Effects of Density Variations in Turbulent Diffusion Flames

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Most of industrial or natural gaseous flows involve density heterogeneities that may be responsible for specific physical mechanisms: local accelerations, instabilities, segregation processes, etc. To be accurate enough, models used for numerical simulations must take these mechanisms into account. Some of these physical processes are the consequence of the mass conservation law that imposes a direct correlation between density and the velocity field. Besides, in low Mach number flows, the density field may also be expressed from scalar quantities such as temperature and/or species mass fractions via the equation of state. Accordingly, such a velocity/scalar interaction leads to direct relationships between turbulent transport terms of scalars and momentum in turbulent flows. Therefore, the objective of this work is to introduce a simple strategy able to evidence these relationships, which may lead to closures for turbulent transport terms taking large density variations effects into account. The strategy presently developed holds for flows where the value of the density can be obtained through the knowledge of a unique scalar quantity. This quantity can be a passive scalar, as pertaining for mixing between two flows featuring different density. It can also be a reactive scalar, such as the progress variable often retained to characterize fully premixed combustion. The present study considers a situation that involves both phenomena: mixing and reactive processes, as encountered in diffusion flames.

1 A relevant scalar for variable density flows

Non reactive flows with variable density occur when several streams having different temperature or composition mix together. If only two streams are involved, temperature and composition can be both obtained through the use of a single normalized scalar, i.e. the mixture fraction ξ. The value of this mixture fraction is defined to be respectively unity and zero in each of the two stream considered. On the other hand, in the case of fully premixed combustion, a normalized reactive scalar is often introduced to represent the evolution of temperature and composition through the flame structure: the progress variable c. The value of this variable is respectively unity and zero in fully burnt gas and fresh reactants. Then, in both types of flows, non reactive and fully premixed reactive, the equation of state may be written:

$$\frac{1}{\rho} = \alpha + \beta f \qquad \text{with} \qquad \alpha = \frac{1}{\rho_{\max}} \qquad \text{and} \qquad \beta = \frac{1}{\rho_{\min}} - \frac{1}{\rho_{\max}}, \qquad (1)$$

where f denotes the normalized scalar ξ in the case of non reactive flows and the normalized scalar c in the case of fully premixed reactive flows. $\rho_{\max}$ and $\rho_{\min}$ are respectively the maximum and minimum values of density in the flow considered. Equation (1) can be also used for diffusion flames where the variable f is neither the mixture fraction ξ nor the progress variable c but the normalized specific volume $\mathcal{V}=1/\rho$: $f=(\mathcal{V} - \mathcal{V}_{\min})/(\mathcal{V}_{\min} - \mathcal{V}_{\max})$. The specific volume is indeed suitable to deal with non premixed flames since physical processes involve both phenomena: mixing and chemical reactions. Accordingly,

two scalar variables are required, one to represent the evolution of the mixing between the two streams, i.e fuel and oxidizer, and another one to represent the evolution of the chemical reactions. However, if chemical reactions are considered infinitely fast when compared to mixing processes, temperature and composition correspond to the chemical equilibrium whatever the level of mixing between fuel and oxidizer. Thus, this assumption allows to retain only the mixture fraction to represent both phenomena, mixing and chemical reactions. Nevertheless, as opposed to non reactive mixing, the specific volume $\mathcal{V}$ is no longer linearly related to the mixture fraction. The specific volume, temperature, density and mass fractions of chemical species can be obtained from chemical equilibrium calculation using for example the chemical software Cantera [1]. Figure (1) shows the chemical equilibrium profiles for the normalized temperature $T(\xi)$ and the normalized specific volume $f(\xi)$ along a modified mixture fraction $\chi = \xi^{(\log(0.5)/\log(\xi_{st}))}$ in order to obtain the stoichiometric conditions at $\chi = 0.5$ whatever the reactants under consideration. These profiles correspond to the structure of local diffusion flames
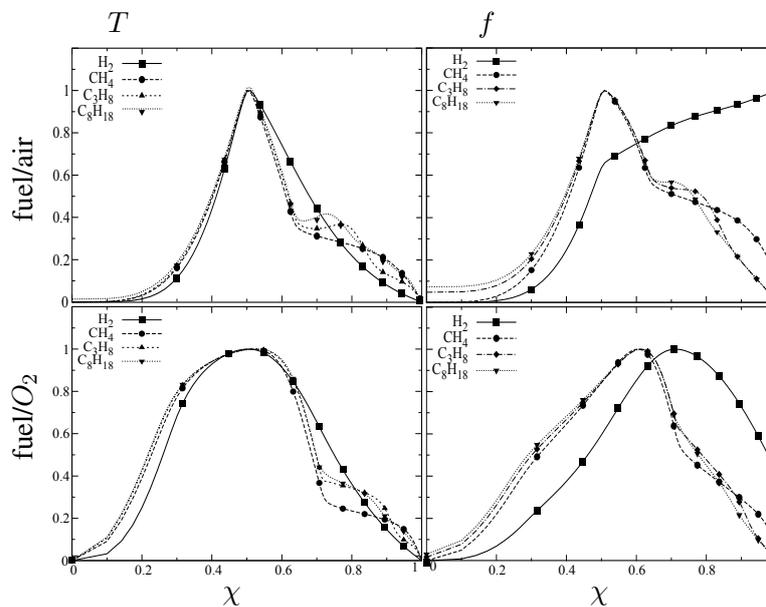

Figure 1: Chemical equilibrium profiles for normalized temperature $T(\xi)$ (left) and normalized specific volume $f(\xi)$ (right) through local fuel/air diffusion flame (top) and fuel/O_2 diffusion flame (bottom).

using four different fuels (hydrogen, methane, propane and octane) and two different oxidizers (air and pure oxygen). As expected, the temperature reaches a maximum value around stoichiometric conditions whatever the fuel and oxidizer considered. However, the normalized specific volume shows the same evolution only for hydrocarbon fuels burning with air. Thus, for these diffusion flames, the normalized temperature can be used to study the effects of density on the flow field. On the contrary, for hydrogen/air flames and fuels burning with pure oxygen, the normalized temperature evolution can differ significantly from the specific volume evolution. In the latter case, the maximum value of the specific volume does not correspond to stoichiometric conditions, as it is shifted towards the rich side. In the former case, this maximum corresponds to pure Hydrogen condition showing a monotonic evolution for the specific volume. Therefore, the normalized specific volume seems a more appropriate quantity than normalized temperature to study the effects of density variations on turbulent transports.

Eventually, whatever the reactants, $\mathcal{V}(\xi)$ is strongly non-linear so that the potential effects of density on the velocity field is conditioned by the values of the mixture fraction. These effects may be very important on the pure air side where the maximum value of the specific volume is reached for very low values of the mixture fraction: $\xi_{st} = 2.85\ 10^{-2}$ for hydrogen and $\xi_{st} = 5.52\ 10^{-2}$ for methane. Thus,

as our goal is to study these effects on turbulent transport phenomena, it seems more relevant to use the scalar variable f, which perfectly represents the evolution of density, rather than a scalar variable for which the definition is based on temperature or composition mass fractions.

An other advantage of the normalized specific volume is that it allows to rewrite easily correlations $\overline{\xi''}$ and $\overline{u''}$ which drives the influence of mean pressure terms in the transport equations for the Reynolds stresses $\overline{\rho u'' u''}$ and scalar turbulent fluxes $\overline{\rho u'' \xi''}$:

$$\overline{u''} = \overline{(\rho u''/\rho)} = \beta \overline{\rho} \widetilde{u'' f''}; \tag{2}$$

$$\overline{\xi''} = \overline{(\rho \xi''/\rho)} = \beta \overline{\rho} \widetilde{\xi'' f''}; \tag{3}$$

where β has been defined in Eq. (1). Equations (2) and (3) clearly show that $\overline{u''}$ and $\overline{\xi''}$ are nothing else than the turbulent scalar flux of f and the co-variance between f and ξ.

In the case of non reactive mixing, $f=\xi$, the relation proposed by Jones [2] is recovered: $\overline{u''}=\overline{\xi''}\widetilde{u''\xi''}/\widetilde{\xi''^2}$. Equations (2-3) are also fully consistent with well-known relations obtained for fully premixed combustion ($f = \xi = c$): $\overline{u''} = \tau(\overline{\rho}/\rho_r)\widetilde{u''c''}$ and $\overline{c''} = \tau(\overline{\rho}/\rho_r)\widetilde{c''^2}$.

Eventually the normalized specific volume is perfectly appropriate to study variable density flows. It can be used for both passive and reactive flows. Its evolution represents temperature variations as well as composition variations and is able to highlight specific combustion behavior: hydrogen-air flame or oxy-combustion. Furthermore, it allows to recover the well-known relation of Jones [2] as well as the useful expressions valid in fully premixed combustion.

2   Turbulent diffusion flame model

The turbulent flame brush considered here is made up of thin diffusion flamelets whose structure is obtained from chemical equilibrium calculations. Besides, the shape of the mixture fraction Probability Density Function (PDF) is supposed to be a β function. Thus, all averaged quantities, the mean density $\overline{\rho}$, mean temperature $\widetilde{T}$ and mean species mass fractions can be calculated from the mean mixture fraction $\widetilde{\xi}$ and its variance $\widetilde{\xi''^2}$. They may be stored in so-called flamelets libraries. Correlations involving the normalized specific volume f can also be put in the libraries: (i) the cross correlation $\overline{\rho \xi'' f''}$ appearing in Eq.(3) and (ii) the variance $\overline{\rho f''^2}$. Profiles through the air/fuel diffusion flame brushes of these quantities for different values of the segregation rate are displayed in Fig.(2).

As expected, for small level of segregation, these mean quantities reach a maximum close to the pure air side of the flame brush. This behavior can be associated with the strong variations of density around stoichiometric conditions, i.e. for low values of the mixture fraction, see Fig. 1.

For large values of the segregation rate, the gas is mainly composed of pure air and pure fuel pockets. Thus, profiles show a bimodal characteristic: parabolic shape with a maximum at $\widetilde{\xi} = 0.5$. Besides, larger values of these correlations are obtained for the case featuring the largest density difference of reactants: hydrogen/air turbulent diffusion flames. On the contrary, when the density difference of reactants is small, the correlations vanishes for large segregation rate.

The most important feature observed in Fig.(2) is the change of sign for the correlation $\widetilde{\xi'' f''}$ across the flame brush. This result is the signature of the maximum observed for $f(\xi)$ profiles, see Fig. 1. Consequently, the monotonic evolution of $f(\xi)$ for hydrogen/air diffusion flames leads to a positive value for $\widetilde{\xi'' f''}$ all across the flame brush. For high level of segregation, the sign of $\widetilde{\xi'' f''}$ does not change across the flame brush. It is positive if the fuel is lighter than oxidizer, i.e. for hydrogen and methane, and negative if the fuel is heavier than oxidizer, i.e. for propane and octane.
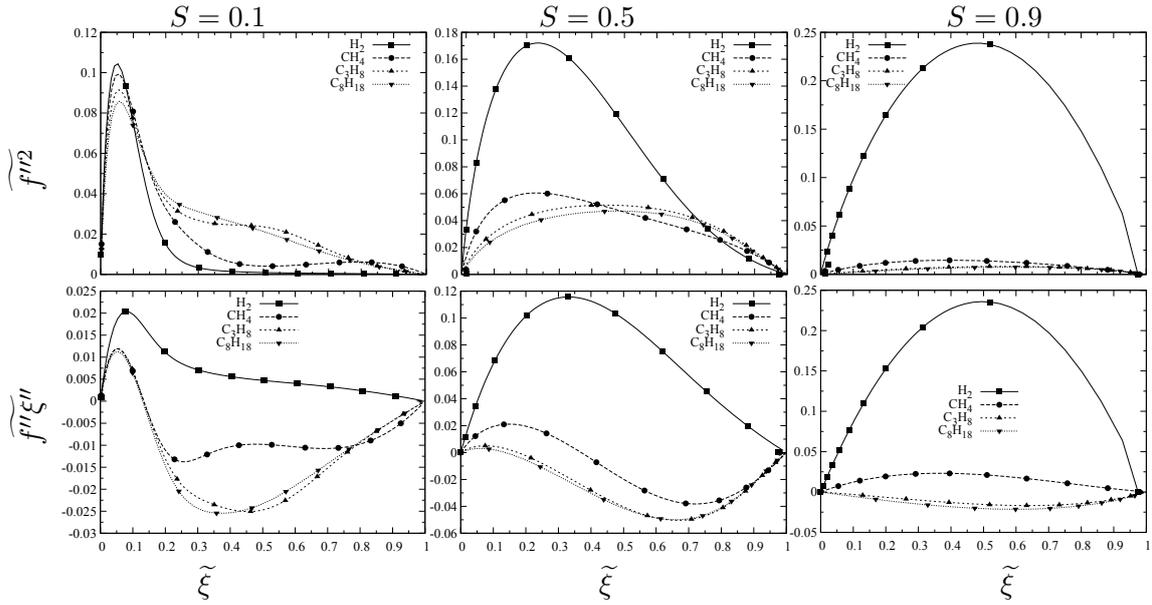
Figure 2: Specific volume variance $\widetilde{f''^2}$ (top) and cross correlation $\widetilde{\xi''f''}$ (bottom) through the air/fuel diffusion flame brushes for three distinct values of the segregation rate: 0.1, 0.5, 0.9 from left to right.

These mean quantities highlight the correlation that exists between mixture fraction and density and are very important to represent effects of density variations upon turbulent transport in diffusion flames. These results shows that these effects may change through the flame brush. Besides, they depend on the level of segregation but also on the fuel and oxidizer considered.

3   Turbulent transport model: velocity splitting procedure

The objective of the present work is to propose closures for the turbulent transport terms, i.e. $\overline{\rho u'' u''}$ and $\overline{\rho u'' \xi''}$ which take effects of density variations into account. The cornerstone of the proposed approach consists in splitting the velocity field into two distinct contributions:

$$\boldsymbol{u} = \boldsymbol{v} + \boldsymbol{w}. \tag{4}$$

The $\boldsymbol{v}$-velocity field is associated with the constant density motions whereas the $\boldsymbol{w}$-velocity field represents the modifications of the flow induced by density variations. In a first approximation, the study focuses on the case of hydrocarbon fuel combustion so that density variations are much more controlled by chemical reactions rather than density difference between fuel and oxidizer. Therefore, the $\boldsymbol{w}$-velocity field can be associated with the local accelerations induced by the flame structures. These structures - via the chemical reactions and the associated heat release - act as a source of density variations so that the norm of the $\boldsymbol{w}$-velocity is defined as proportional to f:

$$\| \boldsymbol{w} \| = s\beta f, \tag{5}$$

where s denotes the chemical consumption rate per unit of flame area $(kg.m^{-2}.s^{-1})$. the quantity s is related to the scalar dissipation rate (SDR) and can be obtained analytically in simplified cases, see for example [3, 4, 5, 6]. It can be evaluated from detailed chemistry calculations as well, by using a chemical kinetic software. It must be pointed out that in the case of a stretched diffusion flame at the limit of extinction, the value of s can be approximated as $s = \rho_r S_L$, so that Eq.(5) becomes fully

consistent with the previous analysis conducted for premixed situations by Robin et al. [7]. Therefore, it is concluded that the results of the corresponding study remain valid, the reactive scalar involved being f instead of c.

The splitting procedure is then applied to the scalar turbulent flux by using Equation (4):

$$\overline{\rho \boldsymbol{u}''\xi''} = \overline{\rho \boldsymbol{v}''\xi''} + \overline{\rho \boldsymbol{w}''\xi''}, \tag{6}$$

where the scalar turbulent fluxes $\overline{\rho \boldsymbol{v}''\xi''}$ and $\overline{\rho \boldsymbol{w}''\xi''}$ are modeled following the recent proposal of Robin et al. [7, 8] and using Eq.(5), so that the formal expression of the scalar turbulent flux can be written as:

$$\overline{\rho \boldsymbol{u}''\xi''} = -\overline{\rho}(\nu_T/\sigma_T)\boldsymbol{\nabla}\widetilde{\xi} + \overline{\rho}s\beta\lambda(1+\psi)\widetilde{\xi''f''}\boldsymbol{M}. \tag{7}$$

The first term of the Right Hand Side (RHS) of Eq.(7) is associated with the passive turbulent mixing of the two reactant streams, and is represented by a gradient law. The second term of the RHS represents the *direct* and *indirect effects* of thermal expansion on the scalar turbulent flux, see Robin et al. [7, 8]. The *direct effects* are induced by the local variations of density. The corresponding modeled expression involves a unit vector $\boldsymbol{M}$ that characterizes the mean orientation of the scalar flux and a parameter λ that measures the associated local fluctuations of orientation, see Robin et al. [8] for more details. The *indirect effects* correspond to the acceleration induced by the flowfield curvature of the streamlines through thermal expansion. They have been modeled by invoking an analogy with the *direct effects* via the introduction of the model parameter ψ. For diffusion flames, such *indirect effects* can become very important because the effects of thermal expansion may be re-oriented towards the main direction of the flow.

Equation (7) also involves the cross correlation $\overline{\rho}\widetilde{\xi''f''}$ already discussed, see Eq.(3) and Fig 2. Then, the behavior of the algebraic model (7) is similar to the one obtained by solving a transport equation for the scalar flux. Moreover, Eq.(7) involving the chemical consumption rate s, we can conclude that even if the mixture fraction is a passive scalar, the only unclosed term of its mean transport equation, i.e. the turbulent scalar flux, will depend on reactive processes.

Consideration of such a splitting procedure allows the turbulent kinetic energy to be modelled as:

$$\overline{\rho k} = \overline{\rho k}_{\boldsymbol{v}T} + \tfrac{1}{2}(s\beta)^2(1+\psi^2)\left[\overline{\rho f''^2} + \widetilde{f}\left(1-\lambda^2\right)\right], \tag{8}$$

where $\overline{\rho k}_{\boldsymbol{v}T}$ represents the turbulent kinetic energy induced by pure mixing processes. We consider here that $\overline{\rho k}_{\boldsymbol{v}T}$ can be evaluated by using the same modeled transport equation as the one retained for non reactive flows. The second term of the RHS of Eq.(8) involves the chemical consumption rate s and the variance of the reactive scalar $\overline{\rho f''^2} = \overline{\rho f''^2} = \overline{f''}$, see Fig. 2. This variance associated with the mean pressure gradient corresponds to the scalar-pressure term of the transport equation for the reactive scalar flux $\overline{\rho \boldsymbol{u}''f''}$ and then is involved in the velocity-pressure term of the transport equation for the turbulent kinetic energy $\overline{\rho k}$, see Eq.(2). Therefore, this velocity splitting procedure is fully consistent with a second order approach and does provide algebraic closures for the turbulent transport terms, as an alternative to solving additional transport equations.

The reactive scalar flux $\overline{\rho \boldsymbol{u}''f''}$ can be modeled employing the same strategy:

$$\overline{\rho \boldsymbol{u}''f''} = -\overline{\rho}(\nu_T/\sigma_T)\boldsymbol{\nabla}\widetilde{f} + \overline{\rho}s\beta\lambda(1+\psi)\widetilde{f''^2}\boldsymbol{M}. \tag{9}$$

It should be noticed that the ratio of the second terms of the RHS of the modeled passive and reactive scalar fluxes, i.e. thermal expansion terms in Eq.(7) and Eq.(9), leads to $\overline{\rho \boldsymbol{u}''f''}/\overline{\rho \boldsymbol{u}''\xi''} = \widetilde{f''^2}/\widetilde{f''\xi}$, which may be rewritten:

$$\overline{\boldsymbol{u}''} = \overline{f''}\widetilde{\boldsymbol{u}''\xi''}/\widetilde{f''\xi''}. \tag{10}$$

This last expression is similar to the one proposed by Jones [2] but more general, i.e. adapted to reactive flows. Moreover, in the case of non reactive scalar mixing, i.e. in situation where $f \equiv \xi$, Eq.(10) becomes strictly identical to Jones' expression.

Finally, the velocity splitting procedure provides algebraic and consistent closures for turbulent transport terms that account for thermal expansion effects. These relationships behave in agreement with the scalar fluxes obtained by using second order approach and they allow to recover and generalize classical second order expressions.
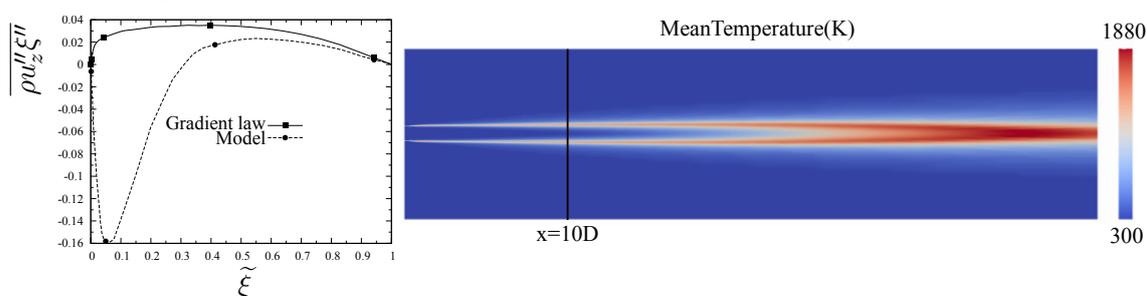

Figure 3: Transverse component of the scalar flux $\overline{\rho u_z'' \xi''}$ trough the mean flame structure at 10 diameters downstream of the injection nozzle (left). Meant velocity, temperature and mixture fraction fields (right).

3   Conclusions

Based on the normalized specific volume, this study of turbulent diffusion flames shows that turbulent transport terms may be strongly affected by the effects of density variations. A closure strategy of turbulent transport terms based on a velocity splitting procedure is proposed and leads to new algebraic models for the turbulent scalar fluxes and the turbulent kinetic energy. These closures have been applied to the calculation of practical turbulent diffusion flames, showing counter-gradient diffusion behavior in a part of the flame brush, see Fig.3.

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