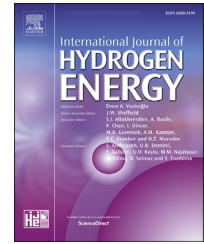


Available online at www.sciencedirect.com

ScienceDirect

journal homepage: www.elsevier.com/locate/hydro

Numerical investigations on flashback dynamics of premixed methane-hydrogen-air laminar flames

Tahsin Berk Kıymaz ^a, Emre Böncü ^a, Dilay Güteryüz ^a, Mehmet Karaca ^b,
Barış Yılmaz ^c, Christophe Allouis ^{a,d}, İskender Gökalp ^{a,e,*}

^a Middle East Technical University, Mechanical Engineering Department, Ankara, Turkey

^b Middle East Technical University, Aerospace Engineering Department, Ankara, Turkey

^c Marmara University, Mechanical Engineering Department, İstanbul, Turkey

^d STEMS-CNR, Naples, Italy

^e ICARE-CNRS, Orléans, France

HIGHLIGHTS

- 2D unsteady computations of laminar hydrogen added methane-air flames are performed to capture flashback dynamics.
- Higher wall temperature increases the boundary layer flashback propensity.
- H₂ addition to CH₄+Air premixtures increases the flashback propensity.
- Flashback dynamics shows asymmetrical flame propagation.

ARTICLE INFO

Article history:

Received 14 March 2022

Received in revised form

19 May 2022

Accepted 24 May 2022

Available online 22 June 2022

Keywords:

Laminar premixed flames

Flame flashback

Hydrogen

Methane

Numerical simulations

OpenFOAM

ABSTRACT

Injecting hydrogen into the natural gas network to reduce CO₂ emissions in the EU residential sector is considered a critical element of the zero CO₂ emissions target for 2050. Burning natural gas and hydrogen mixtures has potential risks, the main one being the flame flashback phenomenon that could occur in home appliances using premixed laminar burners. In the present study, two-dimensional transient computations of laminar CH₄ + air and CH₄ + H₂ + air flames are performed with the open-source CFD code OpenFOAM. A finite rate chemistry based solver is used to compute reaction rates and the laminar reacting flow. Starting from a flame stabilized at the rim of a cylindrical tube burner, the inlet bulk velocity of the premixture is gradually reduced to observe flashback. The results of the present work concern the effects of wall temperature and hydrogen addition on the flashback propensity of laminar premixed methane-hydrogen-air flames. Complete sequences of flame dynamics with gradual increases of premixture velocity are investigated. At the flame flashback velocities, strong oscillations at the flame leading edge emerge, causing broken flame symmetry and finally flame flashback. The numerical results reveal that flashback tendency increase with increasing wall temperature and hydrogen addition rate.

© 2022 Hydrogen Energy Publications LLC. Published by Elsevier Ltd. All rights reserved.

* Corresponding author. Middle East Technical University, Mechanical Engineering Department, Ankara, Turkey.

E-mail address: igokalp@metu.edu.tr (İ. Gökalp).

<https://doi.org/10.1016/j.ijhydene.2022.05.230>

0360-3199/© 2022 Hydrogen Energy Publications LLC. Published by Elsevier Ltd. All rights reserved.

Introduction

The interest in welcoming hydrogen as an energy carrier increases worldwide for combustion and fuel cell applications to decrease global CO₂ emissions. For combustion applications, however, the use of 100% hydrogen is still technologically and logistically immature and requires significant changes in related infrastructures and appliances for hydrogen combustion. Therefore, hydrogen-enriched natural gas applications could be a preliminary approach to facilitate the introduction of hydrogen [1–6].

The addition of H₂ to CH₄-air alters the key combustion parameters as laminar flame speed, flame thickness, flammability limits and adiabatic flame temperature. Presently, there is no homogenized regulation, for example at the EU level, for hydrogen and natural gas blending rates, the so-called gas quality. Therefore, it is essential to determine the safe hydrogen concentration limits in the existing natural gas transmission and distribution networks, together with this mixture's safer combustion and better performances [7].

Premixed combustion of hydrogenated mixtures presents the risk of upstream flame propagation into the premixing section, which is known as the flame flashback phenomenon. Flashback limits depend on various parameters that can be divided into three main categories based on: (1) flow and combustion physics, (2) operating conditions, and (3) flame configuration [8]. Flashback mechanisms and limits are different for laminar and turbulent flames. Flow and combustion physics cover laminar or turbulent flow characteristics, the effects of the fuel composition and the laminar flame speed [9]. Operating conditions include parameters such as pressure, burner material, wall and unburnt gas temperatures [10]. Flame configuration includes parameters such as burner diameter, rim temperature, burner material, and flame confinement [8,11,12]. Lewis and von Elbe studied the burner diameter effect in their pioneering work [11], while Duan et al. [12] investigated the effect of burner confinement on turbulent flashback. These studies show the strong effect of burner wall temperature on flashback propensity, higher temperatures of the burner rim resulting in higher flashback risk. Kurdyumov et al. [13] stressed the importance of modelling the wall heat losses correctly by comparing laminar flashback computations using adiabatic and cold wall conditions.

Eichler et al. [9] studied the comparison of laminar and turbulent flashback formation by using the micro-PIV technique. They observed that higher turbulence intensity and therefore turbulent flame speed cause higher flashback propensity. For turbulent hydrogen-air flames, the effect of wall temperature is previously studied extensively [12,14]. Duan et al. also state that turbulent flame flashback is determined by the burner rim temperature, and that it should be correctly modelled. Later, they studied the effect of the burner material on the flashback of turbulent hydrogen-air flames and concluded that quartz burners are the more flashback prone than metal burners [12,14].

The present work focuses on the laminar boundary layer flashback phenomenon for a fixed burner diameter but varying fuel composition (by adding hydrogen to methane) and wall temperature. Based on the past mostly experimental

work, the present work numerically investigates the flashback dynamics for CH₄-air and CH₄-H₂-air laminar premixed flames. A numerical framework is chosen to determine whether flashback occurs or not for a given combination of fuel composition and bulk inlet velocity. For each of the investigated wall temperature cases (300K and 600K), 10% and 20% volumetric hydrogen are added to methane. In addition, an adiabatic wall case for 20% hydrogen addition rate is investigated for comparison purposes. In total, seven different cases are presented in this work. The computed flashback limits are compared with the experiments of de Vries et al. [15], the experimental correlations proposed by Lewis and von Elbe [11], Putnam et al. [16] and the theoretical correlations of Hoferichter [17].

Premixed laminar flame flashback phenomenology

Household gas appliances, represented here by Bunsen type burners, may experience flame flashback when the laminar flame speed surpasses the bulk cold premixture velocity. Flame flashback may cause severe damage in domestic gas appliances since it can carry the flame to areas of the burner system that are not designed to sustain high temperatures [18,19]. Flashback can happen in different regimes such as core flow flashback, boundary layer flashback and combustion instability induced flashback. This study is focused only on the boundary layer flashback regime.

Lewis and von Elbe [11] developed a comprehensive phenomenological model based on the critical gradient concept after conducting a series of experiments using laminar Bunsen type burners. This model assumes a fully developed laminar velocity profile of the cold premixture at the burner inlet and introduces two critical parameters: the quenching distance (δ_q) and the penetration distance (δ_p), shown in Fig. 1. The quenching distance is the distance from the burner inner wall where chemical reactions are quenched due to heat losses to the wall. The penetration distance is the distance from the wall at which the local laminar flame speed is equal to the local premixture velocity at flashback conditions. Based on the Lewis and von Elbe's model, Putnam et al. [16] proposed that the critical gradient concept can be interpreted by using the cold flow and the flame Peclet numbers. Hoferichter et al. [17] presented a flashback correlation based on the critical gradient concept with stretch effects by using the Markstein length.

In the present work the flashback limits calculated using the aforementioned methods are compared with the flashback limits calculated using our two dimensional computations. To perform these comparisons, we calculated the Markstein length following Bechtold and Matalon [20] which can be used for lean and rich mixtures. The CH₄-H₂ fuel mixture's Lewis number (Le) is calculated by using the species volumetric fractions. Using both the oxidizer and the fuel Lewis numbers, the effective Le is calculated as in Ref. [20]. The quenching distance is calculated by taking the quenching Peclet number as 4.5 according to the experimental work of Boust et al. [21] and assuming to be unchanged with H₂ addition [19]. The penetration distance is obtained following Hoferichter et al. [17] based on study of Gruber et al. [22].

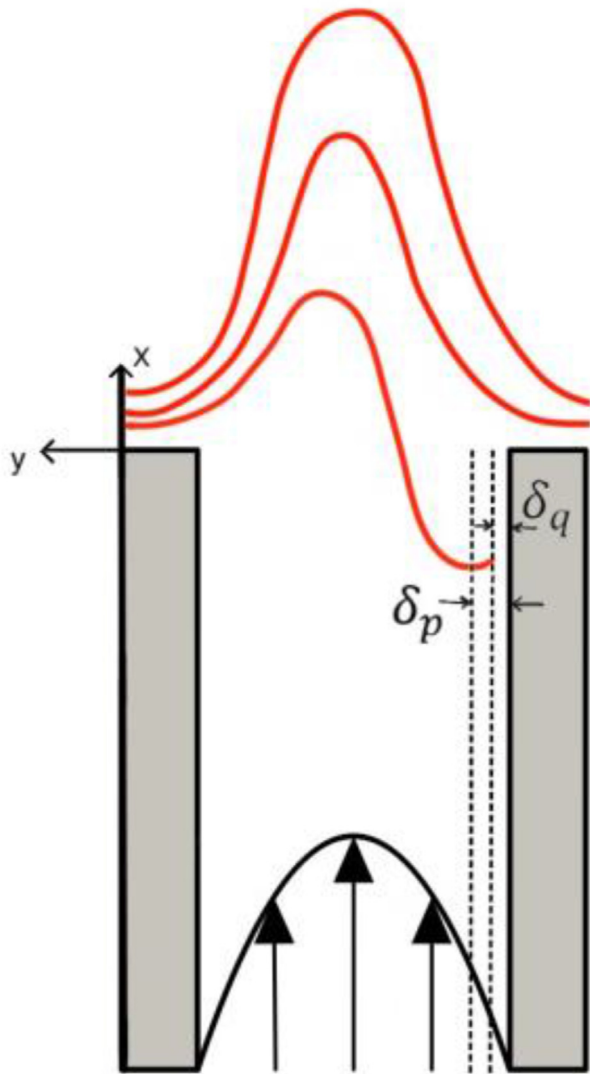


Fig. 1 – Illustration of boundary layer flashback parameters in a laminar premixed flame.

In our numerical work, we attempt to compute the laminar flame flashback dynamics by solving the reactive flow equations and compare the results both with experiments and the above summarized phenomenological and theoretical results.

Numerical modelling

The transient, compressible reacting flow solver 'reactingDNS' developed for OpenFOAM by Zhang et al. [23,24], is used for the laminar flame computations. This solver has a built-in multicomponent species transport model. The finite volume solver employs the PIMPLE [25] algorithm, which combines the PISO (Pressure Implicit with Splitting of Operator) and its extension SIMPLE (Semi-Implicit Method for Pressure-Linked Equations) algorithms. The reaction terms are computed using a reduced GRI-Mech 3.0 mechanism with 218 reactions involving 36 species [26]. Chemical reactions are treated with

the Tabulated Dynamic Adapted Chemistry method [27], which is a combination of two run-time reduction methods, namely the In Situ Adaptive Tabulation [28] and the Dynamic Adaptive Chemistry [29]. An adjustable time step is employed, limiting the maximum Courant number to 0.1 to ensure a stable solution, which leads to a time step of the order of 10^{-6} s. N_2 is the inert species in the computations.

The governing equations in the solver are written in conservative form; they are presented below.

Continuity equation:

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{U}) = 0 \quad (1)$$

Momentum equation:

$$\frac{\partial}{\partial t} (\rho \mathbf{U}) + \nabla \cdot (\rho \mathbf{U} \mathbf{U}) = -\nabla p + \nabla \tau \quad (2)$$

with the viscous stress tensor τ where the bulk viscosity is neglected.

Energy equation:

$$\begin{aligned} \frac{\partial}{\partial t} (\rho h_s) + \nabla \cdot \left(\frac{\rho}{U} h_s \right) + \frac{\partial}{\partial t} (\rho K) + \nabla \cdot (\rho \mathbf{U} K) &= \nabla \cdot \left(\frac{\lambda}{c_p} \nabla h_s \right) + \dot{R}_h \\ + \nabla \cdot \left(\rho \sum_i^N \nabla h_{ki} J_i \right) + \frac{\partial p}{\partial t} & \end{aligned} \quad (3)$$

where h_s is the sensible enthalpy, K is the kinetic energy, and \dot{R}_h is the heat release term due to chemical reactions.

Species transport equation:

$$\frac{\partial}{\partial t} (\rho Y_i) + \nabla \cdot (\rho \mathbf{U} Y_i) + \nabla \cdot (J_i) = \dot{R}_i \quad (4)$$

\dot{R}_i represents the reaction source term and the diffusion flux J_i contains only Fickian diffusion. \dot{R}_i is calculated using Arrhenius equations defined for each chemical reaction modelled in the reduced GRIMECH 3.0 mechanism. \dot{R}_h is calculated using the \dot{R}_i and h_i for species i .

A logarithmic third order polynomial fit is used as in CHEMKIN [30,31] to calculate the detailed transport properties as a function of temperature. This method is also used for modelling the transport properties in turbulent wall flashback studies such as in Eichler et al. [9] and Gruber et al. [32]. Further details on the equations used in the 'reactingDNS' solver can be found in Ref. [24].

Numerical setup

Computational domain

The experimental setup of de Vries et al. [15], a quartz tube burner with 10 mm inner diameter and 1 m length, is chosen as the geometry for the computational domain. A two-dimensional modelling approach is used for the burner and the surrounding ambient air. This assumption does not strictly represent the axisymmetric geometry of the experimental case, it is however chosen to capture asymmetrical flame behavior that result in boundary layer flashback of laminar flames. The last 30 mm of the tube length is considered for the computations where the fully developed flow

conditions are attained (see Fig. 2). This also allows observing the upstream flame propagation dynamics from the exit.

A total number of 102,050 fully structured cartesian cells make up the mesh system which is uniformly confined at the vicinity of the flame front. Since resolving the boundary layer with enough detail is critical in computing flame flashback, the cell size in the radial direction is set to 0.066 mm, giving $y^+ = 0.33$ for the highest bulk inlet velocity case. This cell size is also of the order of the flame thickness for the investigated mixtures. The mesh resolution is further validated by 1D laminar flame speed calculations with the same resolution as the two-dimensional mesh used in OpenFOAM computations. The comparison of one-dimensional computation results with the quasi-steady flame speed analysis using the Cantera solver are in good agreement within ~1% accuracy (see Table 1). Therefore, for unsteady computations our mesh system is considered to provide accurate results for the flame flashback dynamics [33].

Boundary conditions

The computational domain with boundary conditions is shown in Fig. 2. The cold premixture enters the domain inlet with a fully developed Hagen-Poiseuille flow velocity profile as in the considered experimental work [15]. The initial temperature and pressure are taken to be 300 K and 100 kPa, respectively. The domain outlets are assumed to be adiabatic for the temperature boundary conditions. Wave transmissive pressure outlet boundary condition is used at the outlet section to prevent any instabilities caused by incoming waves. The reference pressure for the outlet is set at atmospheric pressure (100 kPa) and the velocity boundary condition at the outlet prevents any backward flow. We implemented both adiabatic and two constant wall temperature conditions. Experimental burner wall temperature measurements are not reported in the work by de Vries et al. [15]. Therefore, we

performed the computations for a cold isothermal wall at 300K and a hot isothermal wall at 600K. The two wall temperature values were chosen to ensure the experimental flashback limits are within the estimates of these two sets of computations. The effect of burner temperature is studied by Kurdyumov et al. [13]; they state that one can expect the experimental conditions would be in between the adiabatic and cold isothermal wall conditions. Our computations show that the flame attaches to the wall for adiabatic wall conditions since there is no heat losses to the burner walls. This is a non-realistic phenomenon, modelled here for demonstration purposes and therefore only constant wall temperature results are presented below in detail.

Results and discussion

Equivalence ratio and laminar flame propagation speed calculations

In the experimental work of de Vries et al. [15], the premixture equivalence ratio changes with hydrogen addition due to their experimental procedure. To compare the numerical results with the experiments, the changes in the equivalence ratio are calculated accordingly, as shown in Table 1. The mass fractions are subsequently calculated to adjust the reactive mixture composition to the experiments. Table 1 also compares the laminar flame velocities computed using Cantera and the present OpenFOAM 1D computations using 'reactingDNS' solver. Both computations are performed using GRIMECH3.0 mechanism. The 1D OpenFOAM simulations have the same mesh refinement as in 2D computations. It is observed that the 1D numerical simulations of S_L present a maximum deviation of about 1% compared to Cantera calculations; they are therefore assumed to be accurate enough for flame flashback computations.

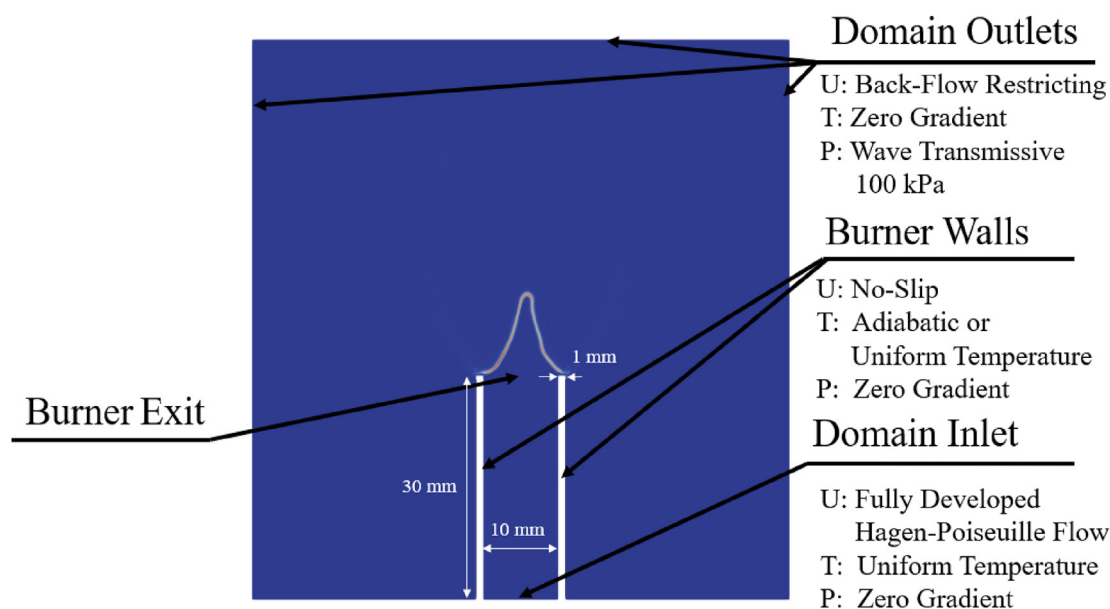


Fig. 2 – Computational domain and boundary conditions.

Table 1 – Initial values for species concentrations.

H ₂ % [mol]	Φ	Y _{H₂}	Y _{CH₄}	Y _{O₂}	Y _{N₂}	S _L	
						Cantera [m/s]	OpenFOAM [m/s]
0	1.3	0	0.071	0.216	0.713	0.237	0.240
10	1.258	0.00093	0.067	0.217	0.715	0.311	0.315
20	1.216	0.0019	0.063	0.217	0.716	0.388	0.393

Temperature and velocity profiles of the stationary flame

Combustion is initiated by imposing a homogeneous temperature field set at 2000K at the burner exit. For a stable CH₄-air flame with no H₂ addition and a bulk inlet velocity of 0.40 m/s, Fig. 3 show the flow streamlines colored by the temperature (Fig. 3a) and by the velocity magnitude (Fig. 3b). When the cold flow reaches the flame front, the streamlines are deflected in the flame local normal direction, and the velocity jump is well observed.

Flashback dynamics

Flashback dynamics and limits are analyzed by conducting numerical simulations of the same premixture composition at the same wall temperature for varying bulk inlet velocities. The computations were started for a stationary flame far from flashback conditions; the inlet velocity is then gradually reduced until flashback occurs. Flashback is considered to take place when the flame front begins to enter the burner tube and travels in the upstream direction. For all cases, the flashback dynamics analysis starts with a stable flame corresponding to the lowest bulk inlet velocity that is not causing flashback for the explored conditions. The bulk inlet velocity of the laminar flame is then reduced (at the time labeled $t = 0$) by a percentage of the laminar flame speed to investigate the flashback dynamics.

An example of the method adopted for the flame flashback dynamics computational analysis is described below for a CH₄-Air mixture at $\Phi = 1.3$ with the wall temperature condition set to 600K (Fig. 4). In the following flashback sequences, the flame front is represented using the normalized heat release rate i.e. the ratio of the computed heat release rate to its maximum value. At the start of the computations, a stable laminar flame far from the flashback point is simulated for a

bulk inlet velocity of 0.48 m/s, twice the computed S_L (0.24 m/s). The bulk inlet velocity is then reduced gradually until leading edge formation is observed. The velocity reduction step values correspond to ~5% of the laminar flame speed. In this example, this corresponds to the ratio of the bulk inlet velocity reduction step (0.012 m/s) to the calculated laminar flame speed (0.24 m/s). For this case, the bulk inlet velocity reduction from 0.38 m/s to 0.368 m/s results in flashback. Once flashback is triggered, the bulk velocity is kept constant and the temporal flame dynamics is computed.

Fig. 4a shows the flame at 0.38 m/s; it is clearly observed that the flame front is not attached to the burner rim. Time is set to $t = 0$ at the instant when the bulk inlet velocity is reduced from 0.38 m/s to 0.368 m/s. 0.195 s after the decrease of the bulk inlet velocity to 0.368 m/s, the flame symmetry is lost (Fig. 4b) and the flame front on the left side of the burner rim becomes parallel to the rim. In Fig. 4c, a leading flame edge is formed, and the flame front starts to propagate in the upstream direction. The quenching distance can be observed near the left wall, where the heat release rate decreases (Fig. 4c and d). The emergence of the penetration distance is also clearly visible in these figures. The tip of the flame front is shifted to the right and the flame becomes a tilted flame (Fig. 4c and d) The tilted flame shape, also observed in the experiments [11,14,15,34] and numerical study by Vance et al. [35], is caused by the adverse pressure gradient in the upstream of the leading edge and the resulting deflection of the streamlines in the opposite direction to the flame [10]. Fig. 4d shows the start of the upstream propagation of the flame front.

In this example, flashback occurs at 0.368 m/s bulk velocity which is 53% higher than the laminar flame propagation speed (0.24 m/s). A flashback initiation delay time of 0.195 s is observed (Fig. 4b). The leading edge formation is observed at 0.278 s (Fig. 4c) and upstream flame propagation at time 0.292 s

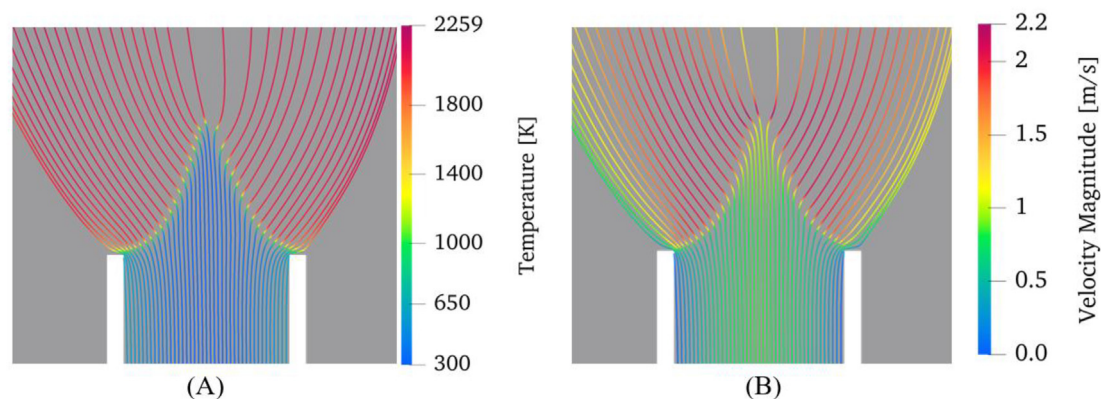


Fig. 3 – Streamlines colored by (A) temperature, (B) velocity magnitude.

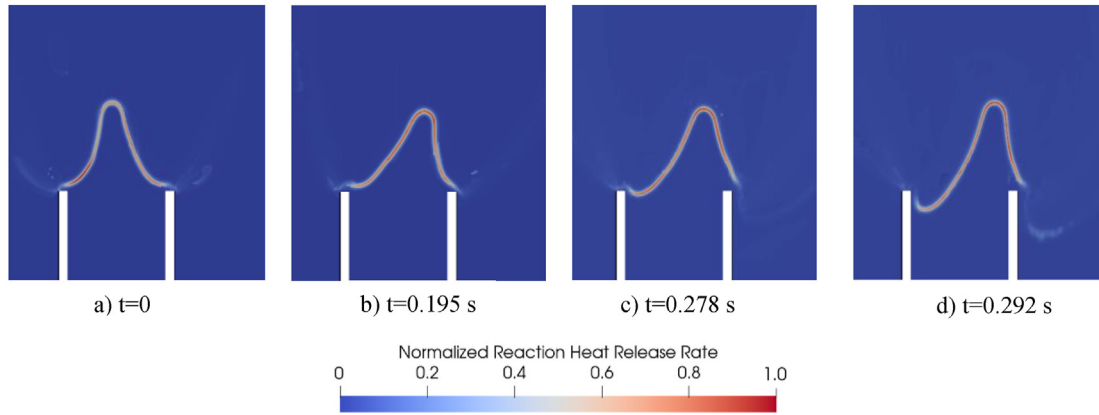


Fig. 4 – Flashback dynamics represented by the normalized reaction heat release rate contours for the methane-air mixture at $\Phi = 1.3$ for $T_{\text{wall}} = 600\text{K}$

(Fig. 4d). We define the characteristic flashback time as the difference between the leading edge formation and the flashback initiation times, which is 83 ms in this case. These characteristic flashback times are two orders of magnitude larger than the laminar flame characteristic chemical time, estimated to be about 0.5 ms for this flame condition, using the flame thickness and the flame propagation velocity values calculated with Cantera.

Similar flame flashback dynamics behavior is observed for the investigated mixtures with hydrogen addition at both 600K and 300K wall temperature cases. However, in the case of CH_4 -air mixture with $\Phi = 1.3$ for 300K constant wall temperature, the flashback dynamics is different.

In this case, the shape of the flame front looks like a flat flame due to low inlet velocity. After decreasing the bulk inlet velocity from 0.180 m/s to 0.165 m/s, the flame front takes a concave shape towards the upstream direction (Fig. 5b) and propagates inside the burner tube (Fig. 5c). Flame quenching can be first seen near the left side of the burner wall. Finally, the flame front fully enters the burner tube from both sides, as seen in Fig. 5d. The characteristic flashback times are about two times larger than the previous case. It can also be noted that in this case, flashback occurs at 0.165 m/s bulk inlet velocity, about 30% lower than the laminar flame propagation

speed (0.24 m/s), confirming the effect of the burner wall temperature.

The effect of hydrogen addition on flashback is shown in Figs. 6 and 7. Fig. 6a represents the stationary flame for the CH_4 - H_2 mixture with 20% hydrogen addition at $T_{\text{wall}} = 600\text{K}$. For this case, the onset of flashback is observed when the bulk inlet velocity is decreased from 1.1 m/s to 0.99 m/s i.e. using the 5% of the laminar flame propagation speed reduction step value as previously. The flame front starts to wrinkle in Fig. 6b. In Fig. 6c, the leading edge is formed, and the flame front starts to travel upstream (Fig. 6d), after a characteristic flashback time of 15 ms.

Fig. 7a represents the same fuel mixture with the wall temperature set at 300K. Under such conditions, it is computed that flashback occurs when the cold flow bulk inlet velocity decreases from 0.46 m/s to 0.44 m/s, i.e., with the same imposed bulk velocity reduction step value of 5% S_L as previously. The flame front is highly asymmetrical in Fig. 7b and it starts to travel in the upstream direction in Fig. 7c, giving a flashback characteristic time of 15 ms, similar to the 600K T_{wall} case. Fig. 7d shows the complete flashback for this case. The leading edge oscillates near the burner rim close to the flashback limit, also observed for all the investigated cases.

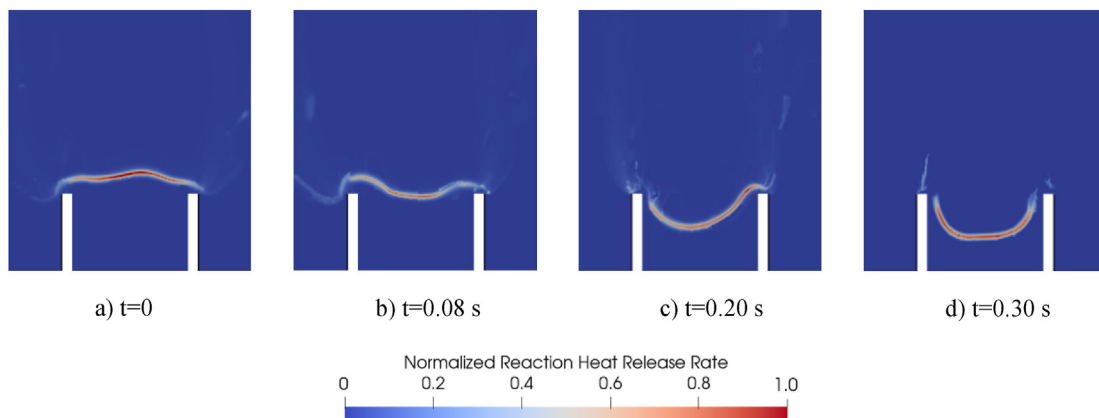


Fig. 5 – Flashback dynamics represented with the normalized heat release rate contours for CH_4 -air mixture with $\Phi = 1.3$ for $T_{\text{wall}} = 300\text{K}$ wall.

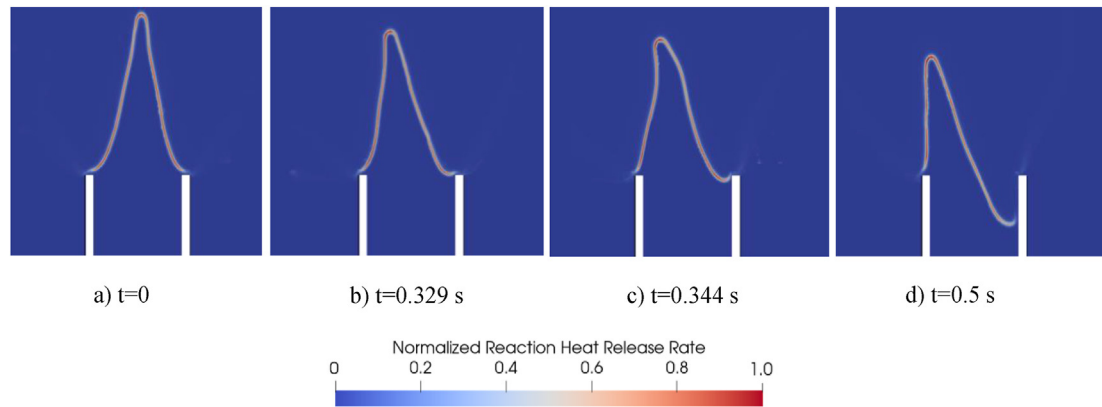


Fig. 6 – Flashback dynamics represented with the normalized heat release rate contours for methane-air flame at $\Phi = 1.216$ with 20% H_2 addition for $T_{\text{wall}} = 600\text{K}$

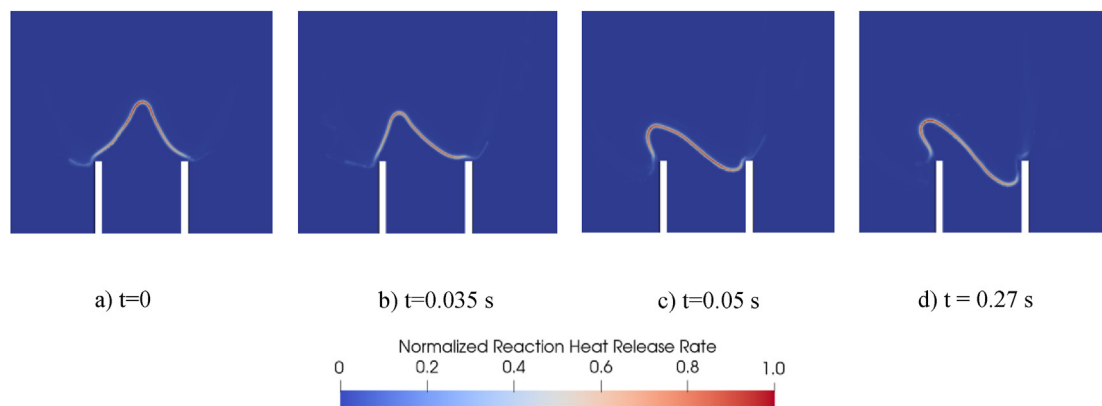


Fig. 7 – Flashback dynamics represented with the normalized heat release rate contours for methane-air flame at $\Phi = 1.216$ with 20% H_2 addition for $T_{\text{wall}} = 300\text{K}$

Hydrogen addition effect on the quenching distance

There are various methods in the literature to estimate the quenching distance. Some examples include using isocontours of %50 of maximum OH^* concentration or %50 of maximum CH^* concentration or the temperature that corresponds to the maximum gradient of the heat release rate [36]. We selected the normalized reaction heat release rate to investigate δ_q and δ_p , since it gives a direct information about the reaction rate. Therefore, the quenching distance is chosen as the nearest point to the wall where the normalized reaction heat release rate is 0.5. Fig. 8 illustrates the quenching and penetration distances, and the leading edge from an instantaneous snapshot of flashback for 20% H_2 blend case with $T_{\text{wall}} = 600\text{K}$. Normalized reaction heat release rate isocontour at 0.5 is also indicated on Fig. 8 with a black line. The midpoint of the burner exit is selected as the origin of the coordinates in Figs. 8 and 9.

For each mixture composition, after the leading edge travels 3 mm upstream from the burner exit, ten consecutive snapshots of the normalized heat release rate are collected with 1 ms time step. Calculated quenching distances are averaged and presented in Table 2. It is observed that the

quenching distance decreases with H_2 addition which agrees with previous studies [8, 35–37]. The mixture with 10% H_2 yields 33% reduction in the quenching distance. A further 10% increase in the H_2 content of the fuel induces a smaller reduction of the quenching distance, indicating a diminishing effect. Hydrogen has faster kinetics and higher reactivity compared to hydrocarbon fuels [8,38]. These properties of hydrogen lead to smaller quenching distances than for hydrocarbon fuels. Thus, even a small amount of hydrogen addition contributes significantly to reduce the quenching distance and hence to increase the flashback propensity.

Wall temperature effect

The effect of burner wall temperature is discussed in this paragraph more comprehensively. The heat transfer to the wall and the resulting temperature distribution along the wall is highly influential on the flashback limits as reported in Ref. [13]. The change in the molecular transport rates and the reactivity due to the near wall thermal boundary layer strongly affects flame dynamics and, consequently, the flame curvature. Numerical computations are conducted with constant wall temperatures of 300K, 600K and for the adiabatic

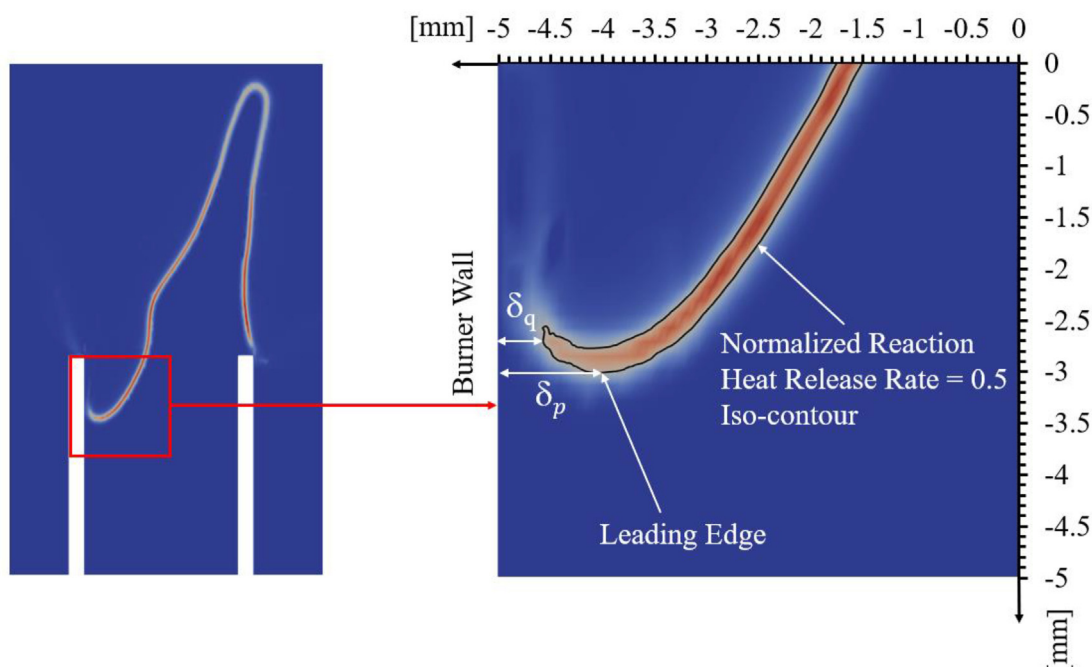


Fig. 8 – Representation of the quenching distance (δ_q) and the penetration distance (δ_p) at flashback for 20% H_2 blend for $T_{\text{wall}} = 600\text{K}$

wall condition. In Fig. 9a–c, heat release rate snapshots of the methane- H_2 -air flame at $\Phi = 1.216$ with 20% H_2 during the boundary layer flashback are shown for the three different wall conditions.

For the 300K wall temperature case, Fig. 9a shows that the reaction rate near the wall is substantially reduced compared to the 600K case shown in Fig. 9b. Quenching and penetration distances were calculated as explained in the previous section. Both δ_q and δ_p decrease with the increase in wall temperature from 300K to 600K. The rate of decrease of δ_q and δ_p are close to each other, 35% and 41% respectively. Although the laminar flame speeds at corresponding conditions are the same, 35% decrease in δ_q results in 125% increase in the critical flashback limit from 0.44 m/s to 0.99 m/s. Thus, explaining the flashback limits using only the laminar flame speed and the quenching distance is not sufficient, especially for high burner wall temperatures. As evidenced in Fig. 9a–b, the curvature of the flashbacking flame near the leading edge is increased. The curvature of the stretched flame leads to a higher local flame speed close to leading edge and hence increases the flashback propensity.

In Fig. 9c where adiabatic wall condition is used, the quenching distance and leading-edge formation are not observed contrary to the constant wall temperature cases, which is in agreement with Kurdyumov et al. [13]. A complete sequence of flashback dynamics for adiabatic wall condition is shown in Fig. 10, for which a significantly different behavior is observed compared to the isothermal wall cases for the same mixture (see Figs. 6 and 7). The flame front is attached to the burner wall which is not the case for isothermal wall conditions and the characteristic flashback times are much shorter. These results reveal that the adiabatic wall temperature condition does not represent the boundary layer flashback phenomenon.

Flashback limits

The computed flashback limits are compared in Fig. 11 with the measurements of de Vries et al. [15] and with the correlations based on the critical gradient concept of von Elbe et al. [11], Hoferichter et al. [17] and Putnam et al. [16]. In the experiments, once the flame is stabilized, the bulk inlet velocity is gradually decreased until flashback occurs. The experimental flashback limit is defined as the bulk inlet velocity U_f when the flame just enters the burner tube.

In Fig. 11, the curves limit the flashback region where the flashback is observed below the curves. Fig. 11a presents the absolute values of the critical flashback velocity. It is observed that the flashback propensity is increased with the addition of hydrogen to the mixture. This is related to the increase of the laminar flame speed and to the decrease of the quenching distance compared to pure hydrocarbon flames [8,35,37].

The predictions made by the critical gradient concept model of von Elbe and the modified model of Hoferichter et al. [17] are close to each other; the modified model predicts flashback limits closer to the experimental results. The critical gradient concept correlations diverge from each other as the hydrogen addition to the fuel mixture increases since flame stretch becomes more important. Putnam's correlation predictions are the furthest away from the experimental results. One reason could be that Putnam's model constructed on the Lewis and von Elbe's concept, is only validated with ethylene/air and acetylene/oxygen mixtures. The Lewis and von Elbe's model is based on the experimental data from natural gas and hydrogen burning in air.

The experimental results lie in-between our numerical results for constant wall temperatures set at 600K and 300K. Comparison of numerical results for 300K and the critical

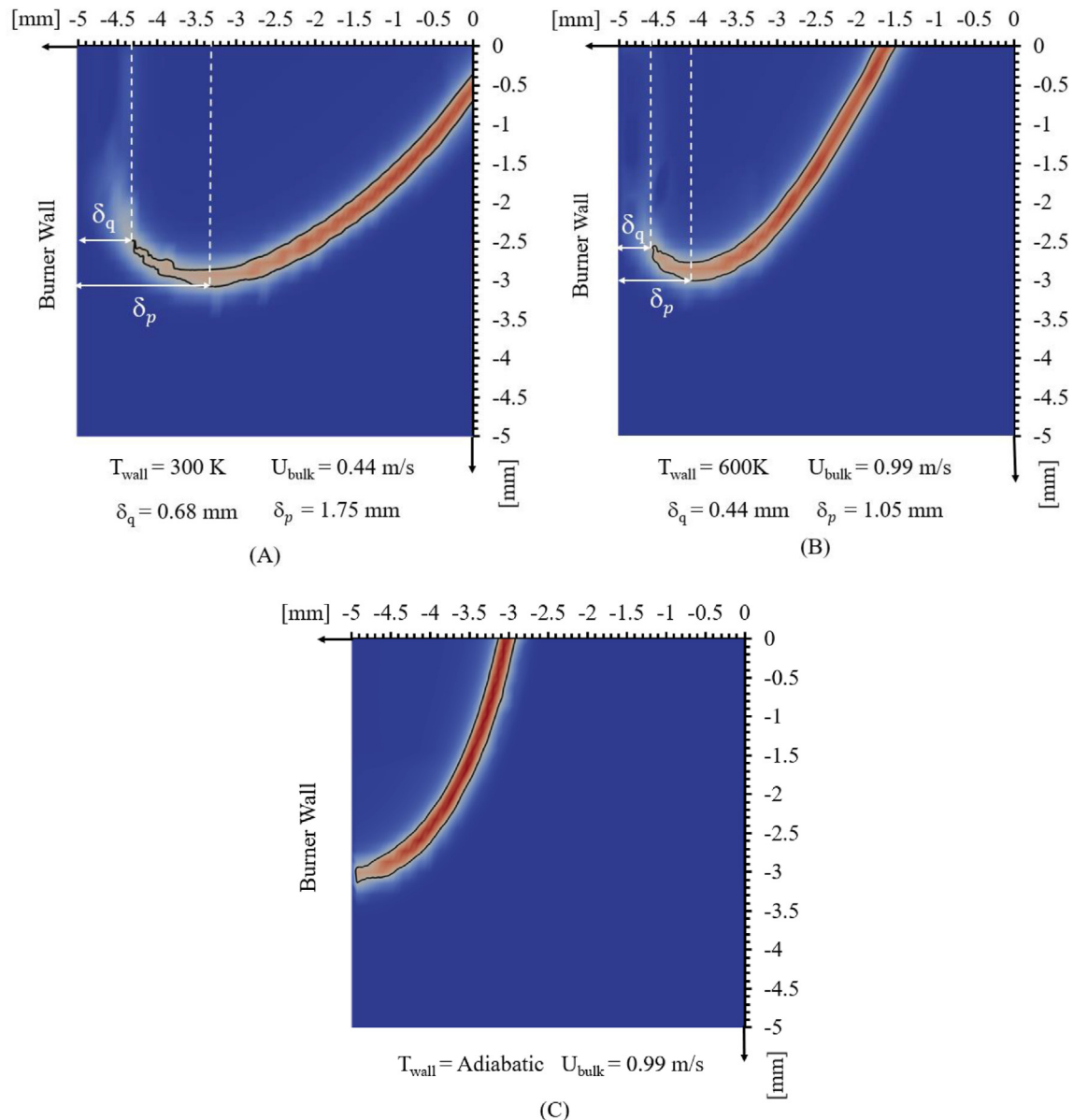


Fig. 9 – Normalized heat release rate contours for different wall temperature conditions for the $\text{CH}_4\text{-H}_2$ - air flame at $\Phi = 1.216$ with 20% H_2 addition.

Table 2 – Variation of the average quenching distance with H_2 addition for $T_{\text{wall}} = 600\text{K}$.

$\text{H}_2\%$ [mol]	δ_q [mm]
0	0.86
10	0.58
20	0.44

gradient concept correlations reveals that flashback limits are close to each other. The results of de Vries et al. [15] are higher than the model predictions for all hydrogen addition rates for 300K wall temperature. This may be related to the quartz burner used in the experiment of de Vries et al. [15]. Because of the low thermal conductivity of the quartz, the wall

temperature in the experiments may have locally increased at the rim. This decreases the quenching distance, thus increasing the difference between the actual quenching distance and the value used in the correlations.

Fig. 11b presents the same data normalized by the computed laminar flame speed S_L for each mixture condition. It should be noted that all correlations and the 300K wall temperature cases underestimate the normalized flashback velocity for a pure methane flame, while the 600K wall temperature computations overestimate it. The normalized critical flame flashback velocity is above 1 for the experimental results and increases with the addition of hydrogen. All correlations and computations for 300K wall temperature show the same trend, especially above 10% molar H_2 addition rate. 600K wall temperature computations also follow the same trend but with higher critical flame flashback velocities. This

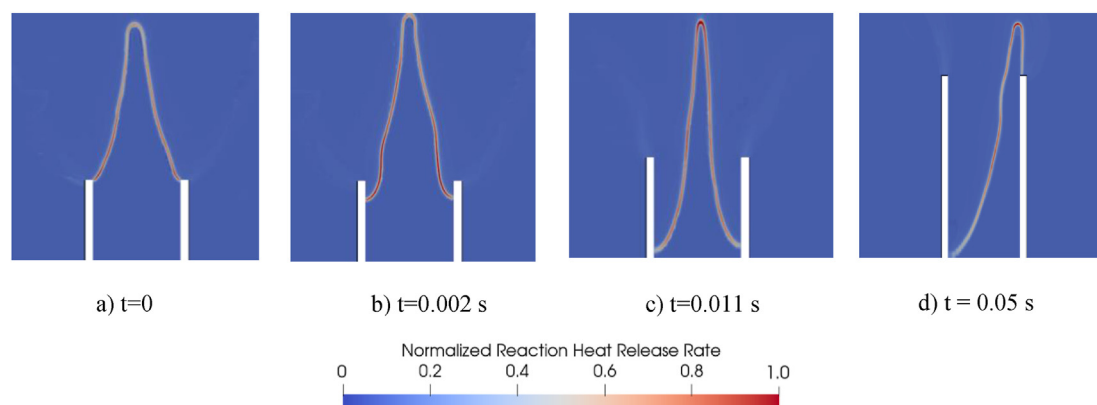


Fig. 10 – Flashback dynamics represented with the normalized heat release rate contours for methane-air flame at $\Phi = 1.216$ with 20% H_2 addition at adiabatic wall condition.

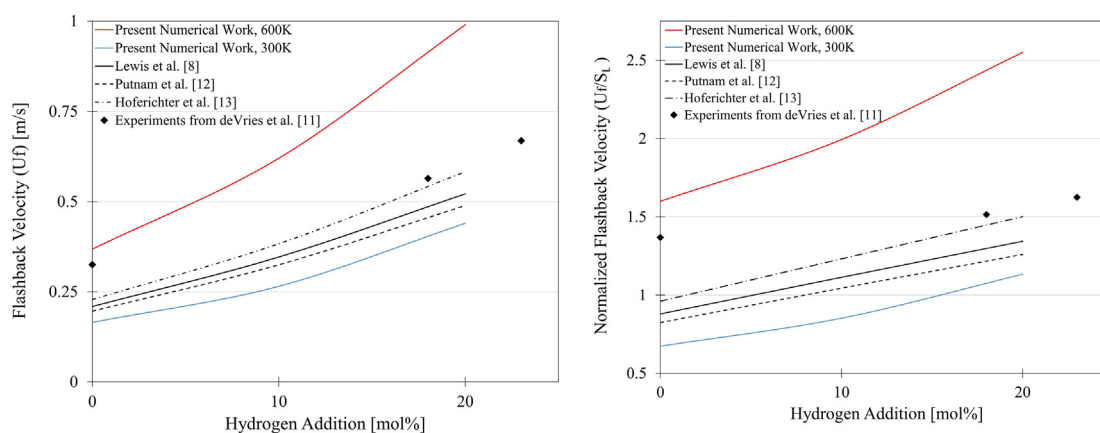


Fig. 11 – Comparison of experimental and calculated flashback limits.

observation seems to challenge the simple definition of the boundary layer flashback critical velocity as only related to the laminar flame propagation speed for hydrogen added methane flames and deserves to be further investigated.

Conclusions

This work investigated numerically the flame flashback limits and dynamics of hydrogen added laminar methane-air flames for the boundary layer flame flashback regime. The numerical simulations were performed using the 'reactingDNS' solver in OpenFOAM. The numerical work is compared to the experiments of de Vries et al. [15]. Computations are performed for CH_4 -air mixtures and different hydrogen addition rates. Flashback limits are determined and compared to the experimental data and the literature correlations based on the critical gradient concept.

The wall temperature effect is investigated by conducting computations for two constant wall temperatures of 300K and 600K. The flashback propensity is found to increase with increasing wall temperature and the hydrogen addition rate. The flashback limits are globally in accordance with the experiments and past correlations.

The differences between the critical flame flashback velocity results for two different isothermal wall temperatures shows the importance of the wall temperature in the flashback phenomenon. The discrepancy between the experimental flashback limits and the numerical ones can be attributed to the use of inaccurate wall temperature conditions. Assuming a uniform wall temperature may not represent the exact physics. Additionally, simplification of the geometry to 2D may induce additional errors in computations.

The main contribution of the complete simulation of the laminar flame flashback process in a simple burner configuration is the detailed information that can be obtained concerning the flashback dynamics without strong modelling hypotheses. Owing to the inherent capabilities of numerical simulations, the flashback conditions can be approached very gradually. As such, the flashback limits can be accurately determined. Here we claim a sensitivity of 5%, which can be largely improved by performing computations for more refined parameter variation ranges.

The numerical simulations of the boundary layer flashback phenomenon under laminar flame conditions will be continued in the future. This study has demonstrated the need of the correct knowledge of the burner wall temperature. Conjugate heat transfer approaches could help to solve this

problem. Inclusion of the Soret diffusion effect into numerical calculations would enhance the accuracy, especially for higher hydrogen content mixtures. The ultimate aim is to establish a detailed numerical data basis for various natural gas and hydrogen blends in order to establish practically important parameters such as the ratio between the flashback critical velocity and the laminar flame speed, the various characteristic time scales of flashback dynamics and their relationship to flow and flame characteristic times. In addition, the dynamic interactions between the burner wall temperature and flashback propensity should be clarified. The observed leading-edge oscillations will be further investigated to understand the dynamics of flashback initiation and propagation. Detailed and systematic experiments should also be performed to validate such a numerical data basis to help establish safe operating ranges for home appliances for various natural gas and hydrogen blending rates.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Acknowledgments

This work is supported by the International Fellowship for Outstanding Researchers Program of TÜBİTAK (Project No: 118C287 and Project No: 118C233). The numerical calculations were performed using TÜBİTAK ULAKBİM, High Performance and Grid Computing Center (TRUBA) resources.

Appendix A. Supplementary data

Supplementary data to this article can be found online at <https://doi.org/10.1016/j.ijhydene.2022.05.230>.

REFERENCES

- [1] Bouvet N, Chauveau C, Gökalp I, Halter F. Experimental studies of the fundamental flame speeds of syngas (H₂/CO)/air mixtures. *Proc Combust Inst* 2011;33:913–20. <https://doi.org/10.1016/j.proci.2010.05.088>.
- [2] Bouvet N, Chauveau C, Gökalp I, Lee S-Y, Santoro RJ. Characterization of syngas laminar flames using the Bunsen burner configuration. *Int J Hydrogen Energy* 2011;36:992–1005. <https://doi.org/10.1016/j.ijhydene.2010.08.147>.
- [3] Yılmaz B, Özdoğan S, Gökalp I. Influence of hydrogen addition on lean premixed methane-air flame statistics. *Proc. of the ASME 10th Biennial Conference on Engineering Systems Design and Analysis* 2010;4:281–7. <https://doi.org/10.1115/ESDA2010-25375>.
- [4] Cohé C, Halter F, Chauveau C, Gökalp I, Gülder ÖL. Fractal characterization of high pressure and hydrogen enriched CH₄-Air turbulent premixed flames. *Proc Combust Inst* 2007;31:1345–52. <https://doi.org/10.1016/j.proci.2006.07.181>.
- [5] Halter F, Chauveau C, Gökalp I. Characterization of the effects of hydrogen addition in premixed methane/air flames. *Int J Hydrogen Energy* 2007;32:2585–92. <https://doi.org/10.1016/j.ijhydene.2006.11.033>.
- [6] Halter F, Chauveau C, Djebaili-Chaumeix N, Gökalp I. Characterization of the effects of pressure and hydrogen concentration on laminar burning velocities of methane-hydrogen-air mixtures. *Proc Combust Inst* 2005;30:201–8. <https://doi.org/10.1016/j.proci.2004.08.195>.
- [7] Gökalp I. A holistic approach to promote the safe development of hydrogen as an energy vector. *Proceedings of the Ninth International Seminar on Fire and Explosion Hazards* 2019;2:21–6. <https://doi.org/10.18720/SPBPU/2/k19-127>. April 2019, Saint Petersburg, Russia.
- [8] Kalantari A, McDonell V. Boundary layer flashback of non-swirling premixed flames: mechanisms, fundamental research, and recent advances. *Prog Energy Combust Sci* 2017;61:249–92. <https://doi.org/10.1016/j.pecs.2017.03.001>.
- [9] Eichler C, Sattelmayer T. Premixed flame flashback in wall boundary layers studied by long-distance micro-PIV. *Exp Fluid* 2012;52:347–60. <https://doi.org/10.1007/s00348-011-1226>.
- [10] Kalantari A, Sullivan-Lewis E, McDonell V. Flashback propensity of turbulent hydrogen-air jet flames at gas turbine premixer conditions. *ASME. J. Eng. Gas Turbines Power* November 17, 2015;138(6):061506. <https://doi.org/10.1115/1.4031761>. June 2016.
- [11] Lewis B, von Elbe G. Stability and structure of burner flames. *J Chem Phys* 1943;11(2):75–97. <https://doi.org/10.1063/1.1723808>.
- [12] Duan Z, Shaffer B, McDonell V. Study of fuel composition, burner material, and tip temperature effects on flashback of enclosed jet flame. *J Eng Gas Turbines Power* 2013;135(12). <https://doi.org/10.1115/GT2013-94822>.
- [13] Kurdyumov V, Fernández-Tarrazo E, Truffaut J-M, Quinard J, Wangher A, Searby G. Experimental and numerical study of premixed flame flashback. *Proc Combust Inst* 2007;31(1):1275–82. <https://doi.org/10.1016/j.proci.2006.07.100>.
- [14] Duan Z, Shaffer B, McDonell V, Baumgartner G, Sattelmayer T. Influence of burner material, tip temperature, and geometrical flame configuration on flashback propensity of H₂-air jet flames. *J Eng Gas Turbines Power* 2014;136(2). <https://doi.org/10.1115/1.4025359>.
- [15] de Vries H, Mokhov AV, Levinsky HB. The impact of natural gas/hydrogen mixtures on the performance of end-use equipment: interchangeability analysis for domestic appliances. *Appl Energy* 2017;208:1007–19. <https://doi.org/10.1016/j.apenergy.2017.09.049>.
- [16] Putnam AA, Jensen RA. Application of dimensionless numbers to flash-back and other combustion phenomena. *Symposium on Combustion and Flame, and Explosion Phenomena* 1948;3(1):89–98. [https://doi.org/10.1016/s1062-2896\(49\)80011-0](https://doi.org/10.1016/s1062-2896(49)80011-0).
- [17] Hoferichter V, Hirsch C, Sattelmayer T. Prediction of boundary layer flashback limits of laminar premixed jet flames. In: *Turbo expo: power for land, sea, and air*, vol. 51050; 2018. <https://doi.org/10.1115/GT2018-75546>. V04AT04A037.
- [18] Lieuwen TC. *Unsteady combustor physics*. Cambridge University Press; 2012.
- [19] Jones DR, Al-Masry WA, Dunnill CW. Hydrogen-enriched natural gas as a domestic fuel: an analysis based on flashback and blow-off limits for domestic natural gas appliances within the UK. *Sustain Energy Fuels* 2018;2(4):710–23. <https://doi.org/10.1039/C7SE00598A>.
- [20] Bechtold JK, Matalon M. The dependence of the Markstein length on stoichiometry. *Combust Flame*

- 2001;127(1–2):1906–13. [https://doi.org/10.1016/S0010-2180\(01\)00297-8](https://doi.org/10.1016/S0010-2180(01)00297-8).
- [21] Boust B, Sotton J, Labuda SA, Bellenoue M. A thermal formulation for single-wall quenching of transient laminar flames. *Combust Flame* 2007;149(3):286–94. <https://doi.org/10.1016/j.combustflame.2006.12.019>.
- [22] Gruber A, Sankaran R, Hawkes ER, Chen JH. Turbulent flame–wall interaction: a direct numerical simulation study. *J Fluid Mech* 2010;658:5–32. <https://doi.org/10.1017/S0022112010001278>.
- [23] Zhang F, Bonart H, Zirwes T, Habisreuther P, Bockhorn H, Zarzalis N. Direct numerical simulation of chemically reacting flows with the public domain code OpenFOAM. *High Performance Computing in Science and Engineering* 2014;14:221–36. https://doi.org/10.1007/978-3-319-10810-0_16.
- [24] Zhong S, Zhang F, Peng Z, Bai F, Du Q. Roles of CO₂ and H₂O in premixed turbulent oxy-fuel combustion. *Fuel* 2018;234:1044–54. <https://doi.org/10.1016/j.fuel.2018.07.135>.
- [25] Holzmann Tobias. *Mathematics, numerics, derivations and OpenFOAM®*. 2019.
- [26] Smith Gregory P, Golden David M, Frenklach Michael, Moriarty Nigel W, Eiteneer Boris, Goldenberg Mikhail, Bowman C Thomas, Hanson Ronald K, Song Soonho, Gardiner Jr William C, Vitali V. Lissianski, and zhiwei qin. http://www.me.berkeley.edu/gri_mech/.
- [27] Contino F, Jeanmart H, Lucchini T, D'Errico G. Coupling of in situ adaptive tabulation and dynamic adaptive chemistry: an effective method for solving combustion in engine simulations. *Proc Combust Inst* 2011;33(2):3057–64. <https://doi.org/10.1016/j.proci.2010.08.002>.
- [28] Pope SB. Computationally efficient implementation of combustion chemistry using in situ adaptive tabulation. *Combust Theor Model* 1997;1(1):41–63. <https://doi.org/10.1080/713665229>.
- [29] Liang L, Stevens JG, Raman S, Farrell JT. The use of dynamic adaptive chemistry in combustion simulation of gasoline surrogate fuels. *Combust Flame* 2009;156(7):1493–502. <https://doi.org/10.1016/j.combustflame.2009.02.008>.
- [30] Kee RJ, Dixon-Lewis G, Warnatz J, Coltrin ME, Miller JA. *A Fortran computer code package for the evaluation of gas-phase multicomponent transport properties*, vol. 13. Sandia National Laboratories Report SAND86-8246; 1986. p. 80401–1887.
- [31] Ansys CHEMKIN 17.0 (15151), ANSYS Reaction Design: San Diego, vol. 20.
- [32] Gruber A, Chen JH, Valiev D, Law CK. Direct numerical simulation of premixed flame boundary layer flashback in turbulent channel flow. *J Fluid Mech* 2012;709:516–42. <https://doi.org/10.1017/jfm.2012.345>.
- [33] Kurdyumov VN, Fernández-Tarrazo E. Lewis number effect on the propagation of premixed laminar flames in narrow open ducts. *Combust Flame* 2002;128(4):382–94. [https://doi.org/10.1016/s0010-2180\(01\)00358-3](https://doi.org/10.1016/s0010-2180(01)00358-3).
- [34] Dam B, Choudhuri A. Flashback propensity of syngas fuels. ASME 2009 Power Conference; 2009. <https://doi.org/10.1115/power2009-81011>.
- [35] Vance FH, de Goey LPH, van Oijen JA. Development of a flashback correlation for burner-stabilized hydrogen-air premixed flames. *Combust Flame* 2022;2022:112045. <https://doi.org/10.1016/j.combustflame.2022.112045>.
- [36] Zirwes T, Häber T, Zhang F, Kosaka H, Dreizler A, Steinhausen M, Hasse C, Stagni A, Trimis D, Suntz R, Bockhorn H. Numerical study of quenching distances for side-wall quenching using detailed diffusion and chemistry. *Flow, Turbul Combust* 2021;106(2):649–79. <https://doi.org/10.1007/s10494-020-00215-0>.
- [37] Ebi D, Bombach R, Jansohn P. Swirl flame boundary layer flashback at elevated pressure: modes of propagation and effect of hydrogen addition. *Proc Combust Inst* 2021;38(4):6345–53. <https://doi.org/10.1016/j.proci.2020.06.305>.
- [38] Crabtree RH. Aspects of methane chemistry. *Chem Rev* 1995;95(4):987–1007. <https://doi.org/10.1021/cr00036a005>.