A multi-mixture fraction closure for dilute turbulent diffusion flame

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1 Introduction

The conserved scalar or mixture fraction concept was originally derived for two-feed systems with one oxidizer stream and one fuel stream [1,2]. Under the assumptions of unit Lewis numbers and large Damköhler number values, the conserved scalar model provides a very efficient basis for calculating turbulent diffusion flames that are handled through the single knowledge of the mixture fraction PDF approximated for instance with presumed beta functions. The mixture fraction variable also plays a central role in laminar diffusion flamelet models [2], the above conserved scalar model being interpreted as the most basic flamelet structure. However, as soon as dilution or *third stream* effects come into play, such formalisms that rely on the mixture fraction concept should be revisited [3,4]. The three-feed situation occurs for instance when a stream of oxygen enriched air is introduced for the purpose of achieving larger temperature levels. Such a situation clearly exceeds the conserved scalar basis. Further works is also required to represent dilution effects. From a general point of view, they are associated with a decrease of the total concentration of reactive chemical species that results from the introduction of additional compounds that will not actively participate to chemical reactions. Water vapor, argon, nitrogen are some among the most typical diluting species that are encountered in practical applications. The description of both laminar and turbulent flames in the presence of such diluting agents is a subject of growing interest and may concern a large number of applications, as those encountered for instance in the field of fire safety [5]. Many fire suppression systems resort to gas pulverization to dilute the reactive mixture while others, such as sprinkler systems, decrease the temperature levels through endothermic vaporization processes together with dilution by water vapor. Some efforts have been already spent to extend available descriptions to the consideration of such dilution effects. For instance, Luo and Beck modified the conserved scalar closure by introducing an oxygen threshold to avoid over-predictions of the combustion rate in fuel rich regions [6]. For fire safety applications, fast chemistry models based on either the Eddy Dissipation Concept (EDC) or the conserved scalar methodology still remain the most classical closures retained to describe non-premixed combustion. However, for large dilution levels, the fast chemistry assumption no longer remains satisfactory to represent the combustion processes. Actually, the level of dilution dramatically influence the chemical behavior which is assumed to follow two possible behaviors depending on the initial proportions of reactive species : it is either considered as infinitely fast or infinitely slow, i.e., extinction. In this respect, the purpose of the present study is (i) to modify the conserved scalar presumed PDF closure to account for the description of a three-feed system (oxidizer, fuel, diluent)

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and (ii) to delineate two chemical-response sub-domains (infinitely fast or infinitely slow chemistry) associated with the consideration of flammability or burning limits [7,8].

This first part of the paper is devoted to the description of a ternary mixture. The corresponding representation is often retained for multi-fuel injection situations as encountered for instance in coal combustion applications [9,10]. The second part of the paper presents a modified model including (i) flammability limits that depend of the mean dilution ratio, (ii) species conservation laws that takes into account the presence of residual unburned gas.

2 Description of the tree origin inlet

In the absence of any diluting species, and assuming both very fast chemistry and negligible Lewis number effects, it is possible to use a single transported scalar to evaluate the mass fractions of all chemical species. The retained scalar is generally the mixture fraction Z defined to be (i) a passive scalar, i.e. not affected by chemical reactions, (ii) linearly related to chemical mass fractions, and whose (iii) value lies between zero (in the oxidizer injection stream) and unity (in the fuel injection stream). However, in the context of combustion involving a diluting stream, the final mixture comes from three distinct origins: the fuel stream, the oxidizer stream, and the diluent. Each of the corresponding mass fractions is represented by a tracer, i.e., a passive scalar quantity. In the following, the three corresponding passive scalars are respectively denoted β_1, β_2, and β_3 and their sum is equal to unity (Fig.1.a). The corresponding framework can be extended to turbulent reactive flows through the consideration of the joint probability density function (PDF) of these scalar quantities (Fig.1.a).

In most of the practical situations described in the above section, mixing between the diluting species and the oxidizer takes place before any significant chemical reactions occurs in such a manner that combustion proceeds between fuel and diluted oxidizer. The resulting domain of definition of the joint scalar PDF reduces to a single line connecting the fuel (β_1) and the diluted oxidizer ($\beta_2 + \beta_3$) (Fig.1.b). Thus, *ad hoc* mathematical functions can be used to presume the PDF shape that can be determined through the single knowledge of the fuel (β_1) tracer average and variance values [9].

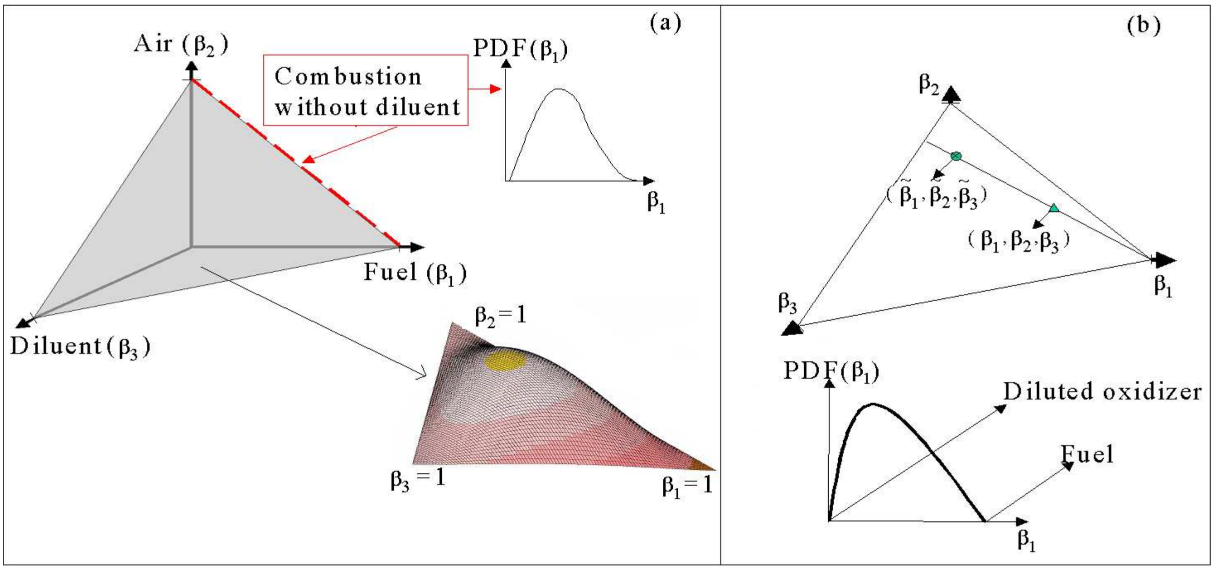

Figure 1.
(a) Ternary diagram of mixture and corresponding PDF shape in the presence or in the absence of dilution.
(b) Reduction of the domain of definition of the PDF to the line connecting fuel and diluted oxidizer.

The assumption of a level of dilution constant and equal to its average value can be expressed through the following equation that describes the linear support of the PDF.

$$\frac{\beta_3}{\beta_2+\beta_3}=\frac{\tilde{\beta}_3}{\tilde{\beta}_2+\tilde{\beta}_3}=X,$$

Along the corresponding line, the stoichiometric mixture fraction of fuel (β_{1S}) can easily be determined from the relationship that exists between its value in the absence of any diluent (β_{1SS}), and the mean level of dilution (X).

$$\beta_{1s}=\frac{1}{1+\left(\frac{1}{\beta_{1ss}}-1\right)\frac{1}{1-X}},$$

In the case of complete reaction, species mass fractions follow piecewise linear relationships (Fig.2).

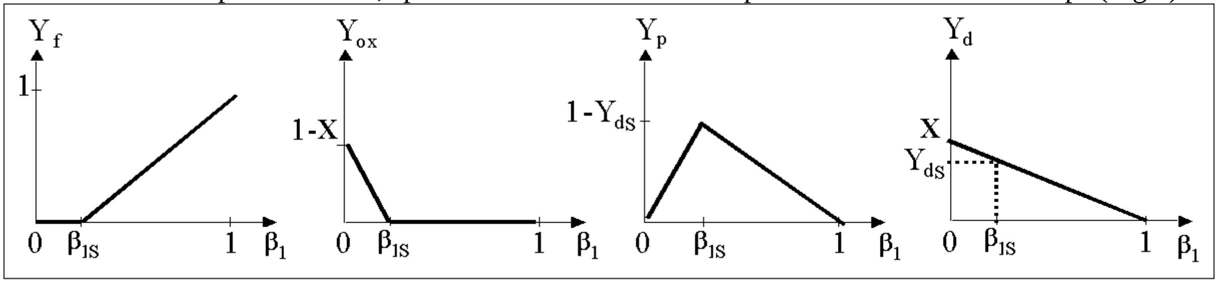

Figure 2. Composition diagrams (β_1, X).

For given values of both of the mixture fraction of fuel and the mean dilution level, the temperature diagram can be easily deduced from the relationships illustrated above in Fig. 2. We will see below how the representation can be extended to the consideration of flammability limits.

3 Turbulent combustion closure including flammability limits

Depending on the concentration of each reactant, the mixture can be flammable or not, and combustion occurs only if the composition in the unburned reactants lies within the flammability limits. In the model described above, the marginal PDF support crosses the corresponding flammability domain thus defining a restricted burning domain whose boundaries will depend on the mean dilution level (Fig.3.a).

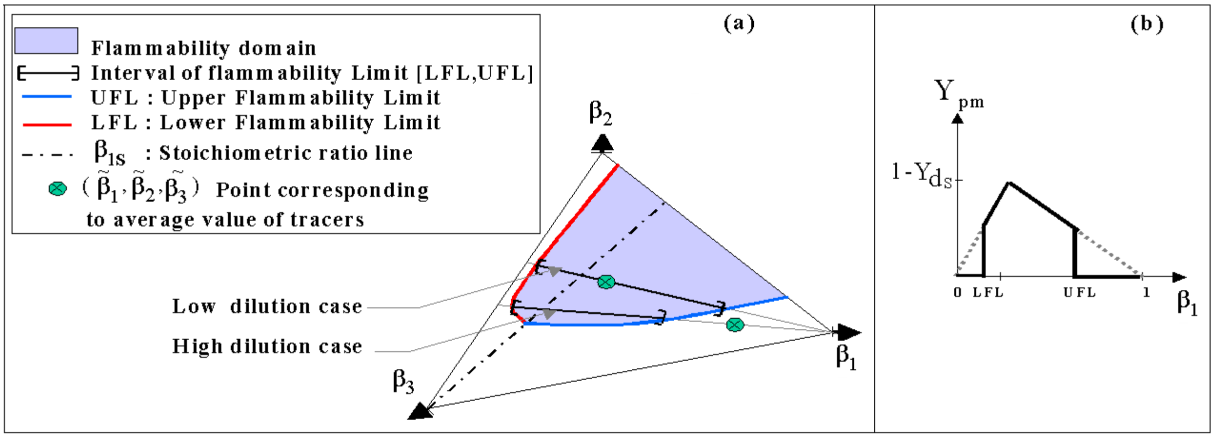

Figure 3. (a) Shrinkage of the burning domain for increasing levels of dilution .
(b) Mass fraction of products liable to be produced in the composition space.

The previous figure displays the evolution of the flammability domain with respect to the mean dilution level (X). The more the oxidizer is diluted, the smaller is the resulting burning interval. The key point is to determine the relationship that can be used to relate the corresponding boundaries to the mean level of dilution. To ensure the progress of chemical reactions, we know that a sufficient amount radicals as well as sufficiently high temperature levels are needed. Based on crossover principles [11], the corresponding effect is taken into account by introducing a critical level of temperature Tcrit=1300K below which combustion no longer takes place. In this manner, the lower flammability limit *(LFL)* increases with the level of dilution up to the stoichiometric value β_{1S} while the upper flammability limit *(UFL)* decreases until it reaches β_{1S}.

Once these two limits are determined, the mass fraction of combustion products liable to be formed *(Y_{Pm})* can be defined in the composition diagram depicted in Fig. 3.b. The mean value $\tilde{Y}_{Pm}$, denoted hereafter as the average concentration of *local potential products*, represents the instantaneous products liable to be formed and regulates the transport equation of the effective products mass fraction *($\tilde{Y}_P$)* which has been retained as the progress variable of chemical reactions. In this way, the irreversible nature of the chemical reaction is introduced through the corresponding production term $\Gamma_{Y_P} = Max\left(\bar{\rho}/\tau \ \left(\tilde{Y}_{Pm} - \tilde{Y}_P\right) \ , \ 0\right)$, that becomes zero if the products concentrations become larger than the local potential products concentration, and, is otherwise equal to a source term that makes $\tilde{Y}_P$ converges towards $\tilde{Y}_{Pm}$ with a relaxation time (τ) smaller than the turbulence integral time scale.

In this case, it is necessary to presume laws for species mass fractions that will be compatible with the boundaries introduced above (Fig. 4) and the products transported. For the diluting species, the evolution law does not change because it does not actively participate to chemical reactions.

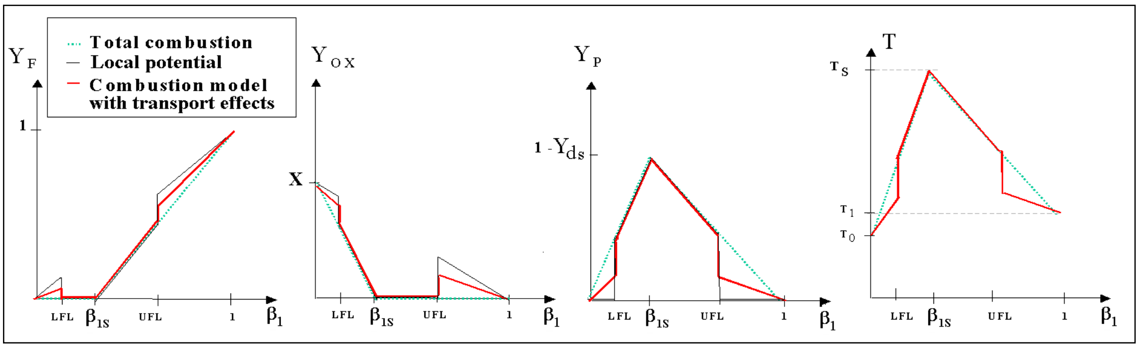

Figure 4. Modified composition diagrams for species mass fractions and temperature.

4 Computational results

The model described above has been implemented in the open-source CFD software package *Code_Saturne*® [12]. *Code_Saturne*® is a parallel general-purpose three-dimensional low-Mach-number CFD code based on a finite volume method. The set of equations considered consists of the averaged Navier-Stokes equations completed with equations for the turbulence modelling and for the additional scalars that have been described above. The time marching scheme is based on a prediction of the velocity field followed by a pressure correction step. Equations for turbulence and scalars are resolved separately afterwards. The discretization in space is based on the fully conservative, unstructured finite volume framework, with a fully colocated arrangement for all variables. The experimental test case retained to assess the computational model corresponds to the statistically steady methane-air jet diffusion flames studied by Prasad et al. [13,14]. A structured grid of 15000 homogeneous cells has been generated. Symmetry axis boundary conditions are applied on the left hand side of the computational domain. The top side (resp. bottom side) of the domain is fixed by an outlet (resp. inlet) boundary conditions. Finally, the boundary condition on the right hand side is approximated by a special boundary condition, which can be either an inlet or an outlet [12].

Figure 5 displays a comparison between experimental data and computational profiles of average temperature performed at different locations downstream of the injection exit. Different dilution conditions have been studied. The reference test-case (a) corresponds to the classical methane-air diffusion flame. The second condition (b) is obtained by a modification of the dilution ratio between oxygen and nitrogen (18% O_2 - 82% N_2). Finally, another kind of diluting agent is studied by incorporating 3 % of water vapor in air, see Fig. 5.c. The agreement obtained between computations and experiments is satisfactory. A very interesting point is that, as expected, the level of temperature decrease obtained from the numerical simulations is found to be sensitive to both the nature and the concentration of the retained diluting agent. The explanation is threefold; first the lessening of oxygen intake reduces the quantities of combustion products. Moreover, the modification of the heat capacity of the mixture induced by the presence of the diluent influences the level of temperature. Finally, the burning domain is reduced and delays the products formation and the associated heat release. For each kind of diluting species, thanks to the finite-rate chemical effects that have been introduced through the consideration of a restricted burning domain, the proposed representation is found able to represent the minimum levels of dilution that are required to obtain the full blow off of the flame, a critical quantity for further developments devoted to fire safety applications.

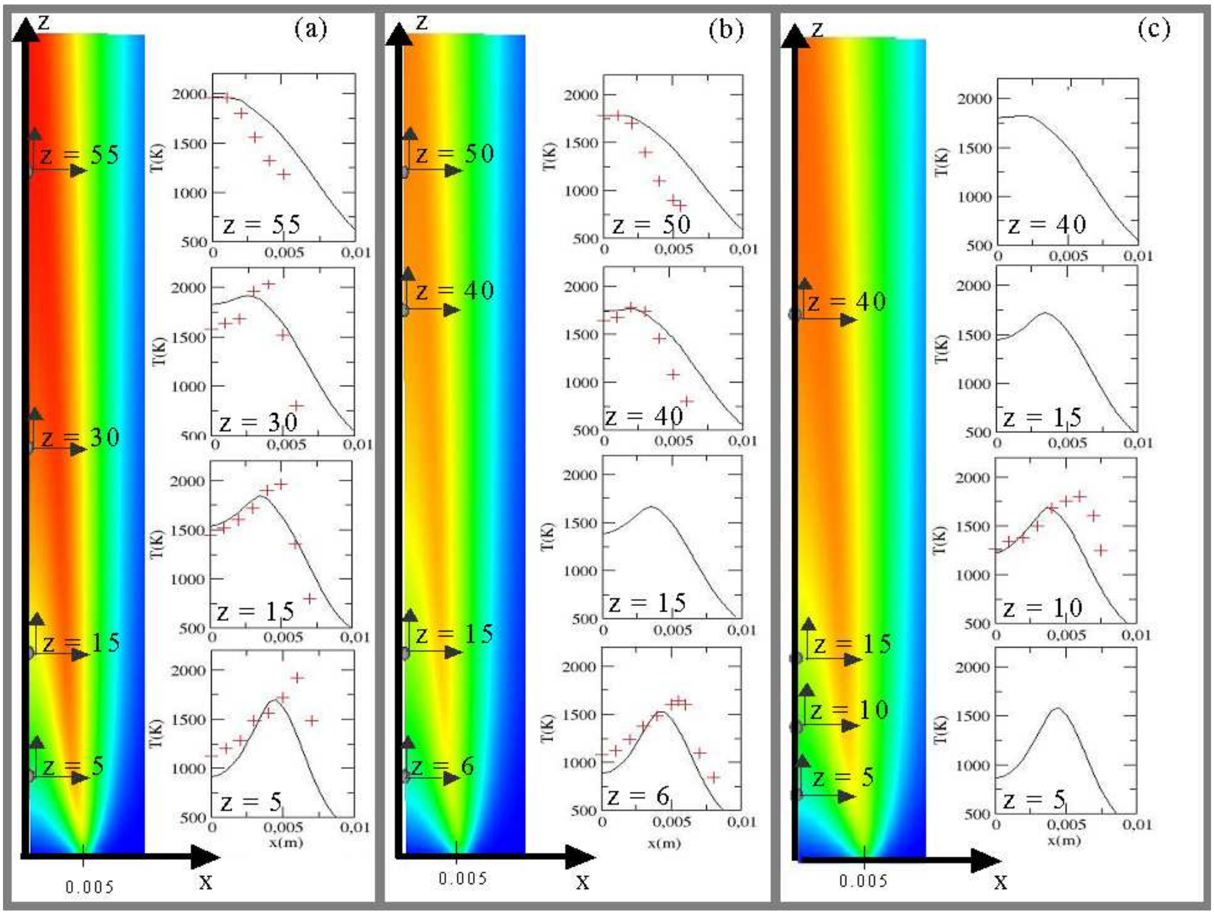

Figure 5. Average temperature field and transverse profiles obtained for (a) pure air, (b) oxygen diluted with nitrogen (18% O_2 - 82% N_2), and (c) air diluted with 3% of water vapor.

Conclusion

Based on the conserved scalar formalism, a generalized description is set forth to represent the limitation of chemical reactions that are induced by dilution effects. The resulting approach is used to simulate the behavior of a diffusion flame in the presence of diluting species. Qualitative as well as quantitative results confirm the relevance of the modelling proposal. The next steps of the study will concern the complete validation of the strategy retained to alleviate difficulties associated with the delineation of the *burning domain* for different conditions. The final objective is to introduce the modelling proposal within a two-phase flow description including gas and evaporating water droplets ; this will make possible the numerical simulations of water mist suppression of non-premixed combustion.

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