Self-Similar Behaviour of Laminar Premixed Flames

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Introduction

Complex chemistry features should be incorporated in turbulent flame simulations, for example to predict pollutant formation. Unfortunately, hydrocarbon combustion schemes involve hundreds of species and thousands of chemical reactions and cannot be handled in practical computations of industrial configurations. Reduced mechanisms have been developed, firstly by hand [1] then from mathematical analysis leading to the Intrinsic Low-Dimensional Manifold (ILDM) [2]. ILDM approach has been improved for premixed flames by tabulating the chemical response of unstrained laminar flames for different equivalence ratios (or mixture fraction) in terms of a progress variable (FPI [3] or FGM [4] formalisms). Unfortunately, these databases may be quite large, even if they depend on a few number of parameters such as progress variable, mixture fraction, total enthalpy (to take into account heat losses), leading to practical problems when computations are conducted on parallel machines: a global implementation of the database may reduce the efficiency of the code (each processor accesses to a single database managed by a master processor, increasing communication times) when local implementation (i.e. a copy of database on each processor local memory) may become prohibitive in terms of memory requirements. To overcome this difficulty, we propose to take advantage of the self-similarity features of the structure of laminar premixed flames.

Self-Similar Behaviour in laminar premixed flames

For a one-dimensional premixed steady flame, the balance equation for the mass fraction Y_K of species k is [5]:

$$\rho_0 S_L \frac{\partial Y_k}{\partial x} = \frac{\partial}{\partial x} \left(\rho D_k \frac{\partial Y_k}{\partial x} \right) + \dot{\omega}_k \tag{1}$$

where ρ_0 is the fresh gases density and D_k the molecular diffusion coefficient. The laminar flame speed S_L depends on the equivalence ratio ϕ , the fresh gas temperature and the pressure. According to the FPI analysis [3], where thermochemical quantities are stored as a function of two variables, the chemical reaction rate $\dot{\omega}_k$ is assumed to depend only on the equivalence ratio ϕ and a progress variable c (c = 0 in the fresh gases, c = 1 in fully-burnt ones).

The laminar flame speed S_L is expressed as $S_L = f(\phi)S_L^0$, where S_L^0 is a reference flame speed, for example chosen for stoichiometric conditions ($S_L^0 = S_L(\phi = 1)$). A convenient assumption

is to split the reaction rate into two contributions:

$$\dot{\omega}_k(c,\phi) = \rho_0 \frac{S_L^0}{\delta_L^0} \underbrace{g(\phi)}_{mixing} \underbrace{h_k(c)}_{reaction}$$
(2)

where g and h_k are two dimensionless functions. $\rho_0 S_L^0 / \delta_L^0$ is introduced for dimensional reasons where the reference length δ_L^0 is the laminar flame thickness for $\phi = 1$. The assumption (2) is sustained by Fig. 1 where the shape of the progress variable reaction rate remains similar when ϕ varies, despite of its amplitude changes through $g(\phi)$.



Figure 1: Reaction rate of the progress variable $\dot{\omega}_c$ plotted as a function of c and ϕ

The balance equation (1) is now rewritten introducing the reduced abscissa $X = (x - x_0)/\delta_l$ where δ_l is the laminar flame thickness and x_0 a reference location:

$$\frac{\partial Y_k}{\partial X} = \left(\frac{D_k^0}{S_L^0 \delta_L^0}\right) \frac{\partial^2 Y_k}{\partial X^2} + \frac{g(\phi)}{f(\phi)^2} h_k(c) \tag{3}$$

using the two classical assumptions $S_L \delta_L \approx S_L^0 \delta_L^0$ and $\rho D_K \approx \rho_0 D_K^0 \approx constant$. The factor $S_L^0 \delta_L^0 / D_k^0$ appears as a flame Reynolds number estimated here for the stoichiometric conditions but assumed to be constant. Integrating Eq. (3) across the flame brush for the progress variable shows that $g(\phi) = f(\phi)^2$ (the integrated reaction rate is directly linked to the laminar flame speed). Then, Eq. (3) reduces to:

$$\frac{\partial Y_k}{\partial X} = \left(\frac{D_k^0}{S_L^0 \delta_L^0}\right) \frac{\partial^2 Y_k}{\partial X^2} + h_k(c) \tag{4}$$

Eq. (4) shows that mass fraction profiles are similar when plotted as a function of the reduced coordinate X, made non-dimensional by the laminar flame thickness δ_L . Then for each species, only one profile should be stored together with the similarity rules, such as the $g(\phi)$ function and maxima, which depend only on the equivalence ratio.

Simulations and Results

The self-similar behaviour of laminar premixed flames is illustrated on Fig. 2(a) where the source term of the mass fraction $Y_c = Y_{CO} + Y_{CO2}$ is plotted for different equivalence ratios in a CH_4 -air flame. Computations have been made using the Premix code [6] with the Qin *et al* kinetic scheme [7].



Figure 2: $Y_c = Y_{CO} + Y_{CO2}$ source term in a laminar premixed methane-air flame plotted for different conditions: $\phi = 0.6$ (·); $\phi = 0.8$ (--); $\phi = 1.0$ (solid line); $\phi = 1.3$ ($\Box\Box$); $\phi = 1.5$ ($\Delta\Delta$).

The reduced reaction rate of Y_c is plotted on Fig. 2(b) as a function of a new abscissa $X = (x - x_0)/\delta_L$, where x_0 is chosen such as the reduced reaction rate is equal to 0.5. Whatever the equivalence ratio, Y_c source term profiles coincide very well, except in burnt gases where small discrepancies appear. Accordingly only one profile, with appropriate scaling relations, have to be tabulated to know other profiles allowing memory space reduction.

This new approach is validated by simulations of lean and rich laminar one-dimensional premixed flames using the source terms extracted from the new table. This table contains stoichiometric profiles for $\dot{\omega}_{Y_c}$ and $\dot{\omega}_{O_2}$ with corresponding relations to estimate the source term for other equivalence ratios. Only two balance equations are solved, for the oxygen and the $Y_c = Y_{CO} + Y_{CO_2}$ mass fractions and results are compared with full complex chemistry calculations (Fig. 3(a) and 3(b)). In all configurations, results match very well. Y_c and Y_{O_2} profils are similar to those obtained from complex chemistry calculations. These calculations validate the new table formulation for major species such as O_2 or CO and CO_2 .



(a) Lean configurations: ($\Box\Box$) is $\phi = 0.9$, ($\nabla\nabla$) is $\phi = 0.7$, ($\triangle\triangle$) is $\phi = 0.5$

(b) rich configuration: $(\Box\Box)$ is $\phi = 1.1$, $(\nabla\nabla)$ is $\phi = 1.3$, $(\triangle\triangle)$ is $\phi = 1.5$

Figure 3: $Y_c(=Y_{CO}+Y_{CO_2})$ and Y_{O_2} profiles. Lines are complex chemistry: solid line is Y_{O_2} and -- is Y_c . Symbols are corresponding calculations with the new table

Conclusion

A new approach for complex chemistry tabulation has been presented taking advantage of the self-similar behaviour of premixed laminar flames which has been introduced theoretically and validated numerically for a CH_4 -air flame. Our future work is to validate this approach for intermediate species such as CH.

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