replicating the whirling component of the flame seen in the experiment with reasonable accuracy. The study yielded the following insights from all of the fuel gas compositions that were examined:

I. Introducing H_2 into the burner enhances the velocity and temperature of the burned gases, which attributed to the H_2's superior combustibility and diffusivity compared to NG/CH_4.
II. The high reactivity of H_2 increases burning rates and shifts the reaction zone, implying that NG-H_2 firing burns faster than pure NG firing.
III. H_2 increases the velocity gradient, potentially pushing the CRZ upstream. Alterations in the CRZ could disrupt the delicate balance of density and velocity gradients, influencing the formation of vorticity by the baroclinic torque and potentially raising the negative axial velocity, risking flame propagation upstream and CIVB flashback.

5. Recommendations

A number of H_2 co-firing cases are required to provide more comprehensive insights into the risk of CIVB flashback with H_2 addition on the NG flame, particularly when the H_2 proportion exceeds 30 %.

Acknowledgement
This work is carried out with the financial support from TNB Research (TNBR) Seeding Fund (SF) (grant number - TNBR/SF 412/2021)

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