Flashback limits of H_2 premixed laminar flames: impact of Soret and multicomponent diffusion

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Abstract

This paper presents a detailed numerical investigation of the flashback limits of hydrogen premixed laminar flames, with a focus on the impact of the Soret effect and multicomponent diffusion. Employing the advanced "1+M" diffusion model, we compare its performance against the traditional mixture-averaged (MA) approach to explore the implications on safety and efficiency of combustion devices, particularly in micro-perforated burners.

Our study highlights the critical role of the Soret effect, which is shown to significantly influence flashback limits, especially under lean conditions. Without accounting for the Soret effect, both MA and "1+M" models underestimate the propensity to flashback, potentially compromising safety. The results demonstrate that, even if the "1+M" model provides more accurate predictions, the MA model's conservative estimates offer a less computationally demanding alternative that still ensures safety against flashback.

The findings emphasize the importance of incorporating accurate diffusion modeling in the design of hydrogen-fueled systems, as it is essential for predicting and mitigating flashback risks.

Introduction

Fossil fuels have been a primary energy source since the industrial revolution, significantly contributing to global greenhouse gas emissions and accelerating climate change. In sectors like residential heating, which heavily relies on natural gas (NG), there is a pressing need for sustainable alternatives. As of 2022, approximately 49% of U.S. households and a similar proportion in Europe use NG for heating, generating considerable CO_2 emissions annually [1]. Transitioning to zero carbon-ready boilers that use green hydrogen (H_2), produced from renewable sources, is seen as a promising solution to harmonize with the variability of renewable energy while mitigating environmental impacts.

However, hydrogen's unique properties, such as high reactivity, flammability limits, and flame speed (about six times that of NG) introduce new challenges in

combustion technology. These properties affect flame propagation and stability, particularly in premixed burner configurations designed for compact combustion chambers. The risk of flashback, where the flame moves upstream into the burner, poses significant safety concerns, and leads to reduced flexibility of practical combustion devices [2].
While traditional theories on flame stabilization provide some insights, they do not fully address the complexities of real-world applications where factors like flame-wall interactions and preferential diffusion play crucial roles. Recent studies [3-6] have emphasized that hydrogen's increased flame speed is not the only factor contributing to flashback. Instead, the interaction between the flame and the burner walls, facilitated by preferential diffusion, is also critical.
In this paper we numerically investigated the enhanced flashback propensity of hydrogen in simplified burner configurations. More specifically, the objective was to better characterize the impact of Soret effect and advanced multicomponent diffusion models (with emphasis on the "1+M" model [7]) on the flashback limits of H_2/air mixtures.

Numerical Methodology

In this study, we investigated the flashback limits in a multi-slit burner configuration, commonly used in domestic boilers. For simplicity, a planar geometry was adopted, in line with the one proposed by Vance et al. [4].
The slit width is W=1 mm, the distance between the slits is D=1 mm, and the plate thickness is t=0.6 mm. The computational domain extends 10 mm downstream and 3 mm upstream from the burner plate. The burner plate is modeled with properties typical of stainless steel used in domestic boilers. Premixed gases are introduced at a uniform velocity with a temperature of 300 K. The mesh comprises rectangular cells, refined near the burner plate and flame front to capture thermal gradients effectively, with ~40,000 cells in the largest configuration.
The flow within the burner is laminar, with Reynolds' numbers ranging from 100 to 1000 under various operating conditions. We employed the laminarSMOKE++ code, which solves conventional transport equations for momentum, species, and energy in laminar flows [8, 9]. The diffusion fluxes are modeled using the conventional mixture-average (MA) formulation or the more accurate "1+M" multicomponent diffusion model, recently proposed in [7]. Boundary conditions include a fixed pressure at the outlet (1 atm) and no-slip conditions on the burner surface. Symmetry conditions to mimic the entire burner setup are adopted along the sides. Radiative heat transfer and gravitational effects are neglected.
The solid region's energy equation is solved in steady-state conditions to decouple it from the gaseous phase dynamics, a method proven effective in similar studies [3-6]. Each simulation begins with a high inlet velocity for stability, then systematically lowers the velocity to determine the minimal specific power that sustains a steady flame without flashback.

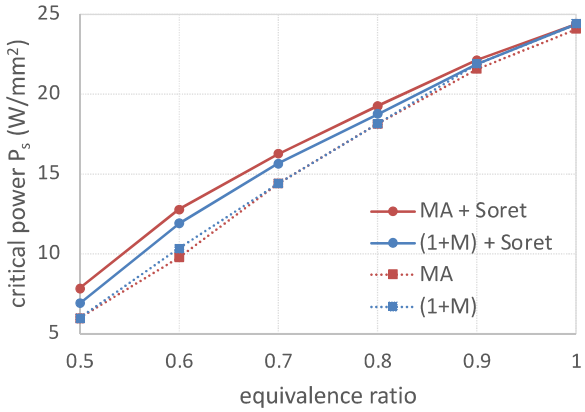

Figure 1. Critical specific power (P_s) at flashback conditions as a function of the equivalence ratio $\boldsymbol{\phi}$.

Results and Discussion

Figure 1 shows the flashback curves, i.e. the critical specific powers (P_S) at critical conditions as a function of the equivalence ratio ϕ, for different diffusion models. As expected, the critical power increases with the equivalence ratio, because of the increased reactivity of the mixture, which enhances the propensity to flashback. If the Soret effect is not included in the calculations, the mixture-averaged (MA) and the 1+M formulations do not show any significant differences. The inclusion of Soret effect increases the critical power, especially at lower equivalence ratios (i.e. lean conditions). Thus, not including the Soret effect in the numerical simulations leads to an underestimation of the flashback propensity and this could be potentially dangerous in applications. No significant differences can be observed between the MA and 1+M formulations at large equivalence ratios. At lean conditions, the two formulations show some deviations: more specifically, the MA formulation tends to slightly overestimate the flashback propensity. In general, the results show that the MA formulation can reproduce quite well the results of the more accurate (but also more expensive) 1+M formulation. Since the MA formulation tends to slightly overestimate the critical power, its adoption for quantifying the flashback propensity can be considered a good alternative to more complex and expensive multicomponent diffusion models (such as 1+M).

The different enhanced flashback propensity due to the Soret effect can be explained and discussed by looking at some specific fields (see Figure 2): temperature, scaled H_2 consumption rate $\hat{\Omega}_{H_2} = \frac{\Omega_{H_2}}{\Omega_{H_2,1D}^{max}}$, scaled H elemental mass fraction $\hat{Z}_H = \frac{Z_H - Z_{H,in}}{Z_{H,in}}$, and scaled enthalpy $\hat{h} = \frac{h - h_{in}}{C_{P,u}(T_b^0 - T_u)}$. In the definitions above, the H_2 consumption rate is scaled with the maximum consumption rate of a 1D adiabatic, flat premixed flame $\Omega_{H_2,1D}^{max}$. The H elemental mass fraction is scaled with the corresponding inlet value $Z_{H,in}$. h_{in} is the inlet specific enthalpy, $C_{P,u}$ and T_u are the specific heat coefficient and temperature at inlet conditions, and T_b^0 the adiabatic flame temperature. $\hat{Z}_H$ can be used to quantify local stratification in composition due to

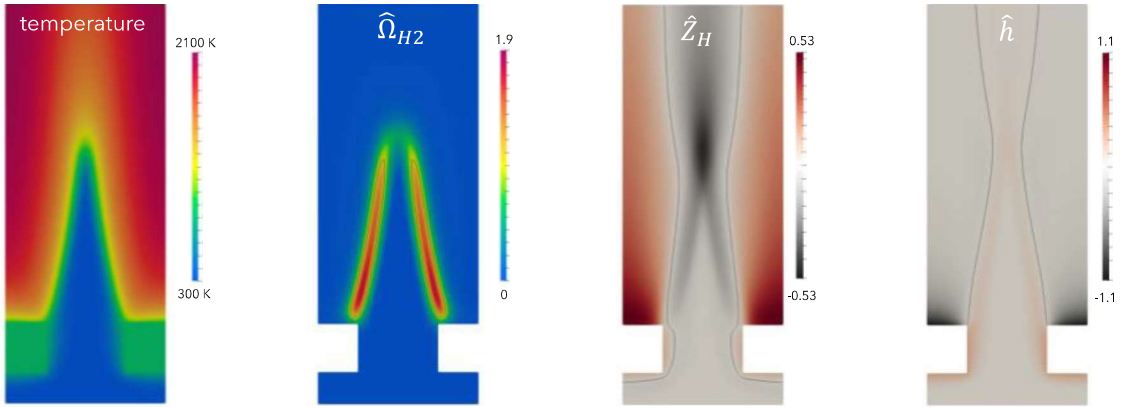

Figure 2. Temperature, scaled H_2 consumption rate $\widehat{\boldsymbol{\Omega}}_{\boldsymbol{H_2}}$, scaled H elemental mass fraction $\widehat{\boldsymbol{Z}}_{\boldsymbol{H}}$, and scaled enthalpy $\widehat{\boldsymbol{h}}$ for $\boldsymbol{\phi = 0.70}$ and P=21 W/mm^2.

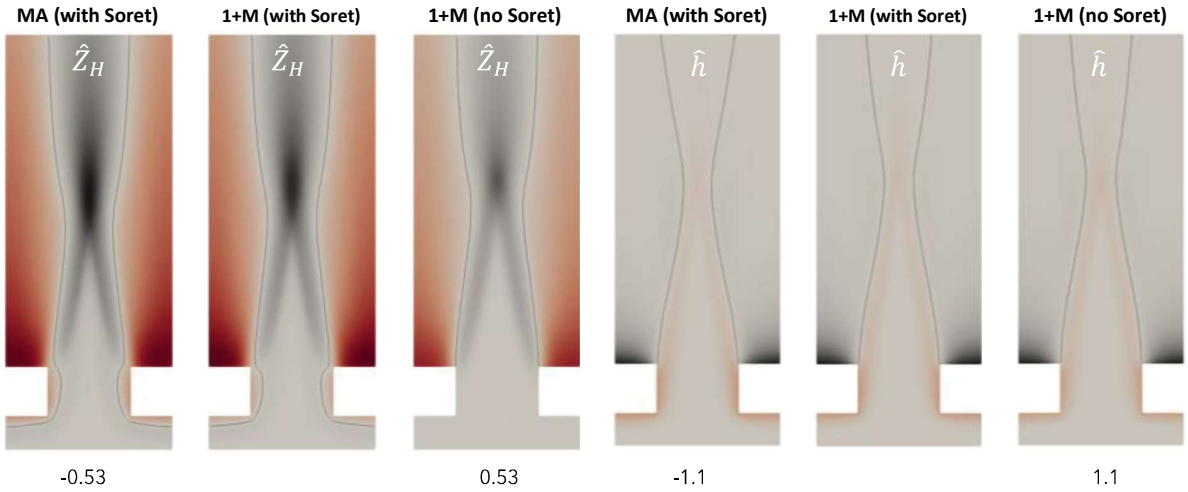

Figure 3. Scaled H elemental mass fraction $\widehat{\boldsymbol{Z}}_{\boldsymbol{H}}$ and scaled enthalpy $\widehat{\boldsymbol{h}}$ for $\boldsymbol{\phi = 0.70}$ and P=21 W/mm^2 when different diffusion models are adopted.

preferential diffusion effects. $\hat{h}$ allows to identify the effects of heat exchange with the burner plate: positive values mean local preheating, while negative values heat loss. From Figure 2, it is clear that the flame burns stronger close to the base and weaker at the tip. This is strictly related to preferential diffusion and stratification of the mixture, which becomes richer close to the burner walls and leaner at the tip. Moreover, there is a significant heat loss along the top wall of the burner. Since the overall system is adiabatic, the heat loss is returned to the gas phase along the lateral and bottom walls, where the inlet mixture is preheated.

Figure 3 shows a comparison between the simulations carried out with the MA and 1+M models (including the Soret effect) and the simulation carried out with the 1+M model without the Soret effect. No significant differences can be observed in terms of scaled enthalpy $\hat{h}$. However, without the Soret effect, no stratification of the inlet mixture can be observed along the bottom and the side walls of the burner, which is on the contrary clearly apparent in MA and 1+M formulations. Indeed, thanks to preheating, Soret diffusion pushes light species (mainly H_2 and H) close to the burner

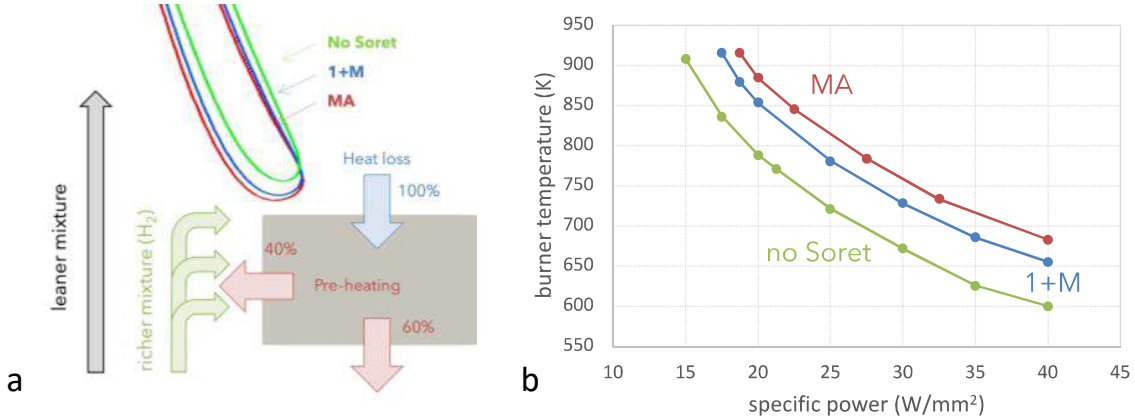

Figure 4. a) Impact of Soret effect and heat loss on flame stabilization ($\boldsymbol{\phi = 0.70}$ and P=21 W/mm^2). The colored curves are the iso-contours of scaled H_2 consumption rate at $\boldsymbol{\hat{\Omega}_{H_2} = 1}$ (adapted from Vance et al. [3]). b) Average burner temperature for $\boldsymbol{\phi = 0.70}$ with different diffusion models.

walls, so the mixture approaching the flame base becomes locally richer. Since the MA and 1+M models including the Soret effect result in richer mixtures, this explains their higher reactivity and thus their higher propensity to flashback.

Figure 4a reports the iso-contours of $\hat{\Omega}_{H_2}$, considered as a measure of the reactivity of the flame. As expected, without Soret effect, the flame burns weaker (being leaner) and the distance between the reactive region and the top wall is larger. When we include the Soret effect (both MA and 1+M formulations), we have the opposite: the flame burns closer to the top wall. The heat loss through the top wall (not here reported) is now larger, thus producing a larger preheating along the side and bottom walls. Higher preheating means stronger Soret diffusion and therefore higher local enrichment of the flame, which then makes the flame stronger. Thus, this is a self-sustained mechanism [3], which is also confirmed by the larger average temperatures reached by the burner, reported in Figure 4b.

Conclusions

This study provides a numerical investigation of flashback propensity of hydrogen premixed laminar flames, elucidating the influence of the Soret effect and advanced multicomponent diffusion models. By comparing the 1+M diffusion model with the conventional mixture-averaged (MA) model, our analysis reveals that neglecting the Soret effect leads to an underestimation of flashback propensity, particularly under lean conditions, which could pose significant risks in real-world applications. The simulations show that while the MA and 1+M models perform similarly under rich conditions, discrepancies emerge at leaner mixtures. The 1+M model provides a more accurate prediction of flashback limits, but the MA model's tendency to slightly overestimate the critical power offers a conservative and less computationally expensive alternative for assessing flashback risks.

The simulations also highlight the importance of considering local composition stratifications and heat transfer effects in predicting flashback behavior. The

inclusion of the Soret effect enriches the hydrogen content near burner walls, increasing local reactivity and thus the propensity for flashback. This indicates a critical feedback mechanism where heat loss at burner walls enhances local preheating and, subsequently, the strength of the flame due to stronger Soret diffusion.

In practical terms, these findings stress the need for incorporating advanced diffusion models and the Soret effect into the design criteria of hydrogen combustion systems to enhance safety and efficiency. For future research, expanding the scope to include varied burner geometries and operating conditions would further refine our understanding of hydrogen's behavior in combustion settings.

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