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Hydrogen Addition Effects on Flashback in a Combustion Chamber

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Abstract
The purpose of this work is to investigate the effects of adding hydrogen to the fuel on the combustion induced vortex breakdown flashback phenomenon in a combustion chamber. An atmospheric research burner is selected for studies and the analysis is performed using numerical simulations. In order to model the turbulence-chemistry interactions, the EDC combustion model is utilized and the GRI 2.11 reaction mechanism is used to investigate the combustion process as carefully as possible. The present studies are performed keeping the exit temperature constant. To do this, by adding any amount of hydrogen to the premixed inlet flow, the methane is decreased by using the trial-and-error until the mass averaged exit temperature remains almost constant. The purpose of applying this limitation is to keep the cycle operational condition unchanged that is important for adding hydrogen to the existing combustion chambers especially from technological viewpoint. In addition, the thermal NOx production is controlled. In the following, the effect of hydrogen addition on the flame thickness and flame shape is investigated and finally, the effect of operating pressure on the flashback behavior is analyzed.

Keywords: Combustion chamber; Flashback; Hydrogen; Methane; Numerical simulation; Swirl number.

Nomenclature

\( E \) = internal energy per unit mass
\( G_k \) = production of turbulent kinetic energy due to velocity gradients
\( J_i \) = diffusion flux of species
\( K \) = turbulent kinetic energy  
\( P \) = pressure  
\( q \) = heat flux  
\( R_i \) = net production rate of species due to chemical reactions  
\( V \) = velocity vector  
\( Y_i \) = mass fraction of species \( i \)  
\( \varepsilon \) = turbulent kinetic energy  
\( \tau \) = density  
\( \tau \) = stress tensor  
\( \nu \) = kinematic viscosity

1. Introduction

Hydrogen, as a carbon-free energy carrier, likely plays a significant role in a world with severe limitations on greenhouse gas emissions [1]. The use of pure hydrogen is so complicated due to different storage and safety issues. Therefore, a gradual transition by adding hydrogen to methane will play an important role in achieving a hydrogen economy [2]. Currently, lean premixed combustion is employed in the gas turbine industry, along with temperature control to minimize the pollutant emissions [3]. The temperature control objective in a lean premixed technology is closely tied to the rate of nitric acid formation, which is effectively limited by the lower flame temperatures which achieved under the lean fuel compositions.

In premixed combustion, adding hydrogen to hydrocarbon fuels extends the range of stable combustion due to the increased flammability limits of the hydrogen [4, 5]. On the other hand, important design criteria for the gas fuel burners include avoiding phenomena such as flashback and flame lift-off. The flame lift-off occurs when the flame stabilizes at a distance farther from the burner exit. On the other hand, flashback occurs when the flame, enters the premixing chamber and propagates upstream, without extinguishing [6]. The flashback phenomenon significantly increases the temperature inside the premixing chamber, which is not prepared for such temperatures and can lead to damage to chamber components.

In fact, the flashback is an inherent feature of all premixed combustion systems, including gas turbine combustion, where the combustible mixture is always present upstream of the combustion zone. In the premixing chamber of gas turbines, it can occur due to at least four different mechanisms [7]: flame propagation in the core flow, combustion instabilities, flame
propagation in the boundary layer, and combustion induced vortex breakdown (CIVB). The speed of the turbulent flame is dependent to the properties of the mixture and the turbulence. This dependence causes uncertainty in defining the speed of the turbulent flame [8]. The magnitude of turbulent flame speed plays a crucial role in triggering the flashback in the core flow and is a function of both turbulent flame interaction and the chemical kinetics [9]. Consequently, fuel composition and turbulence structure are essential parameters for determining the limitations of flashback in the core flow [3].

Characteristic key of the flashback in core flow is the speed of turbulent flame that is often expressed as a function of laminar flame speed and turbulence characteristics. Several correlations have been proposed for turbulent flame speed as a predictive tool for flashback in the core flow by Liu and Lenze [10], Schmid et al. [11], Daniele and Jansohn [12], and Gülder [13]. However, these correlations cannot be universally applied to any fuel, as the turbulent burning velocity depends strongly on the fuel composition [14]. Coats [15] claimed that in most cases, flashback occurs as a result of low-frequency flow instabilities, which has been confirmed by Lee and Ghoniem [16]. They demonstrated that downstream pressure fluctuations, close to the combustion frequency, enhance the instabilities leading to the flashback. But high-frequency oscillations were found to be less effective [8].

The dynamics of methane-air flashback in premixed burners enriched with hydrogen fuel have been investigated both experimentally and analytically using a simplified linear acoustic model by Tuncer et al. [17]. Their findings suggest that to prevent a flashback, low-frequency pressure oscillations should be suppressed. Keller et al. [18] conducted some empirical studies on a combustion chamber equipped with a step to stabilize the flame. Essentially, they attributed the flashback to the reversal of flow caused by large-scale vortex dynamics. Additionally, Thibaut and Candel [19] numerically analyzed the Keller's experiments using Large Eddy Simulation (LES) and found that it associates with very strong oscillations.

The concept of critical velocity gradient, was first introduced by Lewis et al. [20]. Lewis’s critical velocity gradient model disregards the interaction between the flame and the flow, assuming that the flow velocity remains unchanged upstream. Von Elbe and Mentser [21] concluded that the critical velocity gradient is mostly independent of pipe diameter, except in very narrow channels where the flame approaches extinction. But Harris et al. [22] noted that the critical velocity gradient relationship may not be suitable for channels with small widths. In this regard, Huang et al. [23] demonstrated that the critical velocity gradient and flame structure are strongly dependent to the channel width. As the channel width increases, the flame structure in the core flow becomes more pronounced and starts to bend.
Dam et al. [24] investigated the characteristics of different fuel mixtures by increasing the hydrogen mass fraction. They found that the tendency for flashback in the boundary layer increases by an increase in the hydrogen fraction in mixture. Eichler and Sattelmayer [25] studied the flashback phenomenon in laminar and turbulent premixed flames in the boundary layer using both experimental and numerical approaches, confirming that the turbulent flame movement in the boundary layer is a stochastic process. Vance et al. [26] numerically analyzed the effect of increasing hydrogen concentration in methane fuel and the influence of wall temperature. They considered two fixed wall temperatures of 300 K and 600 K, observing a direct relationship between the tendency for flashback and the wall temperature. The CIVB flashback was first identified experimentally and numerically by Fritz et al. [7]. Among other findings, they demonstrated that with an increase in an equivalence ratio, the flame moves upstream in the flow. Tangermann et al. [27] analyzed the CIVB process experimentally and numerically by using LES. Kröger et al. [28] also employed experimental and numerical methods to investigate the mechanisms of CIVB. They used the vorticity transport equation to demonstrate the effects of different terms of the equation on the flashback phenomenon, and attributed the majority of the CIVB to the strain rate. Wendig et al. [29], further explored the influence of swirl number and equivalence ratio. They observed that in a constant swirl number, an increase in equivalence ratio beyond a certain limit leads to the occurrence of CIVB. Noble et al. [30] demonstrated the dependence of flashback on the composition of syngas fuels. From their analysis, it can be generally concluded that reducing the equivalence ratio and increasing the hydrogen concentration can stabilize the flame.

Mansouri et al. [31] used numerical simulations to better understand the flow behavior and flame dynamics at different swirl numbers. They compared three turbulence models and recommended the Realizable k-ε model for such flow fields. Nemitallah et al. [32] investigated the combustion characteristics and stability of hydrogen-enriched rotating flames in methane-oxygen mixtures. Their results indicate that the outer rotation region significantly contributes to flame stabilization at lower hydrogen fractions and diminishes at higher hydrogen fractions. Furthermore, under stoichiometric conditions, an increase in hydrogen concentration leads to a reduction in flame thickness, and the CO emission at an outlet substantially increases at a 50% hydrogen fraction.

Most of the research conducted did not limit the chamber temperature despite the addition of hydrogen, while hydrogen addition will increase the exit temperature of the combustion chamber. In such studies [33-36], the flashback phenomenon, flame shape, or the pollution
will also be affected definitely by the increase in chamber temperature, in addition to the impacts of the presence of hydrogen in the combustion process. The purpose of the present work is to investigate the effects of adding hydrogen to the fuel on the combustion induced vortex breakdown flashback phenomenon in a combustion chamber, keeping the exit temperature almost constant. The purpose of applying this limitation is to keep the cycle operational condition unchanged that is important for adding hydrogen to the existing combustion chambers especially from technological viewpoint. Furthermore, the thermal NOx production will also be controlled in this way.

2. Governing Equations and Numerical Simulation

The continuity equation expresses that mass within a fluid is neither created nor destroyed. It establishes a relationship between velocity and fluid density, ensuring that fluid flow remains continuous and mass conservation is preserved:

\[
\frac{\partial \rho}{\partial t} + \rho \nabla \cdot \mathbf{v} = 0
\]  \hspace{1cm} (1)

The momentum conservation equation (also known as the Navier-Stokes equation) derived from Newton’s second law describes the relationship between pressure, velocity, and viscosity in a fluid. It is expressed in the vector notation as:

\[
\rho \frac{D \mathbf{v}}{D t} = \nabla \cdot \mathbf{\tau}
\]  \hspace{1cm} (2)

In the present work, a combustion chamber is selected for studies where an axisymmetric swirling turbulent flow exists there. So, all three momentum equations must be solved but there is no gradient in tangential direction.

The energy conservation equation is expressed as:

\[
\rho \frac{D E}{D t} = -\nabla \cdot q + \tau_{ij} \frac{\partial u_i}{\partial x_j}
\]  \hspace{1cm} (3)

The k-\( \varepsilon \) standard turbulence model is utilized here where the given equations describe the turbulent energy transfer and dissipation rate as:

\[
\frac{\partial}{\partial t} (\rho k) + \nabla \cdot (\rho \mathbf{v} k) = \nabla \cdot \left( \left( \mu + \frac{\mu_t}{\sigma_k} \right) \nabla k \right) + G_k + G_b - \rho \varepsilon + S_k
\]  \hspace{1cm} (4)

\[
\frac{\partial}{\partial t} (\rho \varepsilon) + \nabla \cdot (\rho \mathbf{v} \varepsilon) = \nabla \cdot \left( \left( \mu + \frac{\mu_t}{\sigma_\varepsilon} \right) \nabla \varepsilon \right) + C_{1t} \frac{\varepsilon}{k} (G_k + C_3 \varepsilon G_b) - C_{2t} \rho \varepsilon^2 + S_\varepsilon
\]  \hspace{1cm} (5)
The turbulent viscosity ($\mu_t$) is calculated from the combination of equations 4 and 5. The constant coefficients in the above equations are given in Reference [37].

For numerical simulation of combustion processes, a set of species transport equations along with the Navier-Stokes equations must be solved for the flow field. In this process, various species and numerous elementary chemical reactions are involved based on the reaction mechanism [38], where the GRI 2.11 mechanism is used in this research. The eddy dissipation concept (EDC) is used here as a combustion model. As a sub-branch of the eddy dissipation model, it allows partial or accurate chemical kinetics to be considered in the calculations. The EDC model assumes that chemical reactions occur in small turbulent structures called fine scales, and then the evolution of species concentrations is calculated by integrating chemistry in these scales. These structures are of the order of Kolmogorov scales.

The volumetric fraction or size of the fine structure is $\gamma^* = \gamma^3$, where $\gamma$ is the ratio of mass in the fine structure region to the total mass, and is expressed as follows:

$$
\gamma^* = \left(\frac{3C_{D_2}}{3C_{D_1}}\right)^{\frac{3}{4}} \left(\frac{\nu}{K^2}\right)^{\frac{3}{4}} = C_\gamma \left(\frac{\nu}{K^2}\right)^{\frac{3}{4}}
$$

(6)

The fine scale time scale $\tau^*$, is defined as follows in the EDC model:

$$
\tau^* = \frac{1}{m^*}
$$

(7)

$$
\tau^* = \left(\frac{C_{D_2}}{3}\right)^{\frac{1}{2}} \left(\frac{\nu}{\varepsilon}\right)^{\frac{1}{2}} = C_\tau \left(\frac{\nu}{\varepsilon}\right)^{\frac{1}{2}}
$$

(8)

$$
m^* = \left(\frac{3}{C_{D_2}}\right)^{\frac{1}{2}} \left(\frac{\varepsilon}{\nu}\right)^{\frac{1}{2}}
$$

(9)

The constant coefficients in the above equations are given in Reference [38]. $m^*$ is the mass exchange ratio between the fine structure and the surrounding mass of the fine structure. In the EDC model, the average reaction rate in each cell is calculated as follows:

$$
R_i = \frac{\rho(y)^2}{\tau^*(1-(y^*)^3)}(Y_i^* - Y_i)
$$

(10)

Where $Y_i^*$ is the mass fraction of the fine structure species after the reaction during the time $\tau^*$.

The simulations are performed using the Fluent software. The SIMPLE algorithm is employed for pressure-velocity coupling of an incompressible flow field and a second-order discretization is used for all governing equations. The grids are refined to ensure that $y^+$ is close to unity for all solid boundaries.

3. Result and Discussion
In the present study, an atmospheric research burner is selected for investigations where an axisymmetric swirling flow exists. Validation is a crucial step in numerical simulations, as it ensures that utilized models and methods most accurately represent real-world phenomena. The dimensions and geometry of the Anacleto et al. [39] combustion chamber which has been empirically studied are depicted in Figure 1.

![Figure 1- Schematic of flow configuration.](image)

The throat diameter of 40 millimeters (D) is used for calculating dimensionless data for comparison. The premixing tube is a cylindrical pipe with an inner diameter of 50 millimeters and a length of 165 millimeters, which includes a convergent-divergent nozzle. The combustion chamber section consists of a cylindrical pipe with an inner diameter of 110 millimeters and a length of 300 millimeters. It should be noted that the origin of the x coordinate is on the axis of symmetry at the beginning of the combustion chamber. In addition, the inlet temperature is 673 K and the inlet mass flow rate is 46 g/s. More details in ref. [39].

For grid independency studies, four different unstructured grids are generated which their resolutions are 43463, 71674, 113052, and 185053. The axial velocity profiles are shown in Fig. 2 where the inlet axial velocity (U₀) is used for non-dimensionalization.

![Figure 2 - Investigating a grid independency for axial velocity profile.](image)
In addition, non-dimensionalized temperature profiles are presented in Fig. 3 where the following equation is used there:

$$c_t = \frac{T - T_u}{T_b - T_u}$$

(11)

In above equation, $T_u$ and $T_b$ represent the temperature of unburned gas and burned gas, respectively. Consequently, the third mesh of 113052 resolutions is chosen to continue the studies here.

![Figure 3](image)

**Figure 3- Investigating a grid independency for temperature profile.**

Then, the results are compared with experimental data of Anacleto et al. [39] in Figures 4-6 to ensure the validity of numerical simulations.

![Figure 4](image)

**Figure 4- Comparison of dimensionless axial velocity profiles.**
There are good agreement between numerical simulation results and experimental data, and discrepancies are inevitable in such a complicated problem. Some of discrepancies can be attributed to the following factors: First, a complexity of combustion process that involves intricate chemical reactions, heat transfer, and turbulence. Accurately capturing all these phenomena in numerical simulations is challenging due to inherent uncertainties and approximations in modeling such complex processes. Then, the measurement uncertainties due to errors which exist in sensors and instruments in experimental studies. Next, assumptions for fuel properties, reaction kinetics, and turbulence models which are often based on empirical correlations. And finally, boundary conditions which play an important
role in the accuracy of numerical simulations, but applying them exactly as what exist in experiments are almost impossible.

Now, the hydrogen is added to the fuel to investigate this turbulent reacting flow features. It is described before, that the constant mass-averaged exit temperature constraint is imposed in present studies. Therefore, by adding any amount of hydrogen to the premixed inlet flow, the methane is decreased by using the trial-and-error until the mass-averaged exit temperature of the combustion chamber remains almost constant. This is performed here using lots of time consuming numerical simulations, and the final computed inlet flow compositions for different hydrogen contents are presented in Table 1.

<table>
<thead>
<tr>
<th>Hydrogen volume fraction in fuel %</th>
<th>( Y_{H_2} )</th>
<th>( Y_{CH_4} )</th>
<th>Equivalence ratio</th>
<th>( T_{exit} ) (K)</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>0</td>
<td>0.028</td>
<td>0.5</td>
<td>1779</td>
</tr>
<tr>
<td>12.76</td>
<td>0.0005</td>
<td>0.0272</td>
<td>0.5416</td>
<td>1782</td>
</tr>
<tr>
<td>18.43</td>
<td>0.00075</td>
<td>0.0260</td>
<td>0.5225</td>
<td>1775</td>
</tr>
<tr>
<td>23.79</td>
<td>0.001</td>
<td>0.0255</td>
<td>0.5175</td>
<td>1776</td>
</tr>
<tr>
<td>28.22</td>
<td>0.00125</td>
<td>0.0253</td>
<td>0.5085</td>
<td>1778</td>
</tr>
<tr>
<td>43.77</td>
<td>0.00225</td>
<td>0.0230</td>
<td>0.4924</td>
<td>1780</td>
</tr>
<tr>
<td>55.66</td>
<td>0.00325</td>
<td>0.0208</td>
<td>0.4685</td>
<td>1779</td>
</tr>
<tr>
<td>64.76</td>
<td>0.00425</td>
<td>0.0184</td>
<td>0.4406</td>
<td>1783</td>
</tr>
</tbody>
</table>

The swirl number is defined here as [17]:

\[
S = \frac{\int_{R_n}^{R_h} \rho \bar{u} \bar{w} r^2 dr}{R \int_{R_n}^{R_h} \rho u^2 r dr}
\]  

(12)

Where \( R_n \) and \( R_h \) are the respective radii of the blade holders and the outer chamber of the rotating device. For the present simulations, the swirl number is 0.805. Considering the results presented in Table 1, the difference between the maximum and minimum exit temperatures is just 8 degrees. So the results will almost pure and will not under the influences of the chamber temperature changes.

First, the effect of hydrogen addition to the fuel on an axial temperature distribution in the combustor is investigated. The results presented in Fig. 7 indicate that by adding hydrogen, the flame flashback tendency is increased and the hot gas section moves upstream more and more. The presence of the hydrogen in fuel augments the chemical reaction rates and moves...
back the flame, although the exit temperature and even the maximum temperature have had little changes.

![Figure 7 - Effect of hydrogen addition on axial temperature distribution.](image)

Among the chemical species involved in the combustion process, Liu et al. [40] demonstrated that the OH species represents the flame structure. Therefore, it is assumed that the highest concentration of OH species is located almost on the flame. Thus, according to Fig. 8, adding hydrogen to methane leads to the movement of the flame location upstream, as what has been shown by temperature field.

![Figure 8 - Effect of hydrogen addition on flame location.](image)
Based on the results obtained from Table 1 and Fig. 8, an interesting observation here is that flashback tendency is amplified by equivalence ratio reduction. This was not the expected result because in the case of a single fuel, an increase in the equivalence ratio amplifies the flashback tendency [7].

Then, the effect of hydrogen addition on the flame thickness is analyzed. As mentioned, the OH species is appropriate to show the flame shape. Here, the flame thickness is assumed to be the difference between the locations of maximum and minimum concentration of the OH species. Figure 9 illustrates the effect of increasing hydrogen concentration in the fuel on the flame thickness. It is demonstrated that as the volumetric percentage of hydrogen increases, the flame thickness decreases. At lower percentages of hydrogen addition to the fuel, its effect on reducing the flame thickness is more pronounced. At higher percentages, the flame thickness becomes almost independent of the amount of hydrogen in the fuel.

![Figure 9 - Hydrogen effect on the flame thickness.](image)

The impacts of hydrogen addition on the flame shape and flashback tendency is explained. Finally, the impacts of operating pressure on those behaviors are investigated. The operating conditions of many combustion chambers are such that they have high inlet pressure and temperature. So, providing these conditions for experimental studies is very complicated and expensive. Accordingly, developing atmospheric test stands to study the combustion chamber behavior has been considered for decades in many research centers. Although the main factor to develop the low pressure test facilities has been the complexity and unavailability of the high pressure ones, their physicochemical characteristics are such that some flow structures are reasonably independent from the operating pressure [41]. Therefore, before using such equipment, it is always necessary to ensure the effect of pressure on the subject under study.
The simulations are performed for pure methane and also for 23% hydrogen addition cases at two different operating pressures. As a result, increasing pressure causes the flame to move upstream and increases the probability of flashback phenomenon. According to Fig. 10, the effect of increasing pressure for methane fuel and also for hydrogen-methane fuel is almost the same. In addition, the results show that although an atmospheric test stand provides qualitatively true results for such studies, but the quantitative results may be wrong.

![Figure 10 - Effect of operating pressure on axial temperature distribution.](image)

**4. Conclusion**

The impacts of hydrogen addition to the fuel on the combustion induced vortex breakdown flashback phenomenon in a research burner are numerically investigated. The EDC combustion model is utilized in order to model the turbulence-chemistry interactions, and the GRI 2.11 reaction mechanism is used to investigate the combustion process of hydrogen-methane-air. The studies are performed keeping the mass-averaged exit temperature constant to keep the cycle operational condition unchanged, which is important for adding hydrogen to the existing combustion chambers especially from technological viewpoint. The effect of hydrogen addition on the flame thickness and flame shape is investigated and finally, the effect of operating pressure on the flashback behavior is analyzed. The results demonstrate that by adding hydrogen and reducing the methane, the equivalence ratio decreases and the flame moves upstream. By defining a hypothetical flame thickness, it is shown that adding hydrogen reduces the flame thickness, but at higher hydrogen percentages, the flame thickness will no longer depend on hydrogen addition. The effect of operating pressure is also
investigated and it is illustrated that increasing the pressure moves the upstream in both pure methane and hydrogen-methane fuels, and atmospheric test stands are not appropriate for quantitative flashback studies.

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• Author contribution: All authors contributed to the study conception and analysis was performed by all of them. All authors read and approved the final manuscript.
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