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The effect of thermal diffusion on stabilization of premixed flames

Faizan Habib Vance*, Philip de Goey, Jeroen A. van Oijen

Mechanical Engineering, Eindhoven University of Technology, Eindhoven, the Netherlands

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ABSTRACT

Soret or thermal diffusion is known to impact combustion mixtures by diffusion of species along a temperature gradient. In this numerical modelling study we show that Soret diffusion can cause considerable local changes in the stabilization of H_2 enriched premixed flames. First we validate two reduced Soret diffusion models with a more complete multi-component model. One model is able to capture the effect of Soret diffusion in the flame zone while the other model captures the effect in the flame zone as well as in the regions where high temperature gradients might exist e.g., near hot burner, side walls. Using the two reduced models along with conjugate heat transfer, we analyze bluff-body stabilized flames and the effect of Soret diffusion in the flame zone and near hot walls. For such flames, heat transfer between the flame and the burner results in local quenching. This heat is recirculated through the burner towards the unburnt gases creating a temperature gradient in the boundary layer around the burner. Because of Soret diffusion, this gradient drives H_2 and even CH_4 towards the burner walls in the unburnt mixture thus creating a local stratification (in the mixture approaching the flame base). As a result of this stratification, the burning rate of the flame near the anchoring location is enhanced, which causes more heat to be lost to the burner. The flame stabilizes at a new location where the strain rate is higher in order to neutralize the enhancement in burning rate and a new balance between flame and flow velocity is found. The effect of this local stratification is shown to be profound only when there is considerable heat loss to the burner such as for flames near flashback.

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1. Introduction

Thermal diffusion plays an important role in H_2 enriched flames. While Fickian diffusion due to a concentration gradient is understood to be the main cause of species diffusion, the effect of Soret or thermal diffusion in such flames cannot be neglected [1]. Soret diffusion caused by thermal gradients results in light species diffusing towards the hotter regions and vice versa for heavier species. These changes in species concentration can have a significant effect on the dynamics of premixed flames. Bongers and de Goey [2] showed that including Soret diffusion in the numerical model resulted in lower adiabatic burning velocities for CH_4 -air and H_2 -air flames. This was also observed by Liang and co-workers [3] in the context of syngas-air flames. They also found that for stretched syngas-air stoichiometric flames, Soret diffusion reduces propagation speed for spherically propagating flames. Ern and Giovangigli [4] simulated Bunsen flames with lean H_2 -air mixtures and showed that the flame angle at the tip was reduced when Soret diffusion was included in the transport model. This

reduction in the local burning velocity was attributed to the reduction in diffusivity of active radicals into the cold region. Further research by the same authors showed that for lean H_2 -air mixtures in a counter-flow configuration, inclusion of thermal diffusion resulted in a significant increase in the flame temperature [5].

The (individual) role of Soret diffusion caused by H_2 and H molecules was investigated in Ref. [6] for freely propagating and counterflow premixed flames. It was concluded that the effect of Soret diffusion caused by H_2 was more pronounced than that of the H radical. The increase in extinction stretch rates were caused primarily by the Soret diffusion of H_2 resulting from the modification of the enthalpy under stretch rates and non-equidiffusion. Zhen et al. [7] advanced the understanding of the role of Soret diffusion of H_2 and H molecules at different pressures and temperatures in 1D and 2D lean H_2 -air flames. They found out that with increasing stretch rate, Soret diffusion of H_2 and H have a competing effect resulting in an initial reduction and then an enhancement in the mass burning rate. This effect increased with an increase in the pressure and decreased with an increase in the unburnt temperature. It was also shown that flame cells with higher curvature were formed when Soret diffusion was included in the model. Effect of Soret diffusion in ignition of H_2 -air flames was recently investigated in Ref. [8]. It was found that Soret

* Corresponding author.

E-mail address: f.h.vance@tue.nl (F.H. Vance).

diffusion can change local stoichiometry and strongly influence ignition behaviour by thermal diffusion of H_2 molecule. Grcar et al. [9] carried out 2D simulations of freely propagating flames with multi-component and mixture-averaged transport models including thermal diffusion. A large discrepancy in the predicted fuel consumption rate prediction existed between the two models. The maximum temperature and $\frac{\nabla T}{T}$ were higher when the multi-component model was used. Based on these observations, they recommended on the importance of the inclusion of the multi-component model in numerical simulations. Although the multi-component transport model is understood to be the most accurate one, its practicality is reduced by the large computational effort it requires. Recently, a reduced thermal/Soret diffusion model has been developed by Schlup and Blanquart [10]. This model is computationally cheaper and was shown to be in good agreement with the results from the multi-component model. In this study we use this reduced model in order to investigate the effect of Soret diffusion on burner-stabilized flames.

While most of the previous studies have focused on the impact of Soret diffusion in the flame zone, its impact on a flame stabilized on a heat conducting burner has not been investigated to the best of our knowledge. The goal of this study is to determine the role Soret diffusion plays on the stabilization of H_2 enriched CH_4 -air premixed flames in the presence of a heat conducting solid body. Previous studies on flame stabilization include numerical investigations (without Soret diffusion) by Kedia and Ghoniem [11,12] that highlighted the importance of inclusion of Conjugate Heat Transfer (CHT) in the simulations by demonstrating its impact on flame stabilization. Michaels and Ghoniem [13] then studied numerically the impact of hydrogen addition into methane flames stabilized on a bluff body with Soret diffusion but did not highlight the effect of Soret diffusion on flame stabilization. They showed that for the same equivalence ratio, flames with more hydrogen in the fuel stabilize at an upstream location where the strain rates are higher. They related this movement of the flame leading edge to the higher extinction stretch rates for increasing H_2 in the fuel. Experimental studies on premixed turbulent bluff body flames with CH_4 -air and CH_4 - H_2 -air blends have been conducted [14–16] showing that the local atomic balance is not conserved because of molecular preferential diffusion even in the case of turbulent flames.

In this study, in order to advance the understanding of flame stabilization, we analyze the effect of Soret diffusion on burner-stabilized premixed flames in the presence of a heat conducting solid. The organization of this study is as follows. First, the reduced Soret diffusion model and a Lewis number based model are validated against a multicomponent model for 1D flat stretched flames, with Soret diffusion. Then, the two reduced models are used for analyzing flat, one-dimensional burner-stabilized flames. A comparison is then made between the profile of local species with and without inclusion of Soret diffusion. Next, two-dimensional bluff body stabilized flames simulated using the two reduced models are compared with results of a model excluding Soret diffusion. The impact of Soret diffusion on flame stabilization is then demonstrated by reducing the inlet velocity until the flame flashes back. Finally, the local mass burning rate and individual contributions to the burning rate are evaluated giving a quantitative understanding of the impact of Soret diffusion on flame stabilization.

2. Governing equations

In this study, a mixture of 40% H_2 and 60% CH_4 by volume is selected for the analysis. This mixture is interesting as it represents a blend of a light and a heavy fuel species, and thus the conclusions made in this study can be applied more generally to a wider class

of fuels. Secondly, this mixture composition could be used as a fuel in a transition towards fossil fuel independent gas grid Hydrogen economy. Chemistry for this CH_4 - H_2 -air mixture is modelled using the DRM19 mechanism [17] which contains 21 species and 84 reactions. The following equations for continuity, species conservation, momentum and energy are solved for a steady, laminar, reactive flow,

$$\nabla \cdot (\rho \mathbf{v}) = 0, \quad (1a)$$

$$\nabla \cdot (\rho \mathbf{v} Y_i) + \nabla \cdot \mathbf{J}_i = \omega_i, \quad (1b)$$

$$\nabla \cdot (\rho \mathbf{v} \mathbf{v}) = -\nabla p + \nabla \cdot \bar{\bar{\tau}}, \quad (1c)$$

$$\nabla \cdot ((\rho E + p) \mathbf{v}) = \nabla \cdot (\lambda \nabla T) - \nabla \cdot (\sum_i h_i \mathbf{J}_i) + \omega_T. \quad (1d)$$

Here $\mathbf{v}$ is the velocity vector, ρ is the density, Y_i are the species mass fractions, ω_i are the species source terms, p is the pressure, T is the temperature, and h_i are the species sensible enthalpy. The stress tensor $\bar{\bar{\tau}}$, total energy E , enthalpy h , species enthalpy h_i and thermal heat release rate ω_T are given by

$$\bar{\bar{\tau}} = \mu \left[(\nabla \mathbf{v} + \nabla \mathbf{v}^T) - \frac{2}{3} \nabla \cdot \mathbf{v} \mathbf{I} \right], \quad (2a)$$

$$E = h - \frac{p}{\rho} + \frac{\mathbf{v} \cdot \mathbf{v}}{2}, \quad (2b)$$

$$h = \sum_i Y_i h_i, \quad (2c)$$

$$h_i = \int_{T_{ref}}^T c_{p,i} dT, \quad (2d)$$

$$\omega_T = \sum_i \frac{h_i^0}{M_i} \omega_i. \quad (2e)$$

Here h_i^0 and M_i is the formation enthalpy and molecular weight of species i . The heat conduction equation is solved inside the solid bluff body using

$$\nabla \cdot (k \nabla T) = 0. \quad (3)$$

Here k is the thermal conductivity of the solid body. The diffusion flux $\mathbf{J}_i$ is given by

$$\mathbf{J}_i = \mathbf{J}_i^F + \mathbf{J}_i^T. \quad (4)$$

Here $\mathbf{J}_i^F = -\rho D_{i,m} \nabla Y_i$ is the Fickian diffusion flux due to species gradients with $D_{i,m}$ the mixture averaged Fickian diffusion coefficients for species i . $\mathbf{J}_i^T = -\rho D_i^T \frac{\nabla T}{T}$ is the Soret or thermal diffusive flux due to temperature gradients with D_i^T being the thermal diffusion coefficient for species i . Mixture properties based on constant Lewis number are used in this study. It has been shown in Ref. [18,19] that the assumption of constant Lewis number based transport properties produces accurate results when compared to that of mixture-averaged properties. The transport properties are calculated based on the following relations [20–22]:

$$\lambda = 2.58 \times 10^{-5} c_p \left(\frac{T}{298} \right)^{0.69} [\text{W m}^{-1} \text{K}^{-1}], \quad (5a)$$

$$\mu = 1.67 \times 10^{-8} c_p \left(\frac{T}{298} \right)^{0.51} [\text{kg m}^{-1} \text{s}^{-1}]. \quad (5b)$$

Here μ , λ and c_p are the mixture viscosity, conductivity and the specific heat capacity $c_p = \sum_i Y_i c_{p,i}$, respectively. Constant Lewis numbers are calculated by simulating one-dimensional flat flames using the multi-component model library EGLIB developed by Ern

Fig. 1. Comparison of S_L with varying fuel equivalence ratio ϕ without Soret diffusion calculated using multi-component and constant Lewis numbers + Eq. (5) transport model at $p = 1$ atm and $T_u = 300$ K.

and Giovangigli [23] using CHEM1D [24]. The constant Lewis numbers are calculated by spatially averaging the local values weighted with the diffusion flux. Two sets of Lewis numbers are calculated based on the inclusion of Soret diffusion in the model. Without Soret diffusion, the Lewis numbers are estimated based on the local Fickian diffusion flux, $\mathbf{J}_i^F$, using the multi-component model by,

$$Le_i = -\frac{\frac{dY_i}{dx}}{|\mathbf{J}_i^F|} \frac{\lambda}{c_p}. \quad (6)$$

A validation of this constant Lewis number model for a fuel mixture with 60% CH_4 and 40% H_2 by volume is presented in Fig. 1. The burning velocity S_L computed using the constant Lewis number approach with calculation of μ and λ from Eq. (5) is plotted against the multicomponent diffusion model for flat unstretched and adiabatic flames with varying ϕ . It can be observed that the prediction of S_L using the reduced model with $Le = \text{constant}$ and Eq. (5) is in excellent agreement with the detailed and (more) expensive multi-component model (and can be subsequently used for detailed calculations in 2D).

Another method to compute the Lewis numbers is to include Soret diffusion in the Fickian model. The Lewis numbers are then calculated based on the total diffusion flux based on the assumption that ∇T and ∇Y_i are correlated in the same manner as in 1D flames,

$$Le_i^* = -\frac{\frac{dY_i}{dx}}{|\mathbf{J}_i^F| + |\mathbf{J}_i^T|} \frac{\lambda}{c_p}. \quad (7)$$

Using this set of fitted Lewis numbers, thermal diffusion can be partially included in the numerical model at no extra cost to the existing constant Lewis number approach, in contrast to the expensive multi-component model. Partial inclusion means that Soret diffusion is modelled only when the temperature and the species gradients are aligned. When this is not the cases, this model will not be able to capture Soret diffusion, for instance, near hot walls. This approach will be validated in the next section and is referred as S(Le) model from here on.

Another approach for inclusion of thermal diffusion at affordable cost has been recently presented in Ref. [10]. In that study, thermal diffusion of H_2 and H was included using the following

relation:

$$D_i^T = -\alpha_i \frac{15}{4} \frac{X_i \mu_i}{\rho \Phi_{i,m}} (1.2 C_{i,m}^* - 1) (1 - Y_i) - Y_i S \text{ [m}^2 \text{ s}^{-1}]. \quad (8)$$

Here X_i and μ_i are the mole fraction and viscosity of species i respectively. S is a scalar enforcing mass conservation for thermal diffusion fluxes. More details and exact expressions for $\Phi_{i,m}$ and $C_{i,m}^*$ can be found in Ref. [10]. The values of α_i are chosen to correct for systematic errors in the derivation of Eq. (8) [10] and is discussed in the next section. The validation of this reduced model is presented in the next section and this model will be referred to as S(RM) in the rest of this study.

To summarize, we will compare the following three transport models in this study:

1. **S(RM)**: The reduced thermal diffusion model with constant Lewis number based mixture properties. Soret diffusion is modelled using Eqs. (6), (8) and (5). This is the most detailed model used in the 2D simulations.
2. **S(Le)**: Constant Lewis number based diffusion properties with Soret diffusion partially included (only when ∇T and ∇Y_i are aligned and correlated as in a 1D flame) using Eqs. (5) and (7). This model is only accurate in the flame zone.
3. **NS**: Constant Lewis number based mixture properties with no Soret diffusion using Eqs. (5) and (6).

Mass conservation is enforced in the numerical models by using Nitrogen as a bath gas for the constant Lewis number models. For the S(RM) model, an additional condition is enforced that the sum of the thermal diffusive fluxes is zero. The S(Le) model is included in this study for separating the thermal diffusion effect in the flame zone from possible thermal diffusion in the unburnt zone near hot walls. Using this model, we can easily distinguish the role of each of these effects on flame stabilization by comparing with results from the S(RM) model. In the next section, these models will be validated against the full multi-component model [23], from here on referred to as MC, for 1D strained and 1D flat burner stabilized flames.

3. Thermal diffusion in 1D flames for model validation

In this section, the effect of thermal diffusion in 1D stretched and burner stabilized-flames will be discussed along with the validation of S(Le) and S(RM) modelling approaches and their effect on the burning rate of the flame. In order to calculate the local burning rate, we define the flame front as an iso-level of the fuel-based reaction progress variable Y at the inner layer of the flame zone. Y is a normalized reaction progress variable given as $Y = \frac{Y_f - Y_{f,u}}{Y_{f,b} - Y_{f,u}}$ with $Y_f = Y_{\text{CH}_4} + Y_{\text{H}_2}$ and subscripts u and b denote unburnt and burnt sides of the flame. The density-weighted displacement speed or mass burning rate is defined as $m = -\rho(\mathbf{v} \cdot \mathbf{n}) = \rho S_D$, where ρ is the density, $\mathbf{v}$ is the local velocity and $\mathbf{n}$ is the flame normal defined as $\mathbf{n} = \frac{\nabla Y}{|\nabla Y|}$. S_D is the flame displacement speed. This definition results from the local kinematic balance in steady flames at the flame front [25]. We will use the flame stretch theory of de Goey and Ten Thije Boonkamp [26] for validating individual contributions of direct stretch and changes in the enthalpy and elemental mass fractions from the reduced models (S(Le) and S(RM)) with the multi-component model MC. Using integral analysis, it was shown that the mass burning rate at the burnt side of the flame front m_b of stretched flames is related to that of the 1D flat unstretched, adiabatic flame m_b^0 by [19]:

$$m_b = m_b^0(\psi_b)(1 - Ka). \quad (9)$$

Here, $\psi_b = (Z_{1,b}, \dots, Z_{N_{e,b}-1,b}, h_b)$ which represents the state at the burnt sides of the flame in terms of element mass fractions Z_j for

Table 1
Sensitivity coefficients for $\phi = 0.52$.

$c_h[\text{gJ}^{-1}]$	c_c	c_H	c_O
5.5	177	788.4	-2.1

$j = 1, \dots, N_e - 1$ elements in the mixture, and the enthalpy h . N_e is number of elements in the mixture. The Karlovitz integral Ka is the non-dimensional stretch rate and given by:

$$Ka = \frac{1}{(\sigma m^0)_b} \int_{s_u}^{s_b} \sigma Y K \rho ds. \quad (10)$$

The mass based stretch rate, K is defined as $K = \frac{1}{M} \frac{DM}{Dt}$, where M is the mass contained inside a control volume in a flame of finite thickness and $\frac{D}{Dt}$ being the substantial derivative [19]. Ka is an integral from the unburnt to the burnt side of the flame along the flame coordinate s . Following [26] we use fuel mass fraction as the progress variable. κ is the curvature of the flame, related to the surface of a small flame segment σ by $\kappa = \nabla \cdot \mathbf{n} = \frac{1}{\sigma} \frac{\partial \sigma}{\partial s}$. These relations hold for weak as well as strong stretch rates [26]. Further, linearisation of Eq. (9) around the adiabatic undistorted state $\psi_b^0 = (Z_{j,b}^0, h_b^0)$ gives for the weak stretch limit [19,26]:

$$\frac{m_b}{m_b^0} = 1 - Ka + \Delta h_b \frac{\partial}{\partial h_b^0} (\ln m_b^0) + \sum_{j=1}^{N_e-1} \Delta Z_{j,b} \frac{\partial}{\partial Z_{j,b}^0} (\ln m_b^0) + h.o.t. \quad (11)$$

The first two terms in Eq. (11) describe the direct stretch effect on the mass burning rate. The third term describes the effect of the change in enthalpy resulting from heat loss and Lewis number effects, while the fourth term describes the effect of preferential diffusion through changes in element mass fractions. Thus, Eq. (11) gives an explicit relation combining the effects of stretch rate, heat loss and preferential diffusion on the mass burning rate of the flame. Eq. (11) can be further written as:

$$\frac{m_b}{m_b^0} = 1 - Ka + \sum_j c_j \cdot \Delta \psi_j + h.o.t. \quad (12)$$

The sensitivity coefficients $c_j = \frac{\partial \ln m_b^0}{\partial \psi_j}$, with $\psi = (Z_1, \dots, Z_{N_e-1}, h)$, are computed by varying the inlet composition and temperature of unstretched adiabatic one-dimensional flames following [19]. The sensitivity coefficients are presented in Table 1 for the selected mixture at $\phi = 0.52$. The sensitivity coefficient of oxygen, c_O has a small value as compared to the hydrogen and carbon sensitivity coefficients. This results from the fuel lean conditions implying that changes in H and C, which make up the fuel composition, have a higher impact on the flame burning rate m . Further details of the methodology can be found in Refs. [19,27].

As the effect of thermal diffusion on premixed flames results in changes in elemental composition and enthalpy, the flame stretch theory can also be used for comparing different contributions in Eq. (12) of the two thermal diffusion models presented in the previous section with the contributions of the multicomponent model. This validation is presented in the next section.

3.1. 1D strained flames

As it is expected that the bluff body stabilized flames are affected heavily by stretch, especially at the flame base region [11,13], we first look at the effect of inclusion of thermal diffusion on 1D flat ($\sigma = 1$) stretched flames using the multi-component model. One-dimensional premixed flames at $\phi = 0.52$ are simulated using CHEM1D and the resulting m_b is scaled with m_b^0 of a flame calculated without Soret diffusion. This scaled m_b is plotted as a function of the Karlovitz integral Ka in Fig. 2. It can be observed that at

Fig. 2. Variation of m_b/m_b^0 with Karlovitz integral Ka for 1D flames at $\phi = 0.52$ with and without Soret diffusion using the multi-component transport model.

Table 2
Lewis numbers without and with Soret diffusion at $\phi = 0.52$.

Species	Le	Le*
H ₂	0.292	0.239
H	0.175	0.165
O	0.697	0.703
O ₂	1.076	1.132
OH	0.712	0.719
H ₂ O	0.848	0.903
HO ₂	1.087	1.079
CH ₂	0.954	0.958
CH ₂ *	0.954	0.958
CH ₃	0.978	0.981
CH ₄	0.987	0.925
CO	1.093	1.091
CO ₂	1.358	1.289
HCO	1.256	1.253
CH ₂ O	1.284	1.282
CH ₃ O	1.313	1.316
C ₂ H ₄	1.314	1.310
C ₂ H ₅	1.426	1.424
C ₂ H ₆	1.444	1.440

zero stretch, i.e., a flat unstretched flame, Soret diffusion decreases the mass burning rate as pointed out in Refs. [2,3]. With increasing stretch rate, it can be seen that m_b/m_b^0 increases for both models, with and without Soret diffusion. The qualitative response is similar for both models but quantitatively the flames burn stronger in the presence of Soret diffusion as is also found in [6] in terms of an increase in flame temperature when Soret diffusion was included for lean H₂-air flames. This results from an enhancement of local stoichiometry under the influence of positive stretch. The maximum increase in m_b/m_b^0 is about 9% at $Ka = 0.3$ when Soret diffusion is not included and almost 18% when it is included in the model as compared to the reference flat flame burning rate.

Next, the Lewis number fitted model S(Le) and the reduced model S(RM) with Soret diffusion are compared with the multi-component model for the 1D strained flames. The constant Lewis numbers for the S(Le) and S(RM) models are shown in Table 2, generated using the multi-component model. It should be noted that the species with major changes in Lewis number when Soret diffusion is included are H₂, H₂O and CH₄. Based on this, the reduced model S(RM) is enabled only for those species whose molecular weight is less than 19 mol g⁻¹ as it includes the dominant species affected by Soret diffusion under the influence of flame

Fig. 3. Numerical mass burning rate and different contributions from Eq. (12) to the mass burning rate versus Ka at $\phi = 0.52$ with three different models. Results for MC, S(RM) and S(Le) are shown with respective text colours.

stretch. The value of α_i in Eq. (8) is kept the same for all species for simplicity and it is found that a value of $\alpha_i = 0.65$ fits the m_b of 1D flat stretched flames. A comparison of m_b/m_b^0 is presented in Fig. 3 along with contributions from the different terms in Eq. (12). It can be observed that there is an excellent agreement in prediction of the mass burning rate by the three models. The individual contributions from direct stretch, enthalpy change and elemental composition changes are also predicted in an excellent manner by the Lewis fitted S(Le) and the reduced S(RM) models. The mass burning rate is significantly increased by the contribution from elemental changes and this increase is partly countered by the direct stretch ($-Ka$) and enthalpy changes. The use of the S(Le) model has the same computational cost as the NS model with constant Lewis numbers. The computation time with the S(RM) is found to be 16% faster than that with the MC model and 20% slower than the S(Le) model.

Profiles of CH_4 and H_2 mass fractions along with the temperature profile for stretched flames at a strain rate of 300 s^{-1} are shown in Fig. 4 for the three different Soret diffusion models, i.e. MC, S(Le) and S(RM), and a model with no Soret diffusion as a reference. It is to be noted that the domain length is larger than that shown here. The unburnt side is located at $x = -5$ mm and the burnt side is located at $x = 20$ mm. It can be observed that fuel species and temperature profiles from the reduced models are in excellent agreement with profiles from the more detailed multi-component model with Soret diffusion. Profiles of intermediate species H and OH and the product H_2O are also shown in Fig. 4 with the x -axis slightly shifted towards the burnt side for a clear presentation. Again excellent agreement can be observed among the different models and thus it can be concluded that the S(RM) and S(Le) models are able to capture Soret diffusion effects in stretched flames.

3.2. 1D burner-stabilized flames

After validation using strained flames, we test the S(Le) and the S(RM) models for 1D flat burner-stabilized flames for the same mixture used in the previous section. Considering the bluff-body problem in the next section, the inlet velocity is chosen to be 9 cm/s and the burner temperature is fixed at 496 K. The porous burner is located between $x = -2$ mm and $x = 0$ mm and has a volumetric porosity of 0.6. The unburnt boundary of the domain is taken at $x = -10$ mm to avoid diffusion across the inlet.

Fig. 4. CH_4 , H_2 , H, OH, H_2O mass fractions and temperature profiles for a 1D flat stretch flame with strain of 300 s^{-1} with three Soret diffusion models and MC-without Soret as a reference.

A comparison of CH_4 and H_2 mass fractions and temperature profiles along x is shown in Fig. 5 without Soret diffusion. Profiles from simulations without Soret diffusion are shown here as a reference for comparison with Soret diffusion effects on burner-stabilized flames. It can be observed that there is an excellent overall agreement between the results from the simulation with the multi-component (MC) model and the simulation with the constant Lewis number based NS model. Results with the inclusion of Soret diffusion are shown in Fig. 6 for three models (MC, S(RM) and S(Le)). Here CH_4 and H_2 profiles show a small dip and then rise in the concentration just upstream of the burner. This results from the Soret diffusion effect caused by the diffusion of species towards the hot burner. However, in this 1D configuration, its impact on the burning rate of the flame is not significant. Mass fraction profiles of the intermediate species H and OH and the product H_2O are also shown in Fig. 6. Again excellent agreement can be observed for all species. The intermediate species are produced and consumed outside the hot burner zone and hence are not significantly affected by thermal diffusion near the hot wall resulting in the S(Le) model being able to predict accurately the species profiles.

It can be observed that the S(RM) captures the diffusion of fuel towards the hot burner in a good manner. The Lewis number fitted model S(Le) is not able to capture this local effect, as could be expected. However, it does capture the Soret diffusion effect in the flame zone as was observed in the previous subsection. The S(Le)

Fig. 8. Numerical scaled heat release rate for $V_{in} = 1, 0.5, 0.375 \text{ m s}^{-1}$ with maximum values shown in white in each subplot. Results are zoomed in on the flame anchoring region. Left column is with No Soret diffusion (NS), centre is with Soret diffusion reduced model S(RM) and right side is Soret diffusion with fitted Lewis numbers S(Le).

modelled with a Neumann type boundary condition implying that there is no change in the field variables in the axial direction. Conjugate heat transfer of the fluid with the solid bluff body (thermal conductivity, $k = 109 \text{ W/m K}$) is also modelled. The steady reacting flow equations are solved on an equidistant structured grid with a $100 \mu\text{m}$ global grid resolution using a finite volume solver, a second-order upwind discretisation scheme and SIMPLE algorithm. A two-level grid refinement is applied based on the temperature gradient resulting in a local resolution of $25 \mu\text{m}$ in the flame zone. These mesh resolutions proved to give grid independent and well resolved solutions. The flame is numerically ignited by specifying a high temperature patch near the rear end of bluff body for $V_{in} = 1 \text{ m s}^{-1}$. The steady solution is used as an initial condition for lower velocity cases until the flame flashes back. Simulations including Soret diffusion are initialized from their respective simulations without Soret diffusion. All simulations presented in this paper are found to converge to a steady state solution.

4.1. Flame shape and structure

Figure 8 shows the heat release rate contours scaled with the maximum value of heat release rate of corresponding 1D flat flames simulated without Soret diffusion. Results are shown for the three models NS, S(RM) and S(Le) as introduced in the previous section. First, the flames at $V_{in} = 1 \text{ m s}^{-1}$ are discussed. All flames appear to burn stronger near the flame base close to the bluff body except for the NS flame. With the inclusion of Soret diffusion, the flame leading edges burn stronger and move closer to the bluff body. This upstream movement happens as the flame starts to burn stronger near the anchoring location resulting from an enhancement in the local burning rate because of stretch induced preferential diffusion effects. The S(RM) flame burns slightly

stronger than the S(Le) flame as indicated by the higher heat release rate. Overall the S(Le) results are closer to the S(RM) model results. However, differences in the maximum burning rate are still observable.

The scaled heat release rate for $V_{in} = 0.5$ and 0.375 m s^{-1} is also shown in Fig. 8. With decreasing velocity, near the flame base, more intense burning can be observed than for the flames at $V_{in} = 1 \text{ m s}^{-1}$. The maximum scaled heat release rate increases with a decrease in inlet velocity for models NS and S(RM) while it remains almost constant for the S(Le) model. The leading edges of the flames move upstream and outwards towards the rim of the burner in the presence of Soret diffusion. The distance between the axis of symmetry and the flame increases as the velocity is decreased and with inclusion of Soret diffusion. At this stage, it can be said that the S(Le) model captures the Soret diffusion effect reasonably well in the cases presented in this section with some larger differences in the maximum values of heat release rate. In order to understand the difference in burning rates predicted by the S(RM) and S(Le) models, we first analyze the heat loss and gain by the solid burner in the next subsection.

4.2. Heat transfer between the flame and the burner

In Fig. 9 the integrated heat flux to the top face of the burner is plotted for the three models, i.e., NS, S(RM) and S(Le) at varying inlet velocities. It can be observed that the flames with Soret diffusion lose more heat to the burner as compared to the flames without Soret diffusion. Flames modelled with S(RM) lose more heat as compared to the S(Le) model and this difference becomes larger as the limit for flashback is approached (low velocity). This larger heat loss results from a stronger burning near the flame base as observed in Fig. 8. Figure 10 shows the iso-contours of 30 and 98%

Fig. 9. Integrated heat flux to the top face of the bluff body.

Fig. 10. Iso-contours of 30 and 99% of the maximum heat release rate for the three models at $V_{in} = 0.375 \text{ m s}^{-1}$.

of maximum heat release rate for $V_{in} = 0.375 \text{ m s}^{-1}$ for the three different models. The flame with only Soret diffusion effects in the flame zone (S(Le)), stabilizes closer to the bluff body and moves further towards the rim of the burner than the NS flame. This results from stronger burning, allowing the flame to stabilize in the region of higher stretch rate and losing more heat to the bluff body than the NS flame. The S(RM) flame stabilizes even closer and moves closer to the rim than the S(Le) flame resulting in higher heat loss to the bluff body. As the system of burner and flow is adiabatic, this heat is transferred back to the flame via the flow at the upstream and side faces of the bluff body causing an increase in the local enthalpy of the unburnt mixture. This causes the max-

imum burning rate to occur at slightly downstream sections of the flames.

The left-most points in Fig. 9 (at the low velocity side) correspond to the velocity limits just before the flame flashes back (and stabilizes at the inlet of the computational domain). It can be seen that the flashback limits change when using different models. The flame without thermal diffusion (NS) stabilizes for the lowest velocities of all the three models (flashback occurred at $V_{in} = 0.25 \text{ m s}^{-1}$), while the S(RM) flame flashes back for the highest inlet velocity (flashback occurred at $V_{in} = 0.3475 \text{ m s}^{-1}$). The limit of the S(Le) flame is in between that predicted by the NS and the S(RM) model as flashback occurred at $V_{in} = 0.3125 \text{ m s}^{-1}$.

Next, temperature distributions in gas and solid burner are discussed. Normalized temperature plots are shown in Fig. 11 with the normalized temperature θ defined as:

$$\theta = \frac{T - T_u}{T_{b,0} - T_u}. \quad (13)$$

Here T_u is the temperature at the unburnt side and $T_{b,0} = 1546.2 \text{ K}$ is the adiabatic flame temperature corresponding to the inlet fuel equivalence ratio. It can be observed that $\theta > 1$ near the flame base for all cases presented here, implying strong Lewis number effects. With decreasing V_{in} , the bluff body temperature increases for all three models. The average bluff body temperature T_s at $V_{in} = 0.375 \text{ m s}^{-1}$ is maximum for the S(RM) flame, then for the S(Le) flame and lowest for the NS flame. This is caused by a stronger burning rate for the S(RM) flame as observed in previous subsections. The pre-heating zones can also be clearly seen near the side walls of the bluff body, increasing in intensity with a decrease in V_{in} and an increase in model accuracy (from NS to S(Le) to S(RM)). In order to further our investigation, we discuss the Soret diffusion fluxes near the flame base and the bluff body in the next section.

4.3. Soret diffusion and local stratification

Due to the existence of temperature gradients near the side and bottom faces of the bluff body, it can be expected that the lighter species diffuse towards the burner walls as it was also observed in Fig. 6. In order to verify this effect, the thermal/Soret diffusion factor, which is the ratio of thermal to Fickian diffusion coefficients given as $a_i = \frac{D_i^T}{D_{i,m}^T}$ are shown in Fig. 12 for $V_{in} = 0.375 \text{ m s}^{-1}$ for CH_4 and H_2 . The values of the thermal diffusion coefficients a_i are usually negative for lighter species and positive for heavier species. This allows lighter species to diffuse towards hot regions and vice versa for heavier species [2,4,29]. The presence of a higher Soret diffusion coefficient in the flame zone (where high temperature gradients are present as well) than in the rest of the domain can be clearly observed in Fig. 12. Here thermal diffusion affects the flame by increasing its burning rate as discussed in Ref. [6] and shown in Fig. 2. It can also be seen in Fig. 12 that outside the flame zone, near the bottom and side faces of the bluff body, where the temperature gradients were observed in Fig. 11, Soret diffusion coefficients are also significant for both CH_4 and H_2 . It appears that both the fuel species diffuse towards the hot burner walls because of Soret diffusion (Soret diffusion coefficients + temperature gradients). In this region, the Soret diffusion coefficient is almost -0.06 for CH_4 and -0.2 for H_2 . This local diffusion of fuel species causes a fuel stratification in the unburnt mixture approaching the flame base that changes the burning rate at different sections of the flame. This is visualized by plotting the local equivalence ratio, ϕ_{local} in Fig. 12 on the right side. The local equivalence ratio is defined as

$$\phi_{local} = \left(\frac{Z_C + Z_H}{Z_O} \right) / \left(\frac{Z_C + Z_H}{Z_O} \right)_{stoic}. \quad (14)$$

Fig. 11. Contour plot of normalized temperature θ for $V_{in} = 1, 0.5, 0.375 \text{ m s}^{-1}$ zoomed-in on the region surrounding the burner with three different models. The first row is with No Soret diffusion NS (a), (b), and (c), the second is with Soret diffusion with fitted Lewis numbers S(Le) (d), (e), and (f) and last row is Soret diffusion with reduced model S(RM) (g), (h), and (i).

Fig. 12. Soret diffusion factor ($a_i = D_i^T / (D_{i,m} Y_i)$) zoomed-in on the region surrounding the burner, for CH_4 and H_2 for $V_{in} = 0.375 \text{ m s}^{-1}$ with S(RM) model along with ϕ_{local} .

where Z_C , Z_H and Z_O are the elemental mass fractions for carbon, hydrogen and oxygen, respectively. From Fig. 12, it can be observed that the maximum of ϕ_{local} occurs just at the burnt side near the flame base region. This indicates a stronger burning rate due to stretch and Soret diffusion induced preferential diffusion effects. One can also observe higher ϕ_{local} near the side walls of the bluff body where Soret diffusion of fuel species results in a richer mixture. This local increase in ϕ causes the flame to burn stronger than the flame from the S(Le) simulation. The effect of this pre-heating induced Soret fluxes on the mixture composition is further

presented in Fig. 14, where mass fractions of CH_4 and H_2 scaled with their respective value at the inlet are plotted as function of radial distance from the side face of the burner towards the outer cold wall (along the white line shown in Fig. 12). The CH_4 and H_2 mass fractions rise as shown in Fig. 12 because of Soret diffusion near the burner side walls. With decreasing V_{in} , an increase in maximum mass fractions of both CH_4 and H_2 can be observed just at the burner side wall. The maximum increase for CH_4 is about 3% as compared to the inlet value for $V_{in} = 0.375 \text{ m s}^{-1}$. For H_2 a significant increase of about 11% in its mass fraction is present for

Fig. 13. Contour plot of ϕ_{local} changes with the inlet value for $V_{in} = 1, 0.5, 0.375 \text{ m s}^{-1}$ zoomed-in on the region surrounding the burner with three different models. First row is with No Soret diffusion NS (a), (b), and (c), centre is with Soret diffusion using fitted Lewis numbers S(Le) (d,e,f) and last row is with Soret diffusion using the reduced model S(RM) (g), (h), and (i).

$V_{in} = 0.375 \text{ m s}^{-1}$. These changes in the unburnt mixture increase the local stoichiometry, resulting in a richer mixture reaching the flame base. This enables the flame to burn stronger as was observed in Fig. 8. In turn, a slightly leaner mixture reaches the flame sections near the immediate downstream region of the flame base. This results in a weaker burning flame at those downstream sections. Plots of changes in ϕ_{local} normalized with the inlet value are shown in Fig. 13. It can be observed that an increase of almost 10% near the flame base can be observed for $V_{in} = 1 \text{ m s}^{-1}$ with all three models. With decreasing V_{in} , the maximum value of ϕ_{local} decreases. But the magnitude of this decrease is different for the three models. At $V_{in} = 0.375 \text{ m s}^{-1}$, the NS flame burns the weakest near the flame base, while the S(Le) and S(RM) flames burn stronger and with a similar local increase in ϕ_{local} . The main difference between the S(Le) and S(RM) flames arises from the higher ϕ_{local} near the bluff body side walls which increases in magnitude with decreasing velocity. This results from the higher pre-heating intensity observed in Fig. 11 showing the combined effect on local burning rate.

At this point, we have identified three sources for an increase in the burning rate of flames with Soret diffusion:

1. A change in local composition and enthalpy because of thermal diffusion in the flame zone, induced by flame stretch (Fig. 2).
2. An increase in local enthalpy resulting from pre-heating via the bluff body side and bottom walls (Fig. 11).
3. A change in local fuel-air ratio at the flame base because of thermal diffusion in the unburnt zone (Fig. 14).

In order to evaluate the role of each of these contributions at different sections of the flame, a detailed investigation of the local mass burning rate is carried out in the next section.

5. Flame burning rate and stabilization

In this section, we quantify the effect of the local changes resulting from thermal diffusion in the flame and the unburnt region along with the changes in enthalpy resulting from pre-heating. Figure 15 shows the variation of mass burning rate, m_b , at the inner layer $Y = 0.9$, as a function of the axial location above the bluff body in the flame front for three different inlet velocities. The mass burning rate is scaled with the mass burning rate m_b^0 of a 1D adiabatic unstretched flame without Soret diffusion.

It can be seen that the mass burning rate for the $V_{in} = 1 \text{ m s}^{-1}$ flames is lower near the flame base due to cooling, then increases to a maximum value and then decreases again slightly at downstream location. The maximum mass burning rate is higher for models with Soret diffusion, i.e., the S(Le) and S(RM) models, as compared to the NS model. The difference in m_b/m_b^0 for S(Le) and S(RM) is only prominent near the flame base location ($z/D \leq 0.5$);

Fig. 14. Mass fractions of CH_4 and H_2 scaled with their respective value at the inlet plotted along the radial direction at $z = -1/2D$ using the S(RM) model.

downstream of the flame base ($z/D > 0.5$), m_b/m_b^0 is identical for both the models. The maximum value of m_b/m_b^0 differs slightly between the S(Le) and S(RM) models as a result of stratification near the burner rim, making m_b/m_b^0 of the flame computed with the S(RM) model higher than the S(Le) flame. With decreasing inlet velocity, the difference between m_b/m_b^0 from the S(RM) and the S(Le) models becomes larger in the flame base region. For $V_{in} = 0.375 \text{ m s}^{-1}$, m_b/m_b^0 is higher at the leading edge ($0 \leq z/D \leq 0.1$) for the S(RM) flame than for the S(Le) flame despite the higher heat loss to the burner. This is the result of the local stratification effect resulting in a richer mixture reaching the flame leading edge. Just downstream of the leading edge ($0.1 \leq z/D \leq 0.5$), the difference in m_b/m_b^0 increases such that for the S(Le) flame, the maximum burning rate is around 40% higher than that for the reference case, while for the S(RM) flame, it is about 55% higher. This increase in local burning rate causes the flame with the S(RM) model to flashback at a higher velocity than the S(Le) flame as was observed in Fig. 9.

Fig. 15. The scaled mass burning rate m_b/m_b^0 plotted along the flame as a function of axial distance of the domain for the 3 different models with $V_{in} = 1, 0.5, 0.375 \text{ m s}^{-1}$.

Fig. 16. An illustration showing the change in flame stabilization location resulting from Soret diffusion induced stratification in the unburnt mixture. Blue lines show heat transport while red lines show mass transport of fuel species. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

6. Discussion and conclusions

A numerical study of bluff body stabilized flames has been conducted for a lean $\text{CH}_4\text{-H}_2\text{-air}$ premixed mixture at different inlet velocities. Flames were stabilized behind a bluff body including conjugate heat transfer between the fluid and the solid burner, and taking into account the Soret diffusion effects and detailed chemical kinetics. In order to include Soret diffusion effects at a reasonable computational cost, a reduced model and a Lewis number fitted model are first validated for 1D stretched flames. With 1D burner-stabilized flames, diffusion of fuel species towards the hot burner was observed. This effect was captured by the reduced model [10] while the Lewis number fitted model was unable to capture this effect. This enabled us to separate the effect of an enhancement in burning rate by Soret diffusion in the flame zone and the effect of Soret diffusion of fuel species towards a hot burner. It is found that Soret diffusion of fuel towards the burner has an impact on the flame leading edge burning rate and thus results in flames flashing back at higher velocity than for other models. A schematic depicting the mechanism of the enhancement in the local burning near the flame base by Soret diffusion phenomena is presented in Fig. 16. The important steps of this mechanism are:

- Because of heat transfer between the flame and the bluff body (flame holder), the flame loses heat which is conducted upstream by the solid body, pre-heating the unburnt mixture.
- This creates a temperature gradient in the vicinity of the bluff body side walls driving both CH_4 and H_2 towards the hot burner wall by thermal diffusion.
- As a consequence, the mixture approaching the flame base becomes locally richer, resulting in an enhancement in the burning rate.
- As the flame base burns stronger, it loses more heat to the bluff body, resulting in more stratification locally (self supporting mechanism).
- The flame finds a new stabilization location such that the higher burning rate is compensated by higher stretch rates.

- Because of fuel stratification, a leaner mixture reaches the downstream section of the flame.
- The local burning rate just downstream of the flame leading edge is enhanced by an increase in the enthalpy, resulting from pre-heating caused by heat loss at the flame leading edge.

For including Soret diffusion in the flame zone, the Lewis number fitted model works well especially when the heat loss to the bluff body and thus the resulting temperature gradients near the side walls are low. This model, which adds no extra cost, can be used in problems where computation time is a constraint and the burner is not subjected to high heat loads. For flames near flashback, the inclusion of Soret diffusion using the reduced model from Ref. [10], which captures the stratification effect near a hot burner, results in a 28% higher inlet velocity limit than that without Soret diffusion. The results discussed in this study indicate a strong need for inclusion of Soret diffusion effects in numerical simulations of fuel mixtures with H_2 or other light species, where quantitative predictions of flashback limits are the objective.

Declaration of Competing Interest

The authors declare that they do not have any financial or non-financial conflict of interests.

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