Approximating the chemical structure of diffusion and partially premixed laminar counter-flow flames using FPI (Flame Prolongation of ILDM)

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The emergence of stricter environmental regulation promotes the intensive use of numerical modeling to progress in burner design. A large variety of approaches exist to tackle the modelling of turbulent flames that are observed in these systems [1]. Some models allow the introduction of complex and detailed chemistry, mostly via a tabulation of the effects of the subtle intermediate chemical paths controlling ignition, extinction and pollutants emission. Along these lines and starting from the knowledge of fully detailed chemical schemes, various methodologies have been proposed to tabulate complex chemistry. One of them, ILDM (Intrinsic Low Dimensional Manifold) [2], is based on a direct analysis of the dynamic behaviour of chemical systems. Relevant subspaces are determined by distinguishing between species linked to fast and slow time scales. A low number of control parameters is then enough to describe the chemical system with certain limitations. Other techniques, like ISAT [3], are based on in-situ generations of look-up tables, which are constructed from the direct solving of the time evolution of the species concentrations.

In many hydrocarbon turbulent combustion problems featuring complex geometries, the large number of transported species involved in the detailed chemical scheme needs to be highly reduced. To overcome some limitations of ILDM appearing when the number of control parameters is below four, the FPI (Flame Prolongation of ILDM) technique was recently proposed by Gicquel et al [4]. FPI was shown to be attractive for capturing the low temperature region of premixed flames, by avoiding in ILDM the use of linear prolongation in the preheat zone that develops ahead of the thin reaction zone. For a given equivalence ratio of the mixture, FPI consists in tabulating the evolution of chemical species and temperature obtained by the calculations of laminar premixed flames; all the concentrations are then related to a progress variable. A similar technique was also developed by Van Oijen et al [5]. This chemistry tabulation was in fact anticipated by Bradley et al [6] for RANS (Reynolds Average Navier Stokes) modelling of premixed turbulent combustion, where the use of burning rates tabulated from premixed laminar flames was introduced and then extended to nonpremixed turbulent combustion.

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Previous works have measured the accuracy of FPI in the case of fully premixed laminar flames, including heat losses [7]. The objective of the work reported in this paper is to estimate whether such a method can be useful for modeling the chemistry of partially premixed and diffusion flames. Because the ultimate objective is to apply the chemistry tabulation to high Reynolds turbulent flows, in this first approach differential diffusion is neglected, Le=1.

The configuration studied is a counter-flow of premixed methane-air mixture against air (Fig. 1-a.). The equivalence ratio ϕ_F of the fresh mixture (at x=$+\infty$) will be varied from stoichiometric mixture ($\phi_F = 1$) up to pure methane ($\phi_F \to \infty$). Following values of ϕ_F and strain rate α, fully premixed or purely non-premixed flames or both together can appear arround the stagnation plane. The strain rate will be varied up to the characteristic quenching value. A one-dimensional formulation is employed to describe the reactive flow. Using the reaction scheme due to Linstedt [8] which involves 29 species and 300 reactions, reference flames are calculated to which FPI results will be compared.

Next an FPI look-up table is constructed from a set of one-dimensional unstrained premixed flames, covering equivalence ratios (or a mixture fraction Z) varying between the lean (Z_l) and rich (Z_r) flammability limits. A progress variable is defined as $Y_c = Y_{CO} + Y_{CO_2}$ [7] and the control parameters of the FPI database are Z and Y_c. All the relevant chemical information are thus available from the knowledge of Z and Y_c by searching in the FPI databases.

As in an ILDM approach reduced to a two-dimensional manifold, FPI supposes that any flame structure can be mapped in the phase subspace (Z, Y_c), whatever is the combustion regime in physical space (x, y). Figure 1-b shows the projection in the phase subspace (Z, Y_c) of a collection of unstrained 1-D premixed flames (vertical dotted lines) with equivalence ratio (mixture fraction Z) and a set of counterflow non-premixed strained flames (curved dashed lines). Each unstrained premixed flame (at a given Z) intersects a non-premixed strained flame at one point of the phase subspace. Modelling the non-premixed strained flame using FPI assumption therefore implies that the chemical structure of both flames are identical at each value of Z. The prediction capabilities of this hypothesis are now investigated.

Two limit cases of the counterflow flame are first considered. In the firstly discussed configuration, the proportion of methane and air of the fresh mixture is stoichiometric ($Z = 0.055$ at $x = \infty$). The CO_2 mass fraction predicted by FPI is compared to the full chemistry calculation and plotted as a function of local value of Z (Fig. 2, left) for different strain rates. The low values of the relative error computed for the temperature and CO_2 mass fraction (Fig. 3, left) demonstrate that FPI provides an interesting approximation of the exact solution, for all levels of strain. Similar results are observed for radical species concentration. Accordingly, source terms are also reproduced properly. Hence in the case of partially premixed flamelets, mixture fraction and progress variable are good candidates to tabulate the chemical response to strain rate variations.

The pure diffusion counterflow flame, featuring a pure fuel free stream ($Z = 1$ at $x = \infty$), is now studied. A similar analysis is performed, Y_{CO2} profiles are plotted as a function of the local value of Z in Fig. 2-right and the relative error is provided in Fig. 3-right. For mixture fraction values in the vicinity of the stoichiometric ($Z_{st} = 0.055$), the FPI response is close to the reference full chemistry solution. However, when Z reaches a critical value on the rich side, a departure between detailed chemistry and FPI appears. This phenomenon is amplified for large values of the strain rate. This suggests that there exists a reaction zone, where both premixed and diffusion flames share the same chemical structure. Outside this zone, a different behaviour governs the species and source term distributions, mainly because of diffusion across the iso-mixture fraction surfaces.

By progressively changing the equivalence ratio of the fuel stream ϕ_F, until errors between FPI and detailed chemistry solution become significant, a validity domain can be defined: For ϕ_F in the range of $[0.8, 2]$, a flame front propagates leading to a partially premixed regime fully reproduced by FPI. In addition for all flames, in the vicinity of the stoichiometric point there exists a thin reaction zone where FPI can be applied, even when $\phi_F > 2$. It is observed that the thickness of the thin reaction zone slightly decays when increasing the strain rate and weakly varies with the equivalence ratio of the feeding fresh mixture.

These observations indicate that a different tabulation strategy rather than FPI should be retained outside the thin reaction zone, where diffusive fluxes dominate. An attempt to include these additional effects in FPI tabulation is under progress.

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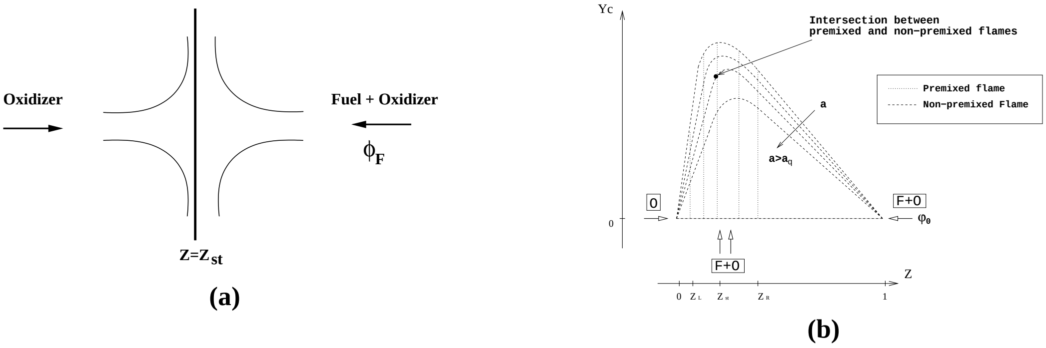

Figure 1: (a): Sketch of counterflow flame. (b): Sketch of premixed ($\phi_F \neq \infty$) and non-premixed ($\phi_F = \infty$) flames expressed in the phase space (Z, Y_c).

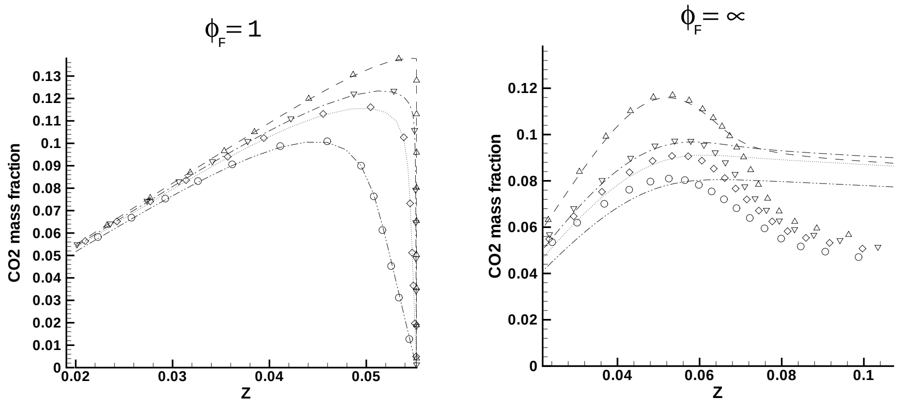

Figure 2: CO_2 mass fraction plotted as a function of local mixture mixture fraction Z for various strain rates for (left) $\phi_F = 1$ and (right) $\phi_F = \infty$. Symbols: FPI tabulation. Lines: full chemistry. Dashed line and triangle up: $10s^{-1}$. Dashed-dot line and triangle down: $158s^{-1}$. Dotted line and diamond: $252s^{-1}$. Dashed-dot-dot line and circle: $398s^{-1}$.

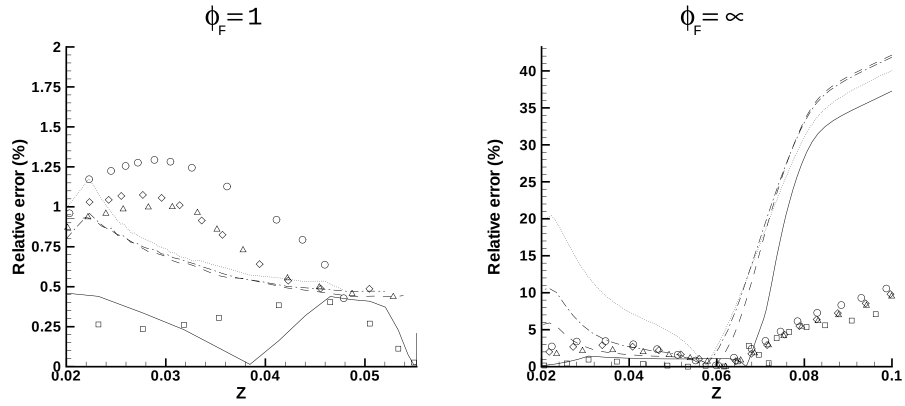

Figure 3: Relative error (detailed chemistry - FPI results) as a function of local mixture fraction Z for various strain rates for (left) $\phi_F = 1$ and (right) $\phi_F = \varsigma\infty$. Symbols: Relative error in temperature prediction. Lines: Relative error in CO$_2$ mass fraction prediction.Dashed line and triangle up: $10s^{-1}$. Dashed-dot line and triangle down: $158s^{-1}$. Dotted line and diamond: $252s^{-1}$. Dashed-dot-dot line and circle: $398s^{-1}$.