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Modelling and simulation of lean premixed turbulent methane/hydrogen/air flames with an effective Lewis number approach

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ABSTRACT

Recent work on reaction modelling of turbulent lean premixed combustion has shown a significant influence of the Lewis number even at high turbulence intensities, if different fuels and varied pressure is regarded. This was unexpected, as the Lewis number is based on molecular transport quantities (ratio of molecular thermal diffusivity to mass diffusivity), while highly turbulent flames are thought to be dominated from turbulent mixing and not from molecular transport. A simple physical picture allows an explanation, assuming that essentially the leading part of the wrinkled flame front determines the flame propagation and the average reaction rate, while the rear part of the flame is of reduced importance here (determining possibly the burnout process and the flame brush thickness but not the flame propagation). Following this argumentation, mostly positively curved flame elements determine the flame propagation and the average reaction rate, where the influence of the preferential molecular diffusion and the Lewis number can easily seen to be important. Additionally, an extension of this picture allows a simple derivation of an effective Lewis number relation for lean hydrogen/methane mixtures. The applicability and the limit of this concept is investigated for two sets of flames: turbulent pressurized Bunsen flames, where hydrogen content and pressure is varied (from CNRS Orléans), and highly turbulent pressurized dump combustor flames where the hydrogen content is varied (from PSI Baden). For RANS simulations, comparison of flame length data between experiment and an effective Lewis number model shows a very good agreement for all these flames with hydrogen content of the fuel up to 20 vol.%, and even rather good agreement for 30% and 40% hydrogen.

1. Introduction

While for laminar premixed flames molecular diffusion processes of heat and of species are known to be important, for highly turbulent flames turbulent mixing is expected to be most dominant. In contrast to this expectation experimental and numerical modelling work indicates also for highly turbulent premixed flames a significant influence of molecular diffusion effects. The following work proposes an explanation of this contradiction with the help of a simple physical picture. Additionally, an extension of this picture allows the derivation of an effective Lewis number closure for fuel mixtures.

Laminar premixed combustion is well known to depend on differential molecular transport effects. For instance thermo-diffusive flame instabilities are explained with the unequality of molecular thermal diffusion α (directed from the burned hot side to the unburned cold side) and molecular mass diffusion D of the deficient reactants (fuel for lean flames) in the opposite direction [1]. The Lewis number $Le = \alpha/D$ describes this ratio. For planar laminar flames the combined reaction and transport processes as well as any Lewis number effects are already included in the laminar burning velocity S_{L0}. For curved flames, a situation with $Le < 1$ (and $D > \alpha$) leads for instance to enhanced reactivity in positively curved flame elements (convex towards the unburned mixture) due to the relative increase of local fuel concentration with only a slight decrease of temperature, while the reactivity is reduced in negatively curved parts of the flame. This leads to the thermo-diffusive instability with self-induced wrinkling of otherwise plane laminar flames. For $Le > 1$, decreased reactivity in the positively curved parts and enhanced reactivity in the negatively curved flames stabilises the plane laminar flame.

For weakly turbulent flows the curvature distribution of premixed flames is typically unsymmetrical due to the dominance of the Huygens effect of flame propagation. Here an influence of non-unity Le values is easily expected.

However, for sufficiently high turbulence levels the curvature distribution reaches a symmetric state (e.g., [2]). So, as both positive and negative flame elements are existing with equal probability, the average of regions with enhanced or reduced reactivity due

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to curvature should vanish, at least in first order. Also turbulent mixing is expected to be dominant compared to the much smaller molecular diffusion effects. Consequently, Lewis number effects are against the expectation here.

Contrary to this expectation, several experimental investigations have shown a dominant role of the Lewis number even in highly turbulent premixed flames [3–5], especially for increased pressure conditions [2].

Additionally, we found in extended numerical studies that an explicit Lewis number dependency in an algebraic reaction rate approach was rather successful to describe a set of about 100 different measured premixed methane, ethylene or propane air flames [6] for pressures up to 1 MPa (10 bar). The Lewis number effect was found to be especially important for increased pressure.

The current work starts with a simple physical picture which in first order explains a possible reason that molecular diffusion effects are still of importance even under highly turbulent conditions. The argumentation is based on the assumption that the leading parts of the turbulent flame brush determine the overall turbulent flame propagation speed, while the rear parts are of minor importance. This assumption has been used in the past from Zel'dovich and Frank-Kamenetskii [7] for laminar spherical flames, and has been extended to a "leading edge concept" by Kuznetsov and Sabel'nikov [8], and is reviewed in [9]. Also the KPP theorem (named after Kolmogorov, Petrovsky and Piskunov) has in so far some similarity as it predicts the turbulent burning velocity as a function of the turbulence characteristics at the leading edge [10,11]. However our approach also includes the local molecular processes near the leading part of the flame.

In a second step this physical picture allows to derive a new relation for an effective Lewis number, if fuel mixtures with different fuel diffusivities are burned. Here, hydrogen/methane flames are investigated, which are of technical importance due to increased flame stability and potentially reduced greenhouse gas (CO_2) emission.

This derived extension of our recently developed RANS reaction model [6] is tested against two different sets of experiments with hydrogen/methane/air flames at increased pressure and systematically increased hydrogen content. For at least up to 20% hydrogen this rather simple physical model is found to be applicable.

It may be noted, that the argumentation of our paper is based on flame curvature. For slightly wrinkled laminar flames, flame strain is believed to have similar effects on the molecular transport balance, where flame elements are situated in positively or negatively strained local flow regions. Assuming here the same probability, the effects of the opposite thermal and species diffusions may cancel out, in first order. Recent DNS studies (e.g., [12]) show instead that preferential alignment effects of the local flame front take place, which leads to unsymmetrical distributions of positive and negative strain (see also [13]). It is likely that this can be seen as an alternative way to explain explicit Lewis number influences [12,14]. For the sake of simplicity we argue only with curvature effects in the following paper, having in mind that similar arguments may be discussed in the frame of strain effects.

2. Experimental test data

Experimental flame data is available from high-pressure flames investigated at CNRS Orléans (France) and from the Paul-Scherrer-Institute (PSI) in Baden (Switzerland). In both cases premixed methane/hydrogen/air flames have been investigated under increased pressure.

2.1. High-pressure Bunsen flame data from CNRS Orléans

Interesting experimental studies were carried out by Halter et al. [15] at CNRS Orléans on a Bunsen-like flame configuration inside a pressurized cylindrical combustion chamber with height 600 mm and diameter 300 mm. For the chosen lean methane/hydrogen/air mixtures, hydrogen was varied in the proportions of 0, 10 and 20 vol.% of the fuel, holding the overall equivalence ratio of the composite premixed mixture constant at 0.6. Grid turbulence was generated by a perforated plate with 2.5 mm diameter holes in a hexagonal array located 50 mm upstream of the burner exit. The flame was stabilized with the help of a small annular hydrogen pilot flame (equivalent to 6 vol.% of the main-stream fuel flow rate).

The mean flow velocity was fixed at 2.1 m/s, axial and radial turbulence intensities u', v' and integral length scale l_x were measured with LDA just above the burner exit (see Table 1, where also the unstretched laminar burning velocity S_{L0} is listed). The operating pressure p was varied between 0.1 and 0.9 MPa (1–9 bar). The flame position along the axial direction of the symmetric line was measured from the statistical evaluation of planar laser scattering images (based on Mie and Rayleigh scattering). The heat release rate was between 2 and 18 kW. The geometrical Reynolds numbers varied between 3500 and 31,500, while the turbulent Reynolds numbers were between 33 and 329.

2.2. Highly turbulent high-pressure flame data from PSI Baden

Griebel et al. [16] conducted experiments on the high-pressure high-momentum jet premixed flame test rig of the Paul-Scherrer-Institute (Baden, Switzerland). The premixed methane/hydrogen/air mixture was preheated to 673 K at 0.5 MPa (5 bar). The overall equivalence ratio was kept constant at 0.5. The thermal power was about 75 kW. The unstretched laminar burning velocities for these mixtures are 0.237, 0.266, 0.296, 0.321 and 0.351 m/s, for hydrogen fractions of 0, 10, 20, 30 and 40 vol.%. The flame was stabilised by an outer recirculation zone created from the sudden expansion of the combustor geometry (dump combustor). The length of the combustion chamber is 320 mm with the inlet nozzle diameter d = 25 mm and an expansion diameter of 75 mm. Inlet grid turbulence was generated on a hexagonal pitch with 3 mm hole diameter, placed 30 mm upstream of the sudden expansion. The inlet mean velocity of 40 m/s, turbulence intensity $u'/U \approx 15\%$ and integral length scale of 2 mm were measured with 2D Particle Image Velocimetry (PIV), and the reacting field was characterised using Planar Laser Induced Fluorescence (PLIF) of the OH radical as a marker of the instantaneous flame front. The inflow geometrical and turbulent Reynolds numbers are $Re \approx 80{,}000$ and $Re_t \approx 1000$, respectively. The latter quantity reached about 2300 in the shear flow region seven diameters downstream. Turbulence intensities, Reynolds numbers and heat release are significantly higher than for the Bunsen flames from Orléans.

Table 1
Experimental inflow conditions (U = 2.1 m/s, ϕ = 0.6) [15].

Conc. of H_2 (h%)	p (MPa)	u' (m/s)	v' (m/s)	l_x (mm)	S_{L0} (m/s)	u'/S_{L0}
0	0.1	0.15	0.12	6.69	0.112	1.36
10	0.1	0.15	0.14	4.30	0.121	1.26
20	0.1	0.16	0.14	3.51	0.132	1.20
0	0.5	0.18	0.14	7.37	0.041	4.36
10	0.5	0.18	0.14	6.97	0.044	4.07
20	0.5	0.19	0.17	6.84	0.048	3.92
0	0.9	0.16	0.11	5.77	0.029	5.32
10	0.9	0.15	0.12	5.45	0.031	4.92
20	0.9	0.16	0.14	5.66	0.033	4.85

3. Reaction model for turbulent premixed flames

3.1. Reaction model

One of the commonly proposed ways to model turbulent premixed flames is based on a reaction progress variable approach. Based on the correlation between major species and temperature, the computation of flames can be simplified essentially by describing the main reactive and thermal processes within one transport equation of the density-weighted mean reaction progress variable $\tilde{c}$ ($\tilde{c} = 0$ in unburned and $\tilde{c} = 1$ in burned mixtures).

$$\frac{\partial}{\partial t}(\bar{\rho}\tilde{c}) + \frac{\partial}{\partial x_k}(\bar{\rho}\tilde{u}_k\tilde{c}) = \frac{\partial}{\partial x_k}\left(\bar{\rho}\frac{\nu_t}{Sc_t}\frac{\partial \tilde{c}}{\partial x_k}\right) + \bar{w}_c \tag{1}$$

Here, the third term describes a simplified turbulent transport model and the fourth term the source of the average reaction progress variable. The numerical scheme is based on the solution of Eq. (1) in combination with the standard averaged Navier–Stokes equations [11,17–20]. The mean reaction rate is modelled as the product of the flame surface density Σ (flame surface-to-volume ratio) and the laminar consumption rate $\rho_u S_{L0}$:

$$\bar{w}_c = \rho_u S_{L0} I_o \Sigma \tag{2}$$

with unburned gas density ρ_u, unstretched laminar burning velocity of the fuel/air mixture S_{L0}, and a correction term I_0 for straining influence. While some modelling approaches describe the spatial development of the flame surface density Σ by an additional transport equation (e.g., [11]), we found very good results for lean methane, ethylene or propane flames with a simple algebraic relation for the product of a flame surface wrinkling ratio $A_T/\overline{A}$ and the gradient of reaction progress variable (Algebraic Flame Surface Wrinkling (AFSW) model, [6]), leading to $\bar{w}_c = \rho_u S_{L0}(A_T/\overline{A})|\nabla\tilde{c}|$. The flame wrinkling ratio (including I_0) is modelled with an algebraic relation, which has been parameterized to fit to about 100 different lean methane, ethylene and propane flames, for 0.1 to 1.0 MPa, experimentally measured by Kobayashi et al. [21]:

$$\frac{A_T}{\overline{A}} = 1 + \frac{0.46}{Le}\,\mathrm{Re}_t^{0.25}\left(\frac{u'}{S_{L0}}\right)^{0.3}\left(\frac{p}{p_0}\right)^{0.2} \tag{3}$$

Here, the turbulence is described by the turbulent Reynolds number $Re_t = u' l_x/\nu$ (with kinematic viscosity ν). An explicit pressure dependency p/p_0 (with $p_0 = 1$ bar) is included. In [6] an explicit dependency on the Lewis number Le of the fuel has been found for the investigated single-component lean fuel–air mixtures. The applicability of this AFSW model has been checked for other flame situations and has also been successfully adopted as a subgrid reaction model for the LES approach [22].

3.2. Physical model to include the Lewis number in the reaction rate

In the development of the above subclosure an important finding was the explicit inclusion of a term for the Lewis number $Le = \alpha/D$ with the fuel diffusivity D. This was an interesting observation, as the importance of molecular transport effects was previously expected to be significant only for laminar or slightly turbulent flames. However, it was found that this Le term in the reaction subclosure accommodates for a variety of fuels [6].

A Lewis number unequal to one is expected to modify the local processes of fuel diffusion towards the flame front and of thermal diffusion away from the flame front. For plane laminar flames this effect is already included in the plane laminar flame speed S_{L0}. For wrinkled flames, however, an enhanced reactivity is expected on the positively curved flame elements and a decreased reactivity

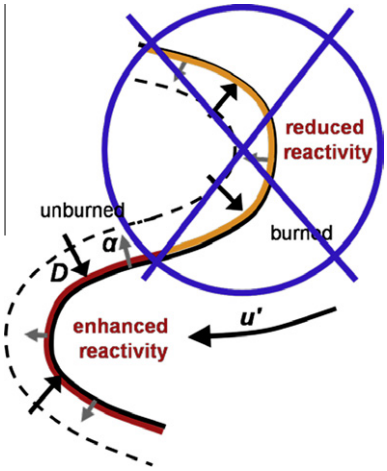

Fig. 1. Physical picture of the Lewis number influence of preferential diffusive transport between heat and fuel species (shown for the case $Le = \alpha/D < 1$). Similar to the "leading edge concept" the processes on the leading side with mostly positive curvature are assumed to be dominant for the flame propagation process and with that for the average reaction rate, while the processes at the rear side of the flame are assumed to affect only the burnout of the flame and the flame brush thickness. This picture explains the significance of the preferential diffusion also for highly turbulent flames.

is expected on the negatively curved flame elements, if for instance the Lewis number is assumed to be below one (Fig. 1). Averaging about positively and negatively curved flame elements, and knowing that the probability distribution for both is similar for sufficiently high turbulence intensity [2], the effect of a nonunity Lewis number on the averaged reaction rate should disappear, as long as the local enhancement and reduction of reactivity scale linear with curvature (first order approximation). However, this is against the observation.

Regarding more closely the detailed influence of the different parts of the premixed flame front, it can be argued that the front side of the wrinkled flame is more important for the overall flame propagation process than the rear side, and with that also for the averaged reaction rate.

In Fig. 1, the consequence of this approach is shown for the case of a Lewis number less than unity. If the leading side of the flame dominates the overall flame propagation, the reduced reactivity on the rear side of the flame is of less influence, compared to the enhanced reactivity on the leading side of the flame. As the leading side is mostly positively curved, for flames with $Le < 1$ a local focussing effect of fuel by molecular diffusion is probably more dominant than the local defocussing effect of the molecular thermal diffusion towards the unburned side of the mixture.

If this physical picture is accepted as interpretation, the observed strong Lewis number dependency of the effective flame propagation rate and with that of the average reaction rate can be understood.

This physical picture has similarities to the "leading edge concept" from Zel'dovich and Frank-Kamenetskii [7] and Kuznetsov and Sabel'nikov [8] as is supported by Lipatnikov and Chomiak [9]. Also here a Lewis number dependency is comprehensible.

It would be interesting to investigate, if the rear side of the flame shows also a visible Lewis number effect. From the physical picture it seems likely, that here the Lewis number may affect the flame brush thickness, as for instance for $Le < 1$ the reactivity on the rear side is reduced, so a longer "burn out" zone and thus a broadened flame brush may be expected here (and the other way round a reduced flame brush thickness for flames with $Le > 1$). We are not aware of experiments to this point, and do not treat this issue in this paper. Very recently, this expected influence of the

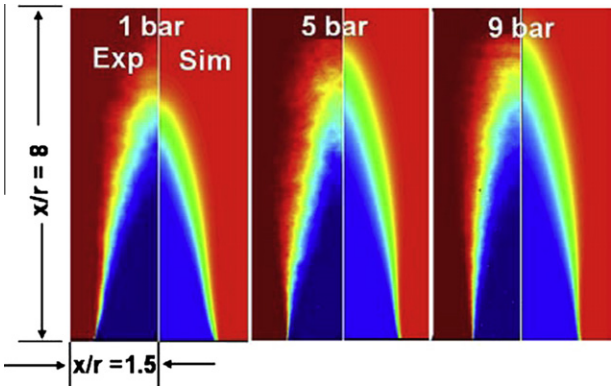

Fig. 2. Contours of Reynolds averaged reaction progress variable $\tilde{c}$ ($0 \leqslant \tilde{c} \leqslant 1$) for pure methane/air flames for equivalence ratio ϕ of 0.6 at 0.1, 0.5 and 0.9 MPa. Left side experiment (Exp), right side the AFSW model simulation (Sim).

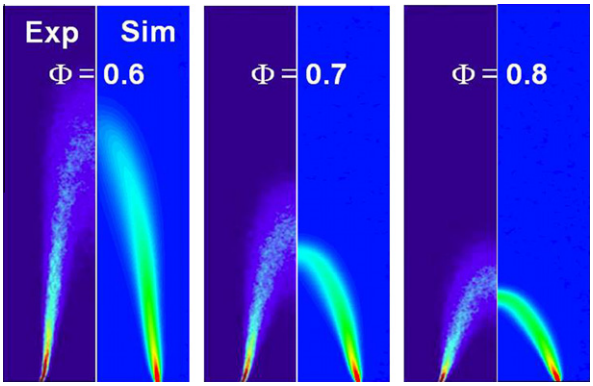

Fig. 3. Contours of gradient of reaction progress variable ($|d\tilde{c}/dx|$) for pure methane flames for ϕ's of 0.6, 0.7 and 0.8 at 1 bar. In each set experimental contours (Exp) are shown on the left side and the AFSW model simulations (Sim) are on the right side. The values range between 0 (blue) and 200 m^{-1} (red). (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

Lewis number on the flame brush width was indeed shown nicely with a comparative DNS study.[1]

3.3. Numerical implementation

In this study, numerical simulations are carried out in two-dimensional cylindrical geometry [23]. Boundary conditions are set up in accordance with the experiments. The pressure–velocity coupling is based on the SIMPLE scheme, with the standard $k-\varepsilon$ model, and the common relations among the physical turbulence parameters u', l_x, and Re_t and the calculated turbulence parameters k and ε are applied (see, e.g., [6]). The AFSW reaction model with the closure (3) is implemented as a user-defined subroutine function. For the enclosed Bunsen flame configuration of CNRS Orléans, a numerical pre-study showed that a reduction of the rather large experimental chamber diameter from 300 mm to 120 mm did not affect the calculated flame position and flame angle, so this was used to reduce computational time. Additionally, in a grid dependency test, we found that the minimum computational mesh size for which the flame height is not affected is 0.25 mm. For the PSI flame simulations, the computational domain size is identical to the experimental dimensions.

4. Results and discussion

4.1. Development of an extended reaction model for mixed fuels

As a first step, the lean premixed pure methane/air flames of Orléans are computed using the AFSW model (Eq. (3)) for the pressures of 0.1, 0.5 and 0.9 MPa. Similar to those cases, where the AFSW model has been developed (see [6]) the pressure dependency of flame position as well as flame brush thickness is simulated in good agreement with the measurements for these near-unity Lewis number flames. Figure 2 shows the contours of the measured and calculated Reynolds averaged reaction progress variable. Note, that the calculated density-weighted reaction progress variables are transformed to Reynolds-averaged values, to be comparable to the measurement.

Also the variation of stoichiometry using the three equivalence ratios of 0.6, 0.7 and 0.8 is predicted well. Figure 3 presents the results for 0.1 MPa where the absolute value of the gradient of the reaction progress variable is shown, indicating the average position and width of the flame brush.

[1] S. Cant, Meeting of the British Section of the Combustion Institute, Cambridge 12/2009.

As the next step, hydrogen/methane flames are investigated. Here, the central question was, if the AFSW model is still applicable. As the Lewis number of the pure fuels in a composite mixture is very different (for example, $Le_{H_2} = 0.29$ and $Le_{CH_4} = 0.955$, [24]), the application of an effective Lewis number Le^* may be appropriate for such fuel mixtures. We tested this with three models.

As a first model A we used a heat release weighted effective Lewis number, as recently proposed by Law and Kwon [25]:

$$Le^* = 1 + [q_{CH_4}(Le_{CH_4} - 1) + q_{H_2}(Le_{H_2} - 1)]/q, \quad (4)$$

Here q_{CH_4} and q_{H_2} is the combustion heat release of the corresponding fuels and q is the total heat release, being the sum of both. For the fuels with 0%, 10% and 20% hydrogen in methane the effective Lewis numbers follow to be 0.955, 0.935 and 0.918, respectively.

In Fig. 4, the predicted flames (plotted as reaction progress variable) are shown for this model A in comparison with the experimental flames for all nine test cases. The experimental flame cone length depends significantly on the percentage of added hydrogen, while the predicted flame shapes remain nearly similar in height. The difference is especially visible for the higher pressure cases. In Fig. 5, the resulting calculated flame heights (defined on the axis as the position with the Reynolds averaged reaction progress variable of 0.5) is shown for model A, for the nine cases. For the sake of comparison, calculations are performed also without the inclusion of the Lewis number term (similar to $Le = 1$ in Eq. (3)). The flame length decreases slightly with hydrogen addition, but this is mainly coming from the small increase of the unstretched laminar burning velocity (0.112, 0.121, 0.132 m/s) with 0%, 10% and 20% H_2 addition. Inclusion of the effective Lewis number according to Model A does not alter this behaviour – in contrast to the experimental observation.

With a modified model B, the effective Lewis number is assumed to be a linear relation between the single fuel Lewis numbers values ($Le^* = x_{CH_4} Le_{CH_4} + x_{H_2} Le_{H_2}$), x_i being the volumetric fractions of fuel species. The resulting flame heights are found to be only slightly different to those for model A, and are therefore not shown here. This model B also does not fit to the experiments.

For the development of a model C for an effective Lewis number, the physical situation near a positively curved flame element towards the unburned lean premixed mixture is analysed more closely (Fig. 6). If compared to the plane unstrained laminar flame situation, a local enrichment of fuel (dominated especially by lighter hydrogen) can be expected for the positively curved flamelet,

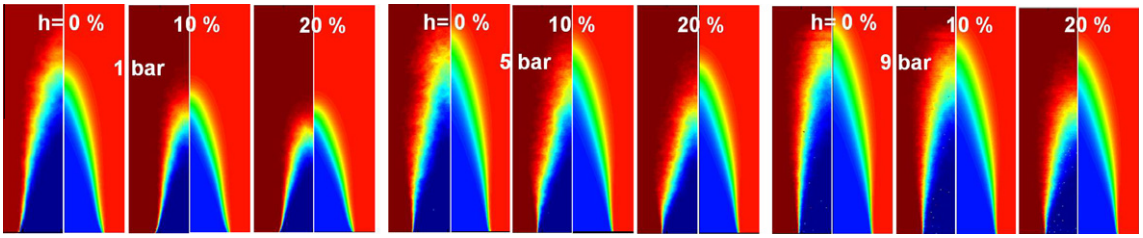

Fig. 4. Contours of reaction progress variable are shown for methane/hydrogen flames with 0, 10, 20 vol.% hydrogen for 0.1, 0.5 and 0.9 MPa ($\phi = 0.6$). Experiment (left) and simulation (right) using the AFSW model combined with model A for an effective Lewis number.

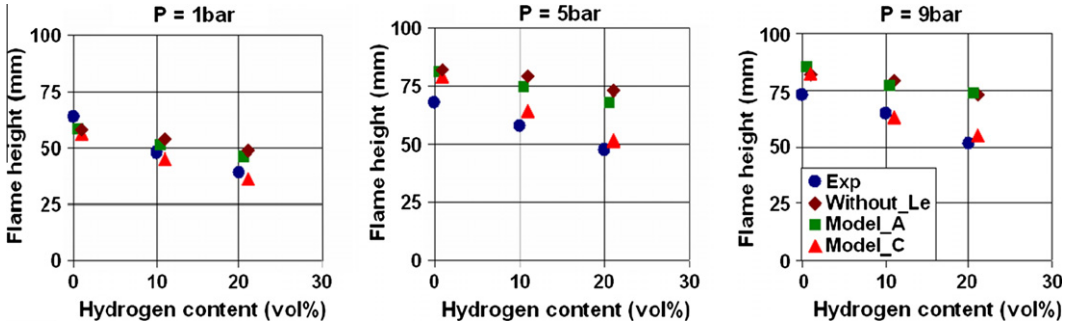

Fig. 5. Orléans Bunsen flames. Comparison between experimental and calculated flame heights for 0, 10, 20 vol.% hydrogen for 0.1, 0.5 and 0.9 MPa ($\phi = 0.6$). Calculations from the AFSW approach are shown without Lewis term and included with those from the two models A and C.

leading to higher reactivity and thus higher local burning velocity. According to the concept that the positively curved leading side of the flame dominates the flame propagation, the overall reaction rate is expected to increase as well. A simple approach to describe this enhancement may be modelled with an effective diffusivity $D^* = x_{CH_4} D_{CH_4} + x_{H_2} D_{H_2}$, with x_i being the volumetric fractions of the fuel mixture. The thermal diffusivity α, is only slightly affected from the hydrogen content in the fuel, as it is a property of the whole fuel–air mixture and thus is dominated by the large nitrogen content.

From this approach, we derived a new model C for a resulting effective Lewis number [26]:

$$\frac{1}{Le^*} = \frac{D^*}{\alpha} = \frac{x_{CH_4} D_{CH_4}}{\alpha} + \frac{x_{H_2} D_{H_2}}{\alpha} = \frac{x_{CH_4}}{Le_{CH_4}} + \frac{x_{H_2}}{Le_{H_2}} \tag{5}$$

with x_i being the volumetric fractions of the fuel mixture. For the three investigated fuel mixtures with 0, 10 and 20 vol.% of H_2, the effective Lewis numbers Le^* are calculated to be 0.955, 0.777 and 0.655, respectively.[2] In Fig. 5, the resulting flame heights are shown, obtained with this model C. As can be seen here, the flame heights are well captured, for both added hydrogen as well as for increased pressure. The comparison of the direct flame shapes are shown in Fig. 7. This new model for the effective Lewis number captures both flame position and flame brush very accurately.

In Fig. 8, the calculated results are presented in the non-dimensional form S_T/S_{LO}, where the turbulent burning velocity $S_T = U \sin\gamma$ is determined from the average flame half cone angle γ and the mean inflow velocity U. The influence of the preferential diffusion of the hydrogen component is clearly visible.

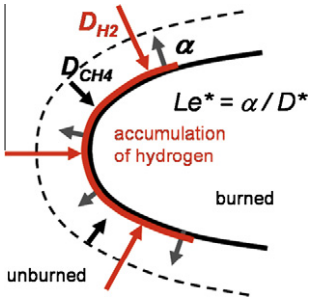

Fig. 6. Physical picture to derive an effective Lewis number for lean fuel mixtures. The weighted average of the fuel diffusivities leads to the effective Lewis number. The positively curved flamelet is assumed to be dominant for the overall reaction rate. Situation is shown for $Le^* < 1$.

4.2. Verification with highly turbulent methane/hydrogen flames

The above developed effective Lewis number approach is applied to the high-turbulence flame data obtained at 5 bar on the PSI burner. It is interesting to test the applicability of these above modified reaction models for this configuration at much higher turbulence intensity and size. Here, experimental data are available for methane/hydrogen mixtures with hydrogen additions from 0% to 40% by volume. For the model C, the resulting effective Lewis numbers are 0.566 and 0.498 for 30 and 40 vol.% of hydrogen content. In Fig. 9, the calculated flame lengths are compared with the corresponding experimental data.

The AFSW reaction rate closure with model C predicts the flame length accurately for the cases with hydrogen content up to 20%, while the model A (and the unity Lewis number approach) over predicts the flame length. For the flames with 30% and 40%

[2] We calculated the Lewis numbers of the pure fuels based on the binary diffusivity of the fuel within nitrogen at 25 °C and based on the thermal diffusivity of the unburned fuel air mixture of the corresponding stoichiometry. Both, fuel diffusivity and thermal diffusivity are known to depend strongly on temperature, however, in first order with the same power law. From that we expected no significant temperature dependency of the Lewis number. See also remark 3.

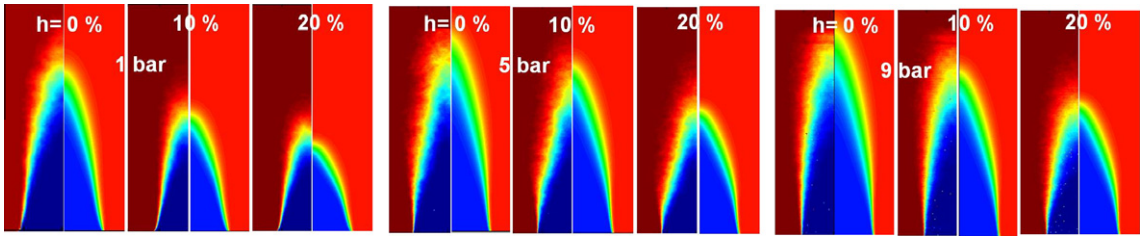

Fig. 7. Orléans Bunsen flames. Comparison between experiment (left) [27], and simulation (right) with the AFSW model and the proposed new model C for the effective Lewis number. Shown are contours of Reynolds averaged progress variable $\tilde{c}$ (between 0 and 1) for methane/hydrogen flames with 0, 10, 20 vol.% hydrogen for 0.1, 0.5 and 0.9 MPa ($\phi = 0.6$).

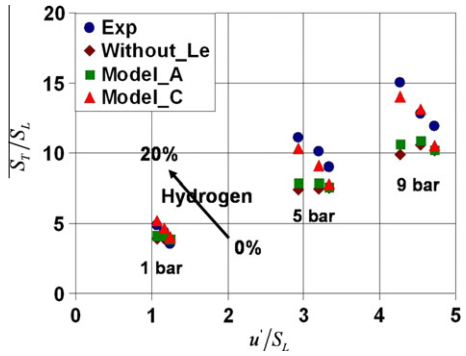

Fig. 8. Orléans Bunsen flames. Comparison of normalised turbulent burning velocity for 0, 10, 20 vol.% hydrogen in methane, for 0.1, 0.5 and 0.9 MPa. Calculations with the modified AFSW approach are shown without and with effective Lewis numbers according to the models A and C ($\phi = 0.6$).

hydrogen content, also the model C begins to show deviations. However, its predictions are comparatively better than that of the other models here, and still show the right trend.[3] In Fig. 10 the flame contours are shown for the cases with pure methane and with 40% hydrogen. The comparison between the experiments and the calculated cases shows that even for the 40% hydrogen case the model C still gives sufficiently good results, while the calculation with model A fails here.

4.3. Discussion

A simple physical picture allows the derivation of an extended reaction rate model for lean methane/hydrogen/air flames. It includes effects of pressure up to 0.9 MPa and it is shown to work well for two sets of experiments with rather different turbulence conditions and Reynolds numbers.

The physical model is based on the assumption that the positively curved flame elements on the leading side of the turbulent flame brush contribute much more to the average reaction rate than the mostly negatively curved flame elements on the rear side of the flame brush. This assumption can explains potentially not only the earlier found explicit dependency of the average reaction rate from the Lewis number (Eq. (3)), but it leads directly to a new proposed effective Lewis number for the mixture of two fuels with different individual Lewis number. Here, it is proposed, to base the effective Lewis number on an effective diffusivity of the two fuels, which is modelled as the weighted average of the individual fuel diffusivities. This simple model works surprisingly well for a large part of the flame conditions where experimental data is available. We see this as a potential confirmation of the mentioned assumption that the leading side of the flame brush contributes more to the reaction rate than the rear side.

It should be mentioned again: if the averaging of the local reaction rates would be done over the total flame brush then the influence of the Lewis number should be nearly zero, as the curvature distribution is typically symmetric for highly turbulent flames and as the expected Lewis number influence is opposite for the positively and negatively curved flame elements (at least, as long a linear relation between curvature and local reaction rate is assumed).

Note, that it was not the aim of the presented study, to develop a fully predictive model for all kind of mixtures and stoichiometries. Instead we wanted to see, how far the rather simple physical idea of preferential diffusion in conjunction with a newly proposed effective Lewis number works.

From this studies we conclude that the limit of our simple model is reached at about 20% or 30% hydrogen added to methane. It is likely that for increased amount of hydrogen other physical and potentially also chemical effects take place additional, being beyond the discussed preferential diffusion processes.

Also it has to be hold in mind that the model is validated for lean mixtures, where experimental data is available. These conditions are of most importance for lean premixed gas turbine combustion. Stoichiometric and fuel rich mixtures have not been investigated. It would be of interest, if here also such simple diffusional models are dominant or if other issues like chemical reaction modifications for turbulent flames are more important.

4.4. Additional remarks

1. After finishing our study we learned that Kröner [28], found independently a similar relation (5) for an effective Lewis number. It enabled him and his co-workers to explain their experiments of flame propagation and flashback in highly turbulent swirling methane/hydrogen/air flames. We see this as a confirmation of the theoretical idea of the importance of the positively curved flame elements for turbulent flame propagation, where the effective diffusivities lead to an effective Lewis number.

2. As mentioned shortly at the end of the introduction, the common understanding of turbulent wrinkled premixed flames assumes the effects of curvature as well as of strain. The paper here discusses only the effects of curvature. Some numerical DNS studies investigated the separate effects of curvature or strain. It is likely, that both are of importance. For instance a recent DNS study [12] finds significant preferential alignment effects of the local flame front with the locally strained flow field and can relate this also to a significant Lewis number influence (although with

[3] After finalizing our calculations one reviewer pointed out that the temperature dependency of hydrogen is not neglectable (leading to a Lewis number of around 0.20 for pure hydrogen for 1600 K, instead of 0.29 we used). Indeed the determination of the transport properties with the temperature near the main radical reaction zone would describe the physical transport processes near the main reaction zone more closely. The effective Lewis number for our cases with 30% or 40% hydrogen would decrease by about 25% and 30%. With that the mean reaction rate and the expected turbulent flame speed would increase correspondingly. Eventually even these cases would be well described with our proposed model (see Fig. 9b).

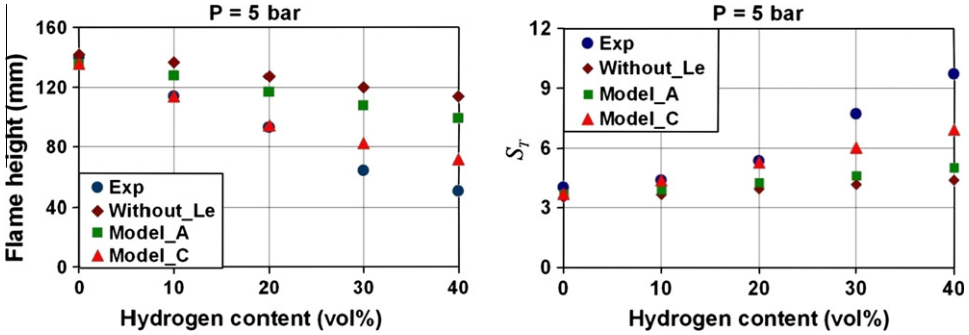

Fig. 9. PSI flames: Comparison of flame height and turbulent burning velocity between experimental and simulated flames for 0, 10, 20, 30 and 40 vol.% of hydrogen at 0.5 MPa (ϕ = 0.5, preheated to 673 K). Flame length and turbulent burning velocity S_T are determined based on the axial position with $\bar{c} = 0.5$. Simulations are obtained using the AFSW reaction closure in combination with an effective Lewis number according to models A and C.

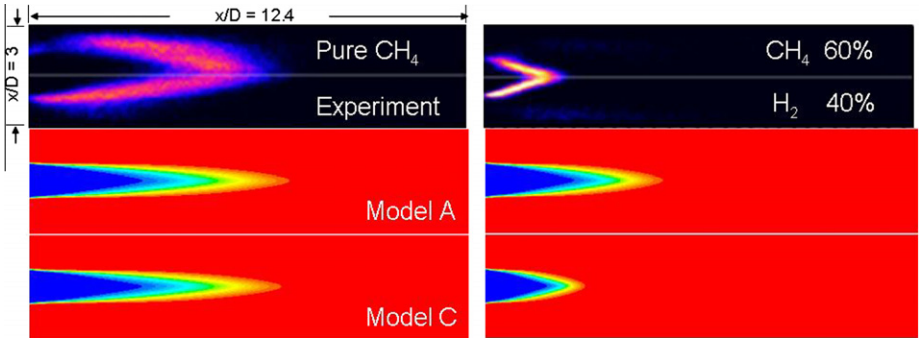

Fig. 10. PSI flames. Shown are experimental [16] and simulated flame heights for pure CH_4 and (40% H_2 + 60% CH_4), for 0.5 MPa and ϕ of 0.5. The AFSW model is modified with model A and model C for the effective Lewis number. For the experimental cases (upper figure) the probability density of the reaction zone is shown qualitatively, indicating the average flame position. The calculated cases (two lower figures) are shown with contour levels of the reaction progress variable $0 \leqslant \tilde{c} \leqslant 1$.

lower turbulent Reynolds number and only a single step reaction). It is likely, that such alignment effects can be seen as an alternative way to explain explicit Lewis number influences even in highly turbulent premixed flames.

3. If our assumption of the dominance of the leading side of the flame brush for the averaged reaction is correct, this should have implications also on other approaches to model turbulent premixed combustion. Eventually this can be of importance also for Markstein number models, where the local reaction rate (local laminar flame speed) is assumed to be a linear relation of positive or negative curvature. The Markstein number should cancel out during the averaging procedure, as long as the positively and negatively curved flame elements are equally weighted. Only if the leading side with mostly positive curvature is more dominant, also in the averaged reaction rate the Markstein number of curvature should be able to remain. We are not aware, if this aspect has been regarded in the past.

5. Conclusion

Previous investigations on reaction modelling of lean turbulent premixed flames with varied fuels and pressure had shown a significant Lewis number influence even for high turbulence intensity. This was insofar against the expectation, as this indicates the strong influence of molecular diffusion processes, while commonly turbulent diffusion is thought to be relevant for highly turbulent conditions instead. A simple physical picture allows an explanation, if it is assumed that essentially the leading part of the wrinkled flame front determines the flame propagation and thus the average reaction rate, while the rear part of the flame has the functionality to be only a burnout zone. Following this argumentation, mostly positively curved flame elements determine the flame propagation and the average reaction rate. Here indeed the effect of molecular diffusion of heat and reactants on the curved flame elements (and with that the Lewis number) are important.

In addition, this simple picture leads to a new proposal for an effective Lewis number for lean methane/hydrogen fuel mixtures, being based on the weighted average of both fuel diffusivities. The applicability of this approach has been tested within an extension of our recently developed RANS reaction model, based on an Algebraic Flame Surface Wrinkling approach (AFSW model).

Two different sets of experimental data have been used to determine the applicability as well as the limit of this concept. Bunsen flames investigated at CNRS Orléans with systematic variation of the hydrogen content up to 20% in lean methane/air flames and with varied pressure up to 0.9 MPa at moderate high turbulence intensity were used to compare three different approaches with effective Lewis numbers. Only the above mentioned approach agreed to the measurement series.

This result was also validated for the flame experiments on the pressurized dump combustor of the Paul-Scherrer-Institute in Baden (Switzerland) at 0.5 MPa where the turbulence intensity is much higher and where again the hydrogen content is varied. Even here, our RANS reaction model in conjunction with the newly defined effective Lewis number worked well for hydrogen concentrations of the fuel up to 20%. For hydrogen concentration of 30% and 40% smaller deviations were observed, which eventually can be even reduced if the transport properties would be determined for the inner layer temperature conditions (see Footnote 3). Beyond this, the limit of the rather simple approach based on diffusional transport seems to be reached. Possibly more complex physico-chemical effects would be needed to model flames with higher amount of hydrogen.

Besides the modelling results within the frame of our special RANS reaction model we see the following more general points:

Firstly, the importance of molecular transport effects even for highly turbulent premixed flames is supported.

Secondly, a new definition of an effective Lewis number for lean fuel mixtures is proposed.

Thirdly, we expect that also for other modelling approaches the concept of the dominance of the leading side of the flame brush (and the lower importance of the rear side) could be significant. Eventually this holds even for models based on Markstein number approaches which would be interesting to investigate.

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