THREE-DIMENSIONAL SIMULATIONS OF FLASHBACK IN PREMIXED HYDROGEN FLAMES WITHIN PERFORATED BURNERS

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Abstract

Predicting flashback in perforated burners for hydrogen substitution in household appliances is crucial yet challenging. Existing studies predominantly employ two-dimensional (2D) simulations due to lower computational demands, but these may not capture the actual flame dynamics, leading to potentially inaccurate predictions of flashback limits. This study utilizes three-dimensional (3D) simulations to evaluate the effects of the finite length of the slits on the flashback limits of hydrogen-premixed flames. Both steady-state and transient simulations are conducted to estimate flashback velocities and dynamics in realistic slit configurations. Comparisons with 2D results reveal significant underestimations of flashback limits by 2D models, as these models neglect the slit ends where flashback typically initiates.

Introduction

The growing interest in hydrogen as a clean fuel necessitates innovative designs for household and commercial heating devices. These devices, equipped with perforated burners, must be re-engineered for hydrogen to prevent excessive temperatures and flashback phenomena. Significant differences in the physical properties of hydrogen compared to natural gas challenge these adaptations. Recent research has concentrated on understanding the flashback limits for hydrogen and hydrogen-natural gas mixtures, with studies exploring these phenomena both experimentally and numerically [1-5]. However, most numerical studies have utilized two-dimensional (2D) simulations, which are computationally economical but could fail to capture the complete dynamics of flashback, potentially leading to inaccuracies. This research takes a novel approach by employing three-dimensional (3D) simulations to better understand how the finite lengths of slits affect flashback limits in hydrogen-air flames. We aim to determine the accuracy of 2D models in estimating flashback velocities and the impact of slit length on flame behavior and heat transfer mechanisms. Our comprehensive simulations include both steady-state and transient analyses, comparing 2D assumptions against more realistic 3D configurations to provide a more accurate understanding of flashback dynamics.

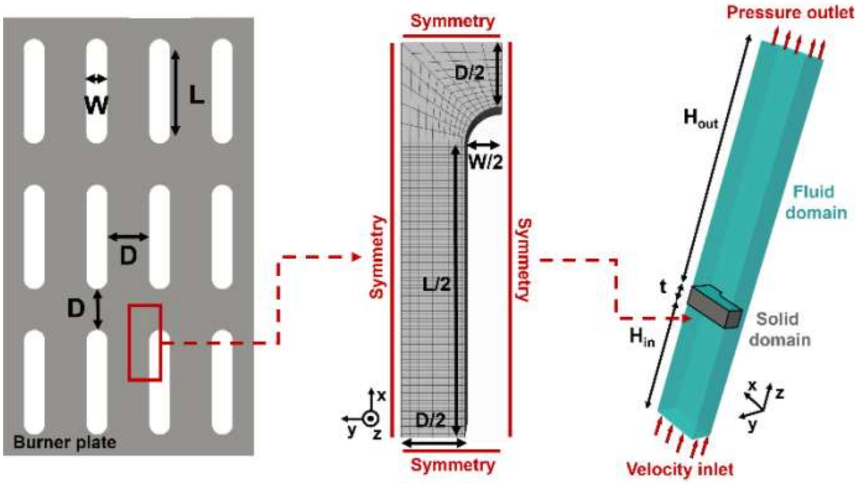

Figure 1. Configuration and computational domain.

Configuration and numerical methods

In this study, we simulate a segment of the perforated plate from a real burner typically used in domestic condensing boilers. We consider 3D configurations representing arrays of holes or slits in various shapes and sizes. The 3D configuration and computational domain are depicted in Figure 1. The computational domain is reduced to a quarter of the entire slit, applying symmetry boundary conditions on the symmetry planes. The numerical fluid domain extends $H_{out} = 4\ mm$ upstream and $H_{out} = 8\ mm$ downstream of the solid plate. The slit width is denoted as W, and the distance between two adjacent slits is D. The length between the centers of the round ends of the slit is denoted as L. With this definition, $L = 0$ corresponds to a circular hole of diameter W. The thickness of the burner plate is $t = 0.6\ mm$, and the slit width is fixed at $W = 0.5\ mm$. The porosity of the burner, $\psi = \mathrm{A_{slit}}/\mathrm{A_{tot}}$, is adjusted by modifying the distance between slits, D, where A_{slit} and A_{tot} represent the perforated and total plate areas, respectively. We examine H2-air mixtures at various equivalence ratios ϕ. Uniform velocity and temperature $T_u = 300\ K$ are imposed at the inlet, and a pressure of $p = 1\ atm$ is imposed at the outlet. At the fluid-solid interface, a no-slip boundary condition is set for the velocity, and zero-mass flux for the species equations, with the fluid and solid domains thermally coupled through conjugate heat transfer (CHT), which accounts for the interaction between the flame and the burner plate. The governing equations include conservation of mass, momentum, and energy, along with transport and reaction equations for the chemical species, solved on a structured grid with a characteristic cell size of 25 μm in the reaction front region. We employ detailed chemistry using a reduced version of the Kee-58 mechanism, which includes 9 chemical species and 22 reversible reactions. The model incorporates full multicomponent diffusion, Soret diffusion, and radiation. The energy equation is solved within the solid domain, which is modeled using properties of stainless steel used in these burners.

Estimation of flashback velocity

This study employs two different solution approaches to address varied objectives. A steady-state approach is used for parametric variations due to its computational efficiency, ideal for extensive studies but unsuitable for analyzing flashback dynamics. In contrast, a transient approach, though computationally demanding, enables the study of these dynamics.

In the steady-state method, a stable flame solution is initially obtained with a high inlet velocity using a pressure-based coupled algorithm with second-order spatial discretization. The inlet velocity is then gradually reduced until the solver cannot converge, indicating the critical velocity for flashback. To determine this velocity accurately, the minimum reduction is set to $\Delta V_{in} = 0.01\ m/s$. The flashback velocity is defined as the cold-flow bulk velocity at the slit entry when flashback occurs, calculated as $V_{FB} = 1/\psi\ V_{in}$ at the flashback occurrence.

For the transient approach, simulations cover the entire slit geometry to address potential asymmetries in flashback dynamics, using a second-order scheme for time discretization and a PISO implicit algorithm. The time step within the fluid domain is 1 μs. The solution methodology remains consistent with the earlier description, maintaining a minimum velocity decrement of $\Delta V_{in} = 0.01\ m/s$.

Results and discussion

In a 2D simulation of a slit array, the domain models a cross-section of the slit, assuming it to be infinitely long, which neglects the slit ends. We aim to identify the minimal slit length for which a 3D slit is closely approximated by a 2D model. We conduct steady-state simulations for 3D configurations with slit lengths ranging from 1 mm to 80 mm, comparing these with a consistent 2D model. All 3D geometries share identical cross-sectional profiles to be represented by the same 2D model. The mixture's equivalence ratio is set at 0.6, and the inlet velocity is adjusted to ensure a uniform cold-flow velocity at the slit entry, standardized at 4 m/s. To illustrate how the burner temperature depends on slit length, Figure 2 plots its volume-averaged value in the solid domain as a function of the slit length, including results from the 2D simulation for comparison. This emphasis on burner temperature is crucial, as it significantly influences the flashback velocity [2].

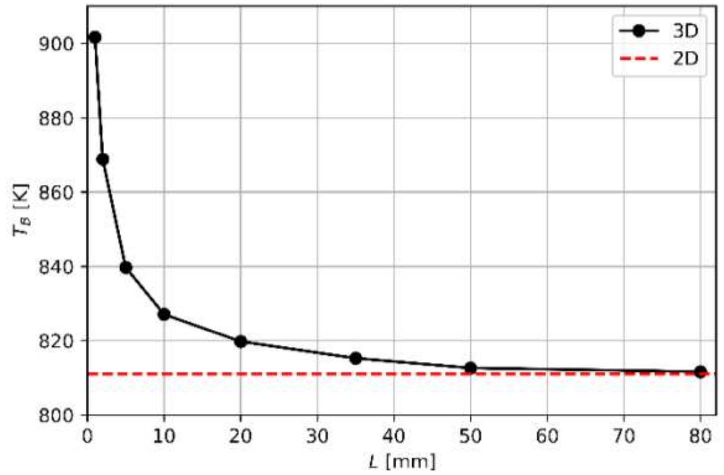

Figure 2. Burner plate temperature as a function of the slit. The dashed line represents the 2D result.

The 2D simulation predicts a burner temperature of 812 K. In contrast, 3D simulations show that at a 1 mm slit length, the burner temperature is 902 K, which decreases to 827 K at 10 mm, eventually aligning with the 2D result around 50 mm. Higher temperatures in shorter slits result from significant heat transfer at the slit ends, where the flame and burnt gases heat the burner plate. As slit length increases, the influence of the ends diminishes, aligning the 3D results more closely with the 2D conditions. The 2D model effectively represents 3D slit behavior only for lengths exceeding 50 mm. However, slits in practical condensing boiler burners typically range from 0 to 5 mm, indicating that 2D simulations may fail to accurately reproduce the behavior of practical devices.

To explore how the finite length of the slit affects the flashback velocity, and compare 3D and 2D models, we calculate flashback velocities using a steady-state approach for three equivalence ratios, $\phi = 0.6$, 0.8, and 1.0. We examine slits ranging from $L = 0$ to $L = 8\ mm$, with $L = 0$ representing a circular hole. To ensure consistent comparisons, we maintain a fixed porosity of $\psi = 0.2$ by adjusting the spacing between slits. In Figure 3, we present the flashback velocities normalized by the 1D unstretched laminar flame speed as a function of slit length. We also include results for a 2D configuration that simulates an infinite slit, matching the width and porosity of the 3D cases. As expected, for both 2D and 3D simulations, the normalized flashback velocity decreases with increasing equivalence ratio, as the flashback propensity is strongly affected by preferential diffusion effects. We observe a rapid increase in the flashback velocity from $L = 0$ to $L = 1\ mm$. However, for $L > 1\ mm$, the influence of slit length on flashback velocity significantly diminishes, reaching an almost constant value. Notably, unlike the burner plate temperatures shown in Figure 2, where 2D results eventually align with 3D values for larger slit lengths, the flashback velocities in 2D do not converge with those in 3D, being underestimated of approximately 50%.

To explain why the flashback velocity is almost independent of slit length, and why these values do not align with those of the 2D case for larger lengths, a deeper understanding of the flashback is needed. To this end, two transient simulations are conducted: one representing a 2D configuration and another for a 3D slit with a length of $L = 2\ mm$. For both configurations, the slit width is specified as $W = 0.5\ mm$ and the porosity as $\psi = 0.2$. An equivalence ratio of $\phi = 0.6$ is set for the inlet mixture. In Figure 4, we illustrate the flashback event for the 2D configurations. The evolution of the temperature profiles is displayed in four snapshots taken during the occurrence of flashback. As the 2D configuration only considers the transversal section of an actual slit, the flashback dynamics can only be

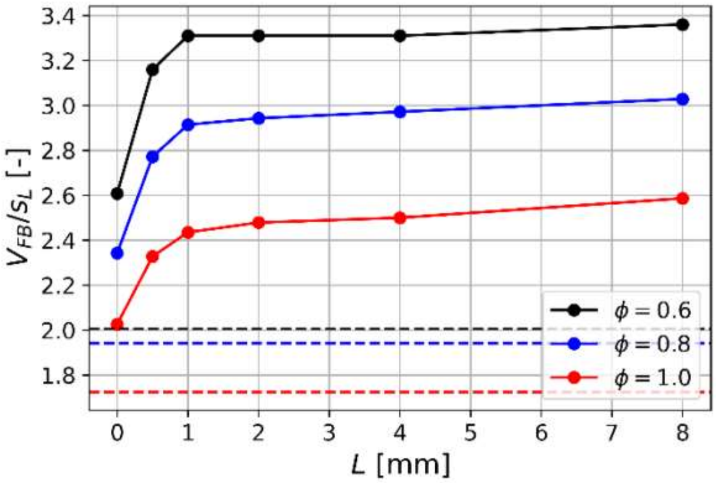

Figure 3. Normalized flashback velocity as a function of the slit length. 2D results are indicated by dashed lines.

represented by the flame crossing the slit starting from the slit side walls. This is imposed by the choice of a 2D domain and could be substantially different from the actual dynamics occurring in a three-dimensional slit.

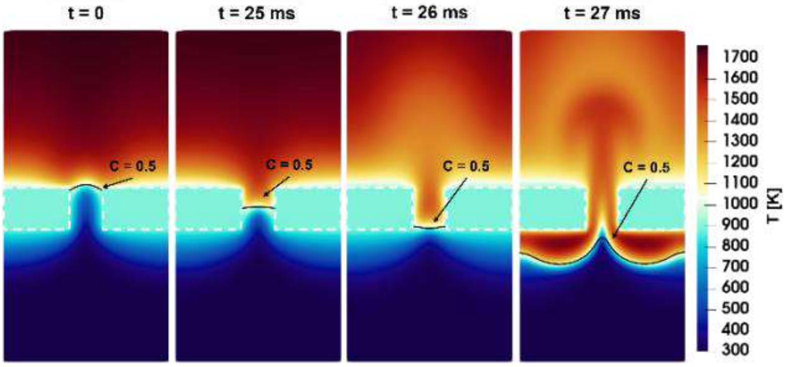

Figure 4. Flashback dynamics in the 2D configuration.

Figure 5 depicts a sequence of four snapshots captured during the flashback occurrence for the 3D configuration. The snapshots illustrate the evolution of the flame front, defined as an iso-surface of progress variable corresponding to $C = 0.5$. The initiation is asymmetric, starting at one end of the slit. From there, the flame front moves backward towards the entrance, traversing the slit entirely on that side, and ultimately driving the entire flashback process. To understand the role of the slit ends and the physical mechanisms involved, a visualization of the last stable flame, is presented in Figure 6. The iso-contour of progress variable at $C = 0.5$ is colored to show temperature (a), local equivalence ratio (b), normalized molecular H_2 consumption rate (c), and displacement speed (d), defined as $S_D = v \cdot n$, where n is the unit vector normal to the iso-surface. A temperature peak is observed at the slit ends where the enclosed geometry enhances heat transfer, resulting in greater pre-heating of the mixture (Figure 6 (a)). In these regions, preferential diffusion effects and Soret diffusion [6] contribute to fuel enrichment of the mixture (Figure 6 (b)). These phenomena lead to an increase in the H_2 consumption rate (Figure 6 (c)), and subsequently, an increase in flame speed, as indicated by the local maxima of displacement speed (Figure 6 (d)). Consequently, this region becomes the initiation zone for flashback, where the local flame speed surpasses the flow velocity, triggering the flashback initiation. The observation of this distinctive dynamics explains why the flashback velocity shows weak dependence on the length of the slit beyond a certain value, as seen in Figure 3. This occurs because the critical region for flashback initiation is consistently located at the slit ends, regardless of the specific value of L. Furthermore, the significant role played by the slit ends underscores that flashback is inherently a three-

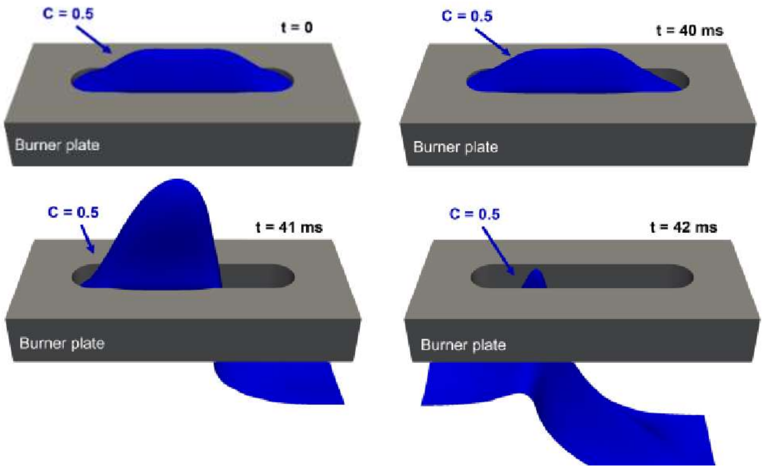

Figure 5. Flashback dynamics in the 3D configuration.

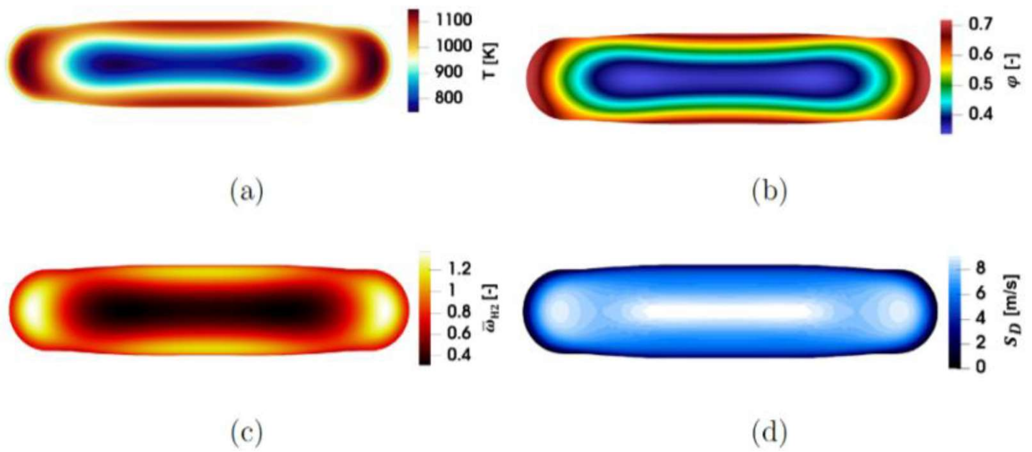

Figure 6. Iso-contour of progress variable (C=0.5) colored by: (a) temperature, (b) equivalence ratio, (C) normalized H_2 consumption rate, and (d) displacement speed.

dimensional phenomenon. Enhanced fuel enrichment and pre-heating at the slit ends cause flashback to initiate at higher inlet velocities compared to 2D configurations. Consequently, the 3D results shown in Figure 3 do not align with those from 2D configurations, where the slit ends are consistently neglected. These results highlight the necessity of using 3D simulations for the accurate estimation of flashback velocities in perforated burners.

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