

Real gas effects in hydrogen/oxygen counterflow diffusion flames

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Abstract

Within this work, the influence of real gas effects on counterflow diffusion flames is characterized. Therefore, the Combustion Simulation Laboratory COSILAB [1] has been extended by real gas relations based on the volume-corrected Peng-Robinson equation of state along with an appropriate modeling of the transport properties. The results indicate that the impact of the real fluid treatment on the local flame structure is limited, although strong property variations take place in the transcritical regime. However, if differential diffusion processes are taken into account, a considerable increase in the flame thickness and a shift of the flame zone towards the oxygen inlet can be detected.

1. Introduction

Modern high performance rocket combustion engines like the first stage engine of the Ariane 5, Vulcain II, are run at high pressures up to 10 MPa while the propellants, usually hydrogen and oxygen, are injected at very low temperatures. For hydrogen, pressure and temperature in the combustion chamber are supercritical, whereas for oxygen, only the pressure is above its critical value. The injection temperature, however, is often significantly below the critical temperature of oxygen ($T_{crit, O_2} = 154.6 \text{ K}$). Under such conditions the mean free path between the molecules in the fluid becomes small enough to allow molecular interactions to become important. This leads to significant deviations from the ideal gas assumption, which entirely neglects intermolecular attraction and repulsion effects. Due to this reason, proper real gas relations for thermodynamic and transport properties as well as for the combustion model need to be incorporated into a CFD simulation.

A very common method in modeling turbulent combustion is the flamelet approach developed by Peters [2]. A counterflow diffusion flame serves as a basis for this combustion model. This configuration is therefore analyzed in here. Particular emphasis is placed on transcritical conditions which are typically encountered in rocket thrust chambers. Due to the one-dimensional character of the counterflow configuration, the resulting flame structures and extinction rates can be assessed without much effort and detailed chemical kinetics can be considered decoupled from the flow field.

Several analyses of counterflow diffusion flames have been performed focusing on low as well as on high pressure conditions. Urzica *et al.* [3] for example investigated laminar flame structures of different methane combinations at both, atmospheric and high pressures. It was found that the pressure as well as the strain rate have a significant effect on flame structure and flame extinction. Pressure effects on non-premixed strained flames were also analyzed by Pons *et al.* [4] who confirmed that the flame thickness is inversely proportional to the square root of pressure. Balakrishnan *et al.* [5] examined flame structures, extinction and ignition limits for H_2 /Air flames at pressures from 0.25 – 10 atm for detailed and reduced reaction mechanisms. Especially thermal diffusion was found to be an important effect for these propellants. Transcritical injection conditions for oxygen/methane flames were studied by Pons *et al.* [6] using the Peng-Robinson equation of state. A modified Soave-Redlich-Kwong equation of state and consistent real gas thermodynamics have been applied by Ribert *et al.* [7] and Kim *et al.* [9]. Ribert *et al.* examined H_2/O_2 diffusion flames in physical space for subcritical and supercritical environments. Significant real effects due to steep property variations were found in the transcritical regime. The resulting influence on the flame structure, however, seems to be limited since the oxygen heats up very rapidly and behaves like an ideal gas when entering the flame zone. Kim *et al.*

in contrast used the flamelet equations formulated in mixture fraction space. Among other things, his study focused on the impact of differential diffusion effects at supercritical pressures.

Within the present study, the influence of real gas effects on the local structure of H_2/O_2 counterflow diffusion flames is investigated at supercritical pressures and very low propellant temperatures. For this purpose, the combustion simulation laboratory COSILAB [1] is extended by implementing general-fluid thermodynamic and transport theories.

2. Theoretical formulation

The physical configuration employed within this study is the axisymmetric counterflow flame shown schematically in figure 1. Two opposing jets of fuel and oxidizer create a stagnation plane with a laminar diffusion flame stabilized at the location of stoichiometric mixture fraction. To ensure a reliable prediction of the flame behavior over the entire regime of thermodynamic states, the basic governing equations are extended by a real gas equation of state with appropriate thermodynamic relations and property evaluation schemes.

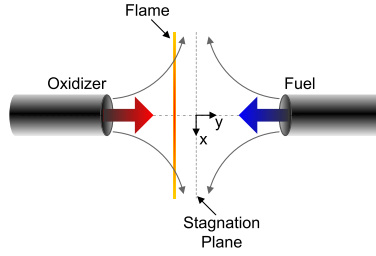


Figure 1: A schematic view of a counterflow diffusion flame configuration.

2.1 Governing equations

Along the axis of symmetry, the one-dimensional balance equations for mass [Eq. 1], radial momentum [Eq. 2], species mass fraction [Eq. 3] and energy [Eq. 4] which are solved by COSILAB are given in physical coordinates x, y as [1] :

$$\frac{\partial \rho}{\partial t} = -\frac{\partial(\rho v)}{\partial y} - 2\rho G \quad (1)$$

$$\rho \frac{\partial G}{\partial t} = \frac{\partial}{\partial y} \left(\mu \frac{\partial G}{\partial y} \right) - \rho v \frac{\partial G}{\partial y} - \rho G^2 + \rho_{+\infty} a_s^2 \quad (2)$$

$$\rho \frac{\partial Y_i}{\partial t} = -\rho v \frac{\partial Y_i}{\partial y} - \frac{\partial}{\partial y} (\rho V_i Y_i) + \dot{\omega}_i \quad (3)$$

$$\rho c_p \frac{\partial T}{\partial t} = \frac{\partial}{\partial y} \left(\lambda \frac{\partial T}{\partial y} \right) - \rho v c_p \frac{\partial T}{\partial y} - \rho \sum_{i=1}^I Y_i V_i \frac{\partial h_i}{\partial y} - \sum_{i=1}^I h_i \dot{\omega}_i \quad (4)$$

Here, the quantity G is defined as $G = u/x$ with the velocity components u, v in x and y direction, respectively. $a_s [s^{-1}]$ is the prescribed, constant strainrate which can be used to generate all flow conditions from the nearly strain free case up to flame extinction. ρ, T, μ and λ are the mixture density, temperature, dynamic viscosity and thermal conductivity whereas Y_i denotes the species mass fractions. The evaluation of the species partial specific enthalpy h_i and the mixture heat capacity c_p is described in section 2.2 below. $\dot{\omega}_i$ is the net mass rate of production of the i^{th} species.

The species diffusion velocity V_i is composed of three parts, the ordinary diffusion velocity V_i^D , the thermal diffusion velocity V_i^T , considered for light species H and H_2 , and a correction velocity V_c [1]:

$$V_i = V_i^D + V_i^T + V_c = -\frac{D_{i,m}}{X_i} \frac{\partial X_i}{\partial y} - \frac{D_{i,m}}{X_i} \frac{\theta_i}{T} \frac{\partial T}{\partial y} + V_c \quad (5)$$

X_i denotes the species mole fractions, $D_{i,m}$ the mixture averaged diffusion coefficient and thermal diffusion ratio θ_i is calculated according to Chapman and Cowling [8] as given in reference [18].

2.2 Thermodynamic properties and equation of state

The thermodynamic properties such as the species partial specific enthalpy can be calculated from the chemical potential μ_i as follows:

$$h_i(T, p, X_i) = -\frac{T^2}{M_i} \left(\frac{\partial (\mu_i/T)}{\partial T} \right)_{p, X_i} \quad (6)$$

Here, μ_i is defined as $\mu_i(T, p, X_i) = G_{0i}^0(T) + R_m T \ln(p/p_0) + R_m T \ln(x_i \varphi_i)$, where G_{0i}^0 is the ideal gas Gibbs free enthalpy of the i^{th} species at reference pressure and φ_i is the fugacity coefficient.

The internal energy as well as the constant pressure specific heat capacity are calculated as the sum of an ideal reference value and a departure function accounting for real gas effects.

$$c_p(T, V_m) = c_v(T, V_m) - T \left(\frac{\partial p}{\partial T} \right)_{V_m}^2 / \left(\frac{\partial p}{\partial V_m} \right)_T \quad (7)$$

The constant volume specific heat capacity is defined as $c_v(T, V_m) = (\partial u / \partial T)_{V_m}$ and the internal energy is derived from

$$u(T, V_m) = u_0(T) + \int_{V_m}^{V_\infty} \left[p - T \left(\frac{\partial p}{\partial T} \right)_{V_m} \right] dV_m \quad (8)$$

Here, the subscript 0 refers to the ideal reference state at low pressure which is evaluated from the NASA polynomials [10]. The departure functions on the right hand side of [Eq. 7, 8] have to be determined using an appropriate equation of state (EOS). As the Peng-Robinson (PR) equation [Eq. 9] [11] is known to be not very accurate in predicting the density in transcritical regions, an additional volume-correction method established by Harstad *et al.* [12] has been applied within the present work.

$$p = \frac{RT}{(V_m - b)} - \frac{a(T)}{V_m^2 + 2V_m b - b^2} \quad (9)$$

Here, V_m is the molar volume and $R = 8.314472 \text{ J/(molK)}$ the universal gas constant. The constants $a(T)$ and b are calculated from empirical relations. $a(T)$ accounts for attractive forces between the molecules in the fluid and is defined as $a(T) = a_0 \cdot \alpha(T)$. The constant a_0 is calculated from the relation $a_0 = 0.457235 R^2 T_c^2 / p_c$ and the temperature dependent function is given by

$$\alpha(T) = \left(1 + \gamma \left(1 - \sqrt{T/T_c} \right) \right)^2 \quad (10)$$

where $\gamma = 0.37464 + 1.54226\omega - 0.26992\omega^2$ is a function of the acentric factor ω . The effects of the reduction of the free volume by the particular volume of the molecules is taken into account by $b = 0.077796 R T_c / p_c$. For the critical points of all substances, the values published by Ribert *et al.* [7] have been applied. They are summarized in table 1.

Table 1: Critical points of all species occurring during the combustion of H_2 and O_2 [7].

	H_2	O_2	H	O	OH	HO_2	H_2O	H_2O_2
T_c [K]	33.2	154.6	404.3	367.4	443.7	487.3	647.3	544.3
p_c [bar]	13	50.4	88.2	76	85.4	82.8	221.2	93.5

Real gas phenomena also have to be considered in the mixing process of pure components. For this purpose, an extended corresponding states principle has been applied in the present study. The multi-component mixture is assumed to behave like a pure real gas component but with coefficients a , b in the EOS modified appropriately through mixing rules. The mixture properties are also calculated using the PR equation of state with parameters calculated from real gas mixing rules. Here, the van der Waals mixing rules [Eq. 11] [13] have been applied. The binary interaction parameters k_{ij} are set to zero as there were no values available.

$$a = \sum_i \sum_j X_i X_j \sqrt{a_i a_j} (1 - k_{ij}) \quad , \quad b = \sum_i X_i b_i \quad (11)$$

A comprehensive validation of the real gas relations summarized above has been performed by Poschner [14], [15] in previous work.

2.3 Transport properties

Close to the critical point, small changes of state evoke strong variations of the transport properties such that quantities like the thermal conductivity and the dynamic viscosity experience steep gradients. Due to this reason, an accurate evaluation of the transport properties for both, the pure components and the mixture is of vital importance for a reliable prediction of real gas flows. Within this work, the dynamic viscosity η as well as the thermal conductivity λ are estimated based on an approach established by Chung [16]. It calculates the dynamic viscosity for dilute gases η_0 from

$$\eta_0 = (4.0785 \cdot 10^{-5}) \frac{(MT)^{1/2}}{V_c^{2/3} \Omega^*} F_c \quad (12)$$

where V_c is the critical molar volume, T the temperature and M the molecular weight. The correction factor F_c accounts for the polyatomic molecular structure of the fluid while Ω^* is the reduced collision integral. For dense fluids, equation [Eq. 12] is extended to the correlation [Eq. 13] including the effects of temperature (index k) and pressure (index p)

$$\eta = \eta_k + \eta_p \quad (13)$$

with $\eta_p = 36.344 \cdot 10^{-6} (MT_c)^{1/2} / V_c^{2/3} A_7 y^2 G_2 \exp(A_8 + A_9/T^* + A_{10}/T^{*2})$ and $\eta_k = \eta_0 [1/G_2 + A_6 y]$. This model has been validated for pressures up to 3447 bar and temperatures ranging from 70 K to 973 K. All parameters which are not explicitly given here are calculated as described in reference [16].

Similarly to the dynamic viscosity, the thermal conductivity for dense fluids is evaluated from

$$\lambda = \lambda_k + \lambda_p \quad (14)$$

where the temperature effects are taken into account by $\lambda_k = \lambda_0 [1/H_2 + B_6 y]$ and the pressure effects are given as $\lambda_p = [3.039 \cdot 10^{-4} (T_c/M)^{1/2} / V_c^{2/3}] B_7 y^2 H_2 T_r^{1/2}$. T_c denotes the critical and T_r the reduced temperature. The thermal conductivity for dilute gases λ_0 is estimated from equation [Eq. 15] with the correlation Ψ as given by Chung [16]:

$$\lambda_0 = 7.452 \frac{\eta_0}{M} \Psi \quad (15)$$

This method has been validated for pressures up to 1247 bar and temperatures from 80 K to 973 K. For both properties, the appropriate mixing rules recommended by Chung *et al.* [16] have been applied.

For the binary diffusion coefficients, the approach proposed by Fuller [17] is used as given in reference [13].

$$D_{ij} = \frac{0.00143 T^{1.75}}{p M_{ij}^{1/2} [(\sum_v)_i^{1/3} + (\sum_v)_j^{1/3}]^2} \quad (16)$$

Here, M_{ij} can be calculated from $M_{ij} = 2 / [(1/M_i) + (1/M_j)]$ and $\sum_v$ is the sum of the atomic diffusion volumes for each component. The mixture averaged diffusion coefficient of one component into the mixture is estimated using Bird's law given in reference [18]. To circumvent mathematical difficulties in the limit of the mixture becoming a pure species, equation [Eq. 17] is applied along with adding a small number $\delta = 10^{-12}$ to the actual species mole fraction. $\bar{M}$ denotes the mean molar mass of all species.

$$D_{i,m} = \frac{\sum_{j=1, j \neq i}^n (X_j M_j)}{\bar{M} \cdot \sum_{j=1, j \neq i}^n (X_j / D_{ij})} \quad (17)$$

Pressure effects are taken into account by an approach recommended by Takahashi [19]. Here, $(Dp)_R$ is the product of diffusion coefficient D and pressure p to its product at low pressures $(Dp)_R = (Dp)/(Dp)_0$. The index r indicates reduced quantities. Model uncertainties may arise when the mixture temperature is smaller than unity [7].

$$\frac{(Dp)_R}{(Dp)_{R,l}} = f(T_r, p_r) \quad (18)$$

Species diffusion caused by a temperature gradient (Soret-effect) is taken into account as described in reference [1] and [18] for the light species H and H_2 . Again, θ_i denotes the thermal diffusion ratio which is given in Chapman and Cowling [8]. Heat diffusion due to concentration gradients (Dufour-effect), however, is neglected in this study.

$$D_i^T = \rho \frac{Y_i}{X_i} D_{i,m} \theta_i \quad (19)$$

2.4 Boundary conditions and numerical method

The general boundary conditions which are applied in COSILAB for a counterflow diffusion flame problem formulated in a stagnation point flow are listed in table 2 [1]. The stagnation plane is defined by $v_{y=0} = 0$.

Table 2: Boundary conditions used in COSILAB [1].

Boundary	G/a_s	T	Y
$y = -\infty$	$(\rho_{+\infty}/\rho_{-\infty})^{1/2}$	$T_{-\infty}$	$Y_{-\infty}$
$y = +\infty$	1	$T_{+\infty}$	$Y_{+\infty}$

The governing equations presented in section 2.1, subject to the above boundary conditions, are discretized on a mesh of grid points, and the resulting system of nonlinear equations is then solved by an optimized, mixed transient-steady Newton's method to arrive at a steady-state solution. In particular, in applying Newton's method a damping strategy is employed which allows the Jacobians to be re-evaluated only periodically. To resolve the local gradients of the dependent variables accurately, self-adaptive gridding is implemented into the numerical procedure. For a more detailed description of the numerical method, ref. [1] should be consulted.

3. Results and Discussion

Based on the numerical framework established above, this study analyzes the influence of modeling real fluids, differential and thermal diffusion as well as the effect of pressure on the detailed structure of H_2/O_2 counterflow diffusion flames for trans- and supercritical thermodynamic states. As this work is performed in the scope of the development of a real gas laminar flamelet combustion model for the application within CFD simulations, special emphasis is placed on calculations with the conditions used for the RCM-3 test case from the Mascotte test rig V03 operated at ONERA [20], [21]. With a temperature of $T_{H_2} = 287\text{ K}$ and at a combustion chamber pressure of $p = 60\text{ bar}$, hydrogen is injected here at a supercritical state. The state of oxygen, however, is transcritical due to an injection temperature of $T_{O_2} = 85\text{ K}$.

The presentation of the results is subdivided into three parts. First, the validation of the real gas treatment is reviewed for the thermodynamic and transport properties of pure oxygen. Secondly, the detailed structure of the counterflow diffusion flame is investigated for typical rocket combustion conditions. Especially, differential diffusion effects and their impact on the flame structure are examined. The pressure influence as well as the influence of thermal diffusion is finally assessed for the real fluid approach in the last section.

3.1 Validation of thermodynamic and transport properties

An accurate modeling of the thermodynamic and transport properties is crucial for a reliable prediction of real gas flows. It provides the basis for analyzing the detailed structure of the counterflow diffusion flame. The real gas formulations outlined above for the thermodynamic and transport properties have already been validated against NIST data [22] as published in previous work performed by Poschner [14], [14]. The main results for pure oxygen are reviewed again in figures 2 and 3 for the supercritical pressures 60 bar and 100 bar . However, the injection of hydrogen into the rocket combustion chamber typically occurs at pressures and temperatures which are above their critical values and thus at a supercritical state. Comparing the ideal and the real gas thermophysical properties of hydrogen at these conditions, only small differences were found [14]. The validation of the hydrogen properties is therefore not included here.

For the calculation of the oxygen density, the Peng-Robinson EOS with volume correction fits the NIST data very well. Particularly the application of the volume correction prevents the over-prediction for subcritical temperatures $T < T_{crit, O_2} = 154.6\text{ K}$ which has been encountered for the simple Peng-Robinson equation [14]. The ideal gas EOS, however, is not able to predict the transition from transcritical to supercritical conditions correctly. At the injection temperature of oxygen $T_{O_2} = 85\text{ K}$ the density is underestimated by a factor of about 4 and 2.5 for the 60 bar and the 100 bar case, respectively. Likewise, the Peng-Robinson EOS predicts the heat capacity at constant pressure c_p sufficiently well. By default, c_p is evaluated from the NASA polynomials [10] for the ideal gas approach. Since these polynomials only depend on the temperature, the pressure influence cannot be captured here.

The validation of the transport properties is shown in figure 3. Here, Chung's formulation for dense fluids is used for the real gas approach [Eq. 13, 14] while his correlation for dilute gases is applied for the ideal gas assumption [Eq. 12, 15]. Of course, the pressure influence cannot be reproduced by the ideal gas approach, neither for the dynamic

viscosity nor for the thermal conductivity. For the real gas model, the effects of pressure as well as the transition from sub- to supercritical temperatures is predicted in close agreement to the NIST [22] data.

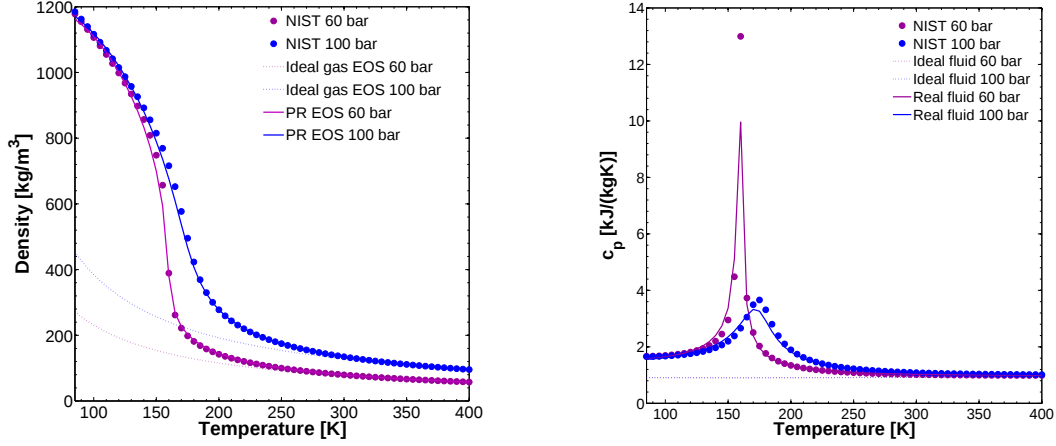


Figure 2: Validation of predicted thermodynamic properties against NIST data [22] for supercritical pressures.

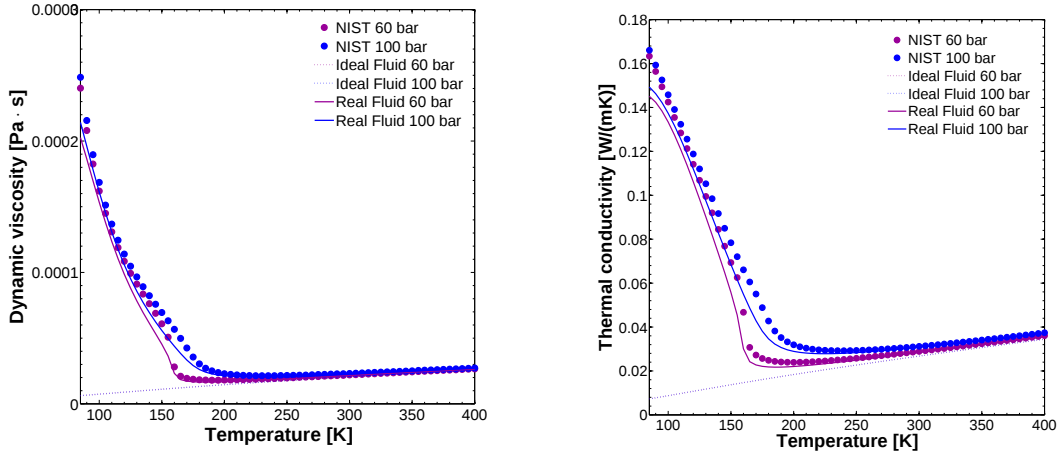


Figure 3: Validation of predicted transport properties against NIST data [22] for supercritical pressures.

3.2 Structures of counterflow diffusion flames

In order to analyze the influence of real fluid modeling on the local structure of hydrogen/oxygen counterflow diffusion flames, the reaction mechanism developed by Ó Conaire [23] is employed. It contains the 8 reacting species H , H_2 , O , O_2 , OH , H_2O , HO_2 and H_2O_2 with 19 reversible reactions. The validation against experimental data has been performed successfully for temperatures ranging from 298 K to 2700 K and pressures from 0.05 – 87 atm [23]. The influence of applying different detailed reaction mechanisms was tested by Ribert [7]. As the results were found to be almost identical for all applied mechanisms, only the Ó Conaire mechanism is considered here.

Within the present work, the 4 different approaches listed in table 3 were used for a detailed analysis of the counterflow diffusion flames. The first of them use the ideal gas equation of state (EOS) along with an ideal treatment of thermophysical properties (*Ideal 1, 2*), whereas for the remaining two, the volume corrected Peng-Robinson EOS has been applied together with an appropriate modeling of thermodynamic and transport properties (*Real 1, 2*). In both cases, one simulation is carried out with unity Lewis number while the other includes differential diffusion effects. The Lewis number is defined as the ratio of thermal to mass diffusivity [Eq. 20]. The Soret-effect is considered only for the real fluid approach (*Real 2*) by applying equation [Eq. 19].

$$Le_i = \frac{\lambda}{\rho c_p D_i} \quad (20)$$

Table 3: Simulation settings used to analyze the counterflow diffusion flames.

Approach	Ideal 1	Ideal 2	Real 1	Real 2
EOS	ideal gas	ideal gas	vol. corr. PR	vol. corr. PR
c_p, h_i	NASA polynom.	NASA polynom.	real fluids: [Eq. 6, 7]	real fluids: [Eq. 6, 7]
λ, η	dilute gases: [Eq. 12, 15]	dilute gases: [Eq. 12, 15]	dense fluids: [Eq. 13, 14]	dense fluids: [Eq. 13, 14]
Le	1	Le_i	1	Le_i
$D_{i,j}$	$\lambda/(\rho c_p)$	Fuller [Eq. 16]	$\lambda/(\rho c_p)$	Fuller + p. corr. [Eq. 16, 18]
D_i^T	-	-	-	[Eq. 19]

The results are presented in figures 4 and 5 as function of the axial distance y [mm]. On the left hand side, the profiles resulting from the approaches *Ideal 1* and *Real 1* are given for a Lewis number equal to unity. On the right hand side, differential diffusion effects are considered (approaches *Ideal 2* and *Real 2*). The strain rate is set to 1000s^{-1} . As stated above, the pressure as well as the inlet temperature of fuel and oxidizer are set according to the Mascotte RCM-3 test conditions with $p = 60\text{bar}$, $T_{H_2} = 287\text{K}$ and $T_{O_2} = 85\text{K}$. All diagrams are based on the stagnation point ($v_{y=0} = 0$) as the common reference position.

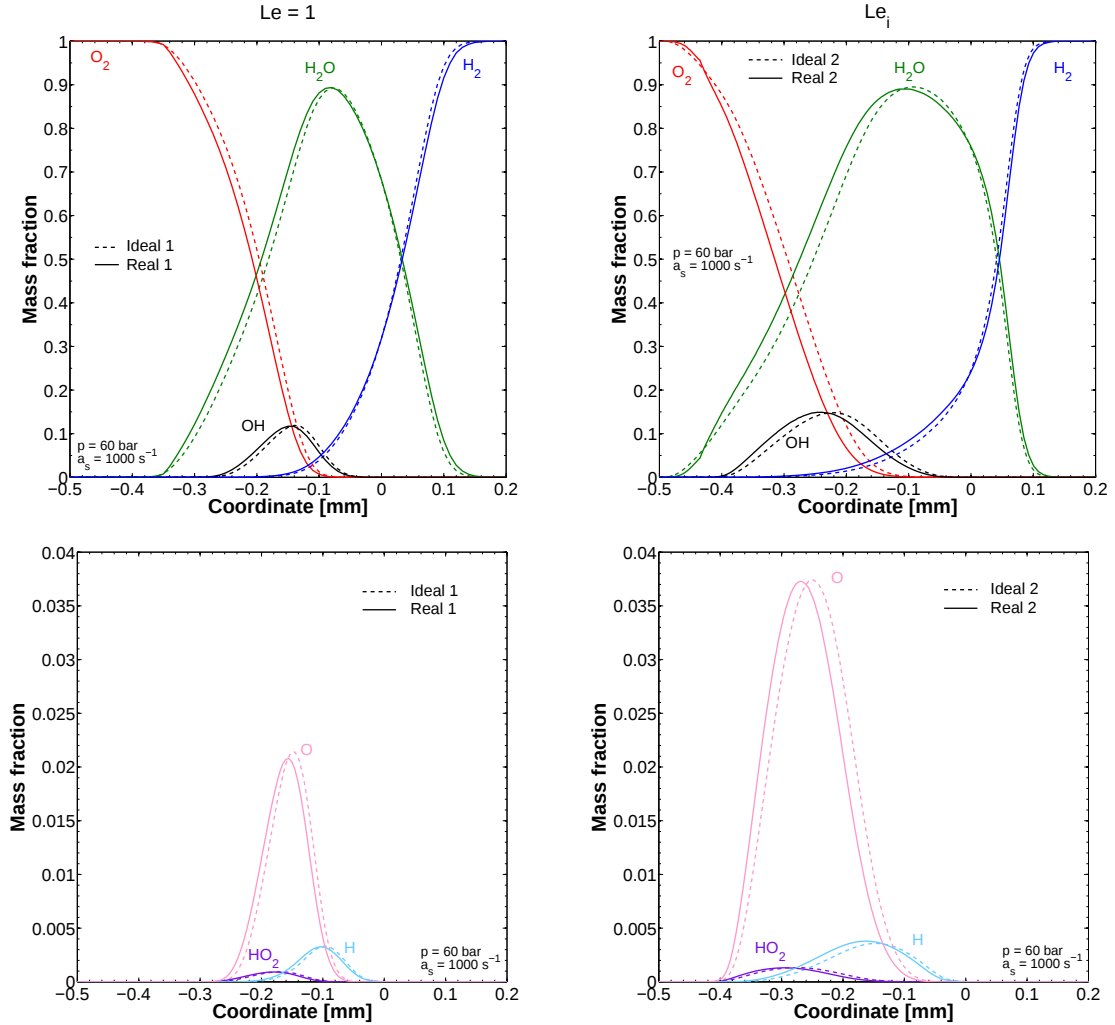


Figure 4: Distribution of major (top) and minor species mass fraction (below) for the settings listed in table 3.

Comparing the ideal and the real treatment for the unity Lewis number approach first (figure 4, 5 left), only small differences are found for the species mass fractions and the temperature distribution. As expected from the analysis of the oxygen thermodynamic properties above (figure 2), the oxygen density is highly underestimated applying an ideal gas equation of state. The diffusion coefficients calculated with equation [Eq. 20] and $Le = 1$ are identical for all species. They are shown for both approaches in figure 5 below. Due to the different modeling of thermodynamic and transport properties, the profile of the real gas diffusion coefficient (*Real 1*) is shifted slightly towards the oxygen side. Similarly, this causes the species mass fraction and temperature distribution also to move towards same side. However, the overall influence of the real gas treatment assuming a Lewis number of unity seems to be limited.

On the right hand side of figure 4 and 5, the same quantities are compared including differential diffusion effects. Here, the shift of species mass fraction and temperature distribution towards the oxygen inlet is much more evident than for the unity Lewis number cases. Larger deviations can also be detected for the density gradient and the temperature profile in the cold oxygen rich region. When the oxygen heats up, almost identical profiles are found for the density and the temperature distribution within the flame zone.

The major species Lewis numbers are presented in 5 below. Here, significant differences between the ideal and the real fluid approach can be found particularly close to the oxygen inlet. As a reason, the disability of the ideal gas approach (*Ideal 2*) to capture the steep gradients in the species' thermophysical properties during the transition from trans- to supercritical state can be identified. Also, the Lewis number of hydrogen is much smaller than unity, indicating that the mass diffusion is significantly enhanced over the thermal diffusivity. It varies only slightly around a value of 0.25 while the Lewis numbers of O_2 and H_2O change rapidly within the high temperature flame zone.

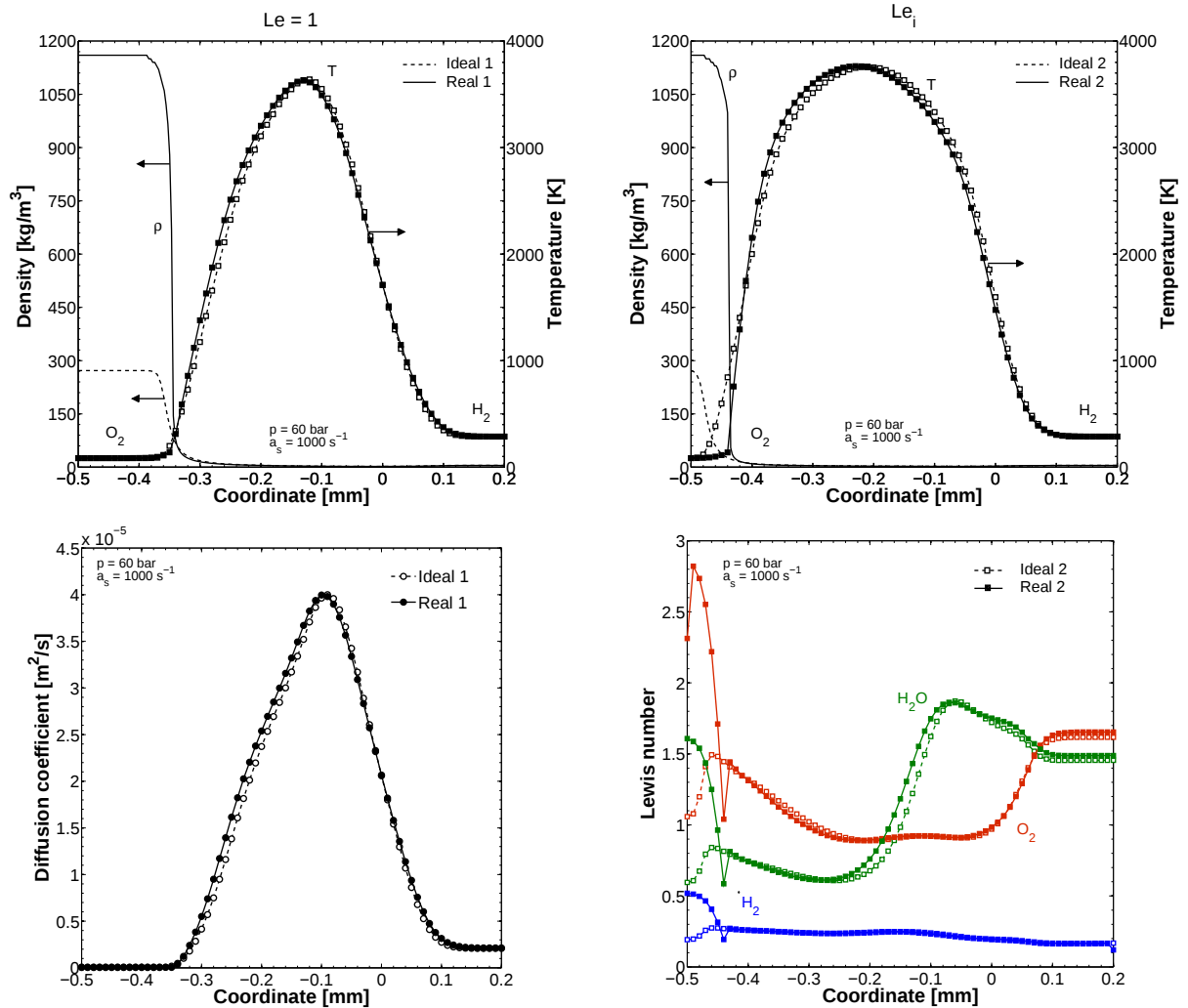


Figure 5: Density and temperature distribution (top) as well as diffusion coefficient and Lewis number (below).

Finally, the local flame structure resulting from the unity and the variable Lewis number method are compared to each other. Two major differences can be observed from the results: First, the flame thickness is increased significantly including differential diffusion effects. Defining the flame thickness according to Ribert [7] as the full width at half maximum of the temperature profile, values of 0.39 mm and 0.28 mm are calculated for the approaches *Real 1* and *Real 2*, respectively. This corresponds to an increase in flame thickness of about 40% based on the unity Lewis number approach. Also the maximum flame temperature is about 135 K higher for the *Real 2* calculation than for the *Real 1* one. Secondly, the profiles of all species mass fractions and especially those of the minor species ones are shifted considerably towards the oxygen inlet if differential diffusion is considered. This can be explained by the high diffusivity of hydrogen which causes more H_2 to diffuse towards the oxygen side and finally results in a shift of the flame zone and an increased flame thickness. The increase in the minor species maximum mass fraction results from the overall higher temperature predicted by applying differential diffusion processes.

3.3 Influence of thermal diffusion and pressure

As the mass diffusion caused by a temperature gradient, also referred to as thermal diffusion or Soret-effect, was found to be an important effect for propellants like hydrogen [5], it is examined in figure 6 below. Therefore, for the major species mass fractions, the density as well as the temperature profile are presented over the axial distance. The *Real 2* approach is used for this purpose with and without modeling thermal diffusion effects according to equation [Eq. 19].

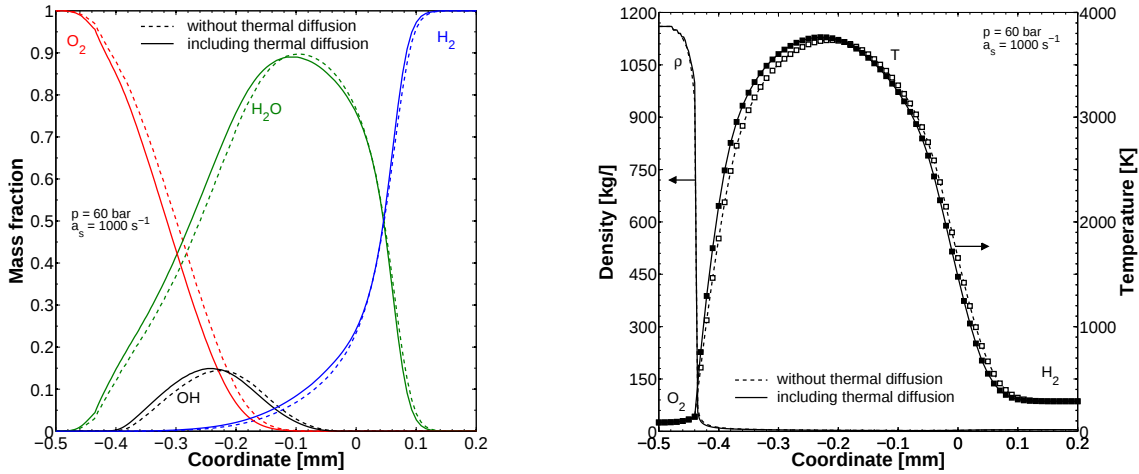


Figure 6: Influence of the thermal diffusion process on the major species mass fractions (left) as well as on the density and the temperature profile (right).

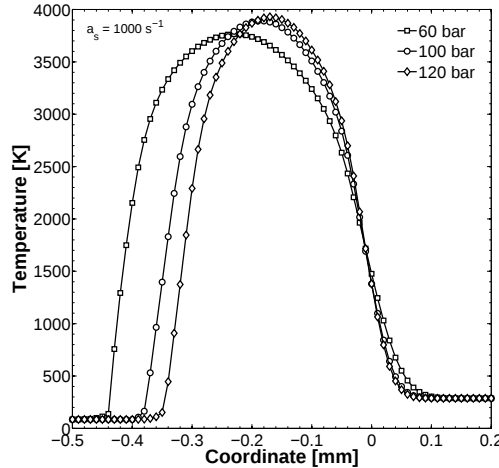


Figure 7: Temperature profiles for the H_2/O_2 counterflow diffusion flame at different supercritical pressures with *Real 2* modeling.

Generally, thermal diffusion causes light molecules to diffuse towards the hot temperature region whereas heavy molecules are driven into the opposite direction. Ribert [7] already observed that the influence of thermal diffusion is slightly enhanced on the oxygen rich side since hydrogen reacts rapidly with other species. This observation is also reflected in figure 6 where e.g. a moderate change of the O_2 mass fraction profile towards the cold oxygen inlet can be detected for the calculation including thermal diffusion. The maximum flame temperature is about 29 K higher for this case whereas almost no influence can be found for the flame thickness.

The local structure of the H_2/O_2 counterflow diffusion flame has also been analyzed for the supercritical pressures of 60 bar, 100 bar and 120 bar. The results are presented in figure 7. Again, the inlet temperatures of the propellants are set according to the Mascotte RCM-3 test case conditions with $T_{H_2} = 287\text{ K}$ and $T_{O_2} = 85\text{ K}$. The strain rate is fixed at $a_s = 1000\text{ s}^{-1}$. As numerical setting, the real fluid approach *Real 2* listed in table 3 is employed. With increasing pressure at constant strain rate, the flame is getting thinner and the maximum temperature is increased. Based on the 60 bar profile for example, the maximum flame temperature is about 128 K and 160 K higher for the 100 bar and the 120 bar case, respectively. These results are found to be consistent to observations from other researchers [3], [7].

4. Conclusion

Within the present work, the influence of real gas effects on the local structure of counterflow diffusion flames has been investigated. For this purpose, the combustion simulation laboratory COSILAB has been extended by real gas relations based on the volume-corrected Peng-Robinson equation of state along with an appropriate modeling of the thermodynamic and transport properties. Special emphasis is placed on calculations with the conditions used for the RCM-3 test case from the Mascotte test rig V03 operated at ONERA [20], [21]. Here, the inlet temperatures are $T_{H_2} = 287\text{ K}$ and $T_{O_2} = 85\text{ K}$ while the combustion chamber pressure is $p = 60\text{ bar}$. The results have been discussed for supercritical pressures in terms of applying a real fluid approach and using differential as well as thermal diffusion.

The real gas thermodynamic and transport theories have been validated successfully against NIST [22] experimental data at moderate and high pressures. In particular, the numerical framework established within this study was able to capture the steep property variations close to the critical point. Regarding the local structure of the counterflow diffusion flame, the species mass fraction profiles as well as the density and temperature distributions were found to be shifted towards the oxygen side when applying the real fluid modeling. Compared to the unity Lewis number calculations, this effect was enhanced when differential diffusion processes were included. The ideal gas equation of state failed in predicting the density of oxygen at the transcritical injections conditions correctly. As the oxygen heats up rapidly when entering the flame zone, the overall influence on the flame structure is limited. The greatest deviations were found comparing the unity and the variable Lewis number approach. Here, the profiles were shifted considerably towards the oxygen inlet due to the high diffusivity of hydrogen included in the calculations. For the case investigated, the flame thickness as well as the maximum flame temperature were increased, indicating that modeling differential diffusion processes affects the flame structure significantly. With increasing pressure, a decreasing flame thickness together with a higher maximum of the flame temperature was observed.

Based on the developed method, flamelet libraries including real gas effects can now be generated. For their application, the results have to be mapped into the mixture fraction space by solving an appropriate transport equation for a suitably defined mixture fraction. Finally, the flamelet library may be used along with the laminar flamelet combustion model.

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