

Using self-similar properties of turbulent premixed flames to downsize chemical tables in high performance numerical simulations

Denis Veynante¹, Benoît Fiorina¹, Pascale Domingo², Luc Vervisch²

¹Laboratoire EM2C, UPR 288 CNRS,
Ecole Centrale Paris, 92295 Chtenay-Malabry, France

²LMFN-CORIA, UMR 6614 CNRS,
Technopôle du Madrillet, 76801 Saint-Etienne du Rouvray, France

1 Introduction

In a recent paper, Ribert *et al.* [1] have evidenced a self-similarity behavior of hydrocarbon premixed laminar flames: species mass fractions and reaction rates may be reduced to collapse on single curves, using a limited set of parameters. For example, in the framework of two dimensional chemistry FPI tabulation [2], the species k reaction rate $\dot{\omega}_k(c, Z)$ is expressed as a function of a progress variable c and a mixture fraction Z but may be rewritten as:

$$\dot{\omega}_k(c, Z) = \dot{\Omega}_k(Z) \dot{\omega}_k^+ \left(\frac{c - c_1(Z)}{c_2(Z) - c_1(Z)} \right) \quad (1)$$

where $\dot{\Omega}_k$, $\dot{\omega}_k^+$, c_1 and c_2 are four vectors. This finding allows a strong reduction of the size of chemical databases (a 2D table is replaced by four 1D tables) which is especially important for implementation on massively parallel computers as such databases should be stored in each processor local memory to minimize communications between processors. Ribert *et al.* have limited their investigation to laminar flames, thinking about large eddy simulations (LES) in terms of Thickened Flame model (TFLES, [3]). In the following, the extension to turbulent flames is analyzed in a presumed probability density function formalism, where the mean (RANS) of the filtered (LES) rate is expressed as:

$$\bar{\omega}_k(\tilde{c}, S_c, \tilde{Z}, S_Z) = \int_0^1 \int_0^1 \dot{\omega}_k(c, Z) p(c) p(Z) dc dZ \quad \text{with} \quad S_c = \frac{\tilde{c}c - \tilde{c}\tilde{c}}{\tilde{c}(1 - \tilde{c})} \quad ; \quad S_Z = \frac{\tilde{Z}Z - \tilde{Z}\tilde{Z}}{\tilde{Z}(1 - \tilde{Z})} \quad (2)$$

where $p(c)$ and $p(Z)$ are beta probability density functions and S_c and S_Z denote the unmixedness (or the segregation factor) of the progress variable c and the mixture fraction Z respectively.

2 Theoretical analysis

The mass fraction balance equation for species k in a 1D steady state turbulent premixed flames reads:

$$\rho_0 S_T \frac{\partial \tilde{Y}_k}{\partial x} = \frac{\partial}{\partial x} \left(D_T \frac{\partial \tilde{Y}_k}{\partial x} \right) + \bar{\omega}_k \quad (3)$$

where S_T and D_T are the turbulent flame speed and diffusivity. Introducing the reduced abscissa $x^+ = \int_0^x \rho_0 (S_T/D_T) dx$ where $D_T/(\rho_0 S_T)$ corresponds to a turbulent diffusion thickness, gives:

$$\frac{\partial \tilde{Y}_k}{\partial x^+} = \frac{\partial^2 \tilde{Y}_k}{\partial x^{+2}} + \frac{D_T}{(\rho_0 S_T)^2} \bar{\omega}_k \quad (4)$$

Integrating this equation over the spatial direction leads to:

$$\tilde{Y}_k^b - \tilde{Y}_k^u = \frac{D_T}{(\rho_0 S_T)^2} \int_{-\infty}^{+\infty} \bar{\omega}_k dx^+ = \frac{1}{\rho_0 S_T} \int_{-\infty}^{+\infty} \bar{\omega}_k dx \quad (5)$$

where \tilde{Y}_k^u and \tilde{Y}_k^b denote the mass fractions of species k in fresh and fully burnt gases respectively. When $\tilde{Y}_k^b - \tilde{Y}_k^u \neq 0$, Eq. (4) may be made non-dimensionalized as:

$$\frac{\partial \tilde{Y}_k^+}{\partial x^+} = \frac{\partial^2 \tilde{Y}_k^+}{\partial x^{+2}} + \frac{\bar{\omega}_k}{\int_{-\infty}^{+\infty} \bar{\omega}_k dx^+} \quad \text{with} \quad \tilde{Y}_k^+ = \frac{\tilde{Y}_k - \tilde{Y}_k^u}{\tilde{Y}_k^b - \tilde{Y}_k^u} \quad (6)$$

Turbulent flames will display a self-similar behavior if the reduced reaction rate $\bar{\omega}_k^+ = \bar{\omega}_k / \int_{-\infty}^{+\infty} \bar{\omega}_k dx^+$ depends only on the reduced spatial location x^+ (or on the progress variable, which varies monotonically with x^+).

The analysis may be conducted further in the framework of flame surface density modelling, when the mean or filtered reaction rate is written [4]:

$$\bar{\omega}_k = \rho_0 \left(\int_0^1 S_L(Z) p(Z) dZ \right) (\tilde{Y}_k^b - \tilde{Y}_k^u) \Sigma = \rho_0 \left(\int_0^1 S_L(Z) p(Z) dZ \right) (\tilde{Y}_k^b - \tilde{Y}_k^u) \Xi |\nabla \bar{c}| \quad (7)$$

where $S_L(Z)$ is the laminar flame speed depending on the mixture fraction Z , Σ the flame surface density, Ξ the wrinkling factor and \bar{c} , the mean or filtered progress variable. Then:

$$\begin{aligned} \bar{\omega}_k &= \frac{\bar{\omega}_k}{\int_{-\infty}^{+\infty} \bar{\omega}_k dx^+} \left(\int_{-\infty}^{+\infty} \bar{\omega}_k dx^+ \right) = \frac{\Xi |\nabla \bar{c}|}{\int_{-\infty}^{+\infty} \Xi |\nabla \bar{c}| dx^+} \rho_0 \left(\int_0^1 S_L(Z) p(Z) dZ \right) (\tilde{Y}_k^b - \tilde{Y}_k^u) \int_{-\infty}^{+\infty} \Xi |\nabla \bar{c}| dx^+ \\ &= \underbrace{\frac{\rho_0^2}{D_T} \Xi \left(\int_0^1 \Xi d\bar{c} \right)}_{\text{Shape } F(\tilde{c}, S_c)} \underbrace{\left| \frac{\partial \bar{c}}{\partial x^+} \right| \left(\int_0^1 S_L(Z) p(Z) dZ \right)^2 (\tilde{Y}_k^b - \tilde{Y}_k^u)}_{\text{Chemistry } G(\tilde{Z}, S_Z)} \end{aligned} \quad (8)$$

This derivation assumes that the turbulent diffusivity D_T is constant across the flame brush but not an infinitely thin flame as a ‘‘generalized flame surface density’’ may be considered [4]. The filtered reaction rate $\bar{\omega}_k$ may then be split into two contributions. The first one gives the shape of the reaction rate and depends on the distribution of the progress variable c (i.e. on \tilde{c} and S_c). It evolves from a Arrhenius law for single step chemistry in laminar flames to a parabolic function for wrinkled infinitely thin flame fronts. The second contribution depends on chemical parameters (mixture fraction, initial temperature and pressure) but not on the progress variable. Then, $\bar{\omega}_k^+$ depends only on the progress variable (or on the reduced coordinate x^+) and the filtered reaction rate also exhibits self-similarity behaviors. Then:

$$\bar{\omega}_k = \int_0^1 \int_0^1 \dot{\omega}_k(c, Z) p(c) p(Z) dc dZ \approx A_k \dot{\Omega}_{1,k}(\tilde{c}, S_c) \dot{\Omega}_{2,k}(\tilde{Z}, S_Z) \quad (9)$$

3 Results

Eq. (9) is evaluated from a chemical database for methane / air combustion under atmospheric conditions, splitting the reaction rate $\bar{\omega}_k$ into three contributions:

$$\bar{\omega}_k = \max(\bar{\omega}_k) \underbrace{\left(\frac{\bar{\omega}_k}{\max(\bar{\omega}_k)} \frac{\max(\bar{\omega}_k | S_c)}{\max(\bar{\omega}_k | S_c, \tilde{Z}, S_Z)} \right)}_{\mathcal{F}_k(\tilde{c}, S_c, \tilde{Z}, S_Z)} \underbrace{\left(\frac{\max(\bar{\omega}_k | S_c, \tilde{Z}, S_Z)}{\max(\bar{\omega}_k | S_c)} \right)}_{\mathcal{G}_k(S_c, \tilde{Z}, S_Z)} \quad (10)$$

where $(\bar{\omega}_k | a, b, \dots)$ is the value of the mean or filtered reaction rate $\bar{\omega}_k$ for given values of the parameters a, b, \dots . Figure 1 displays the functions \mathcal{F}_c and \mathcal{G}_c corresponding to the reaction rate $\bar{\omega}_c$ of the FPI progress variable defined from combined carbon mono and dioxide mass fractions $Y_{CO} + Y_{CO_2}$ as extracted from the database. The function \mathcal{F}_c depends mainly on the filtered progress variable \tilde{c} and its unmixedness S_c . A slight shift is observed when \tilde{Z} varies, especially when S_c is low (quasi laminar flames) but concerns a few number of profiles close to the flammability limits. As expected, the function \mathcal{G}_c depends only weakly on the progress variable unmixedness S_c and $\mathcal{G}_c(S_c, \tilde{Z}, S_Z) \approx \mathcal{G}_c(\tilde{Z}, S_Z)$

Eq. (9) is tested against the chemical database defining:

$$A_c = \max(\bar{\omega}_c) ; \hat{\Omega}_{1,c}(\tilde{c}, S_c) = \overline{\left(\mathcal{F}_c(\tilde{c}, S_c, \tilde{Z}, S_Z) \middle| \tilde{c}, S_c \right)} ; \hat{\Omega}_{2,c}(\tilde{Z}, S_Z) = \overline{\left(\mathcal{G}_c(S_c, \tilde{Z}, S_Z) \middle| \tilde{Z}, S_Z \right)} \quad (11)$$

where $\overline{(Q|a)}$ denotes the conditional average of the quantity Q for a given value of the parameter a . Figure 2 compares the reaction rate $\bar{\omega}_c$ and its estimation from relations (9) and (11). The agreement is very good as the correlation coefficient between the two reaction rates reaches 0.996. As for laminar flames, this self-similarity behaviour allows to drastically reduce the size of the chemical database: a four-dimension database is replaced here by two two-dimension databases. Moreover, as we will show in the final paper, the two functions $\hat{\Omega}_{1,c}$ and $\hat{\Omega}_{2,c}$ may also be replaced with a good precision by analytical expressions such as:

$$\hat{\Omega}_{1,c}(\tilde{c}, S_c) \approx \alpha_c(S_c) (\tilde{c})^{\beta_c(S_c)} (1 - \tilde{c})^{\gamma_c(S_c)} \quad ; \quad \hat{\Omega}_{2,c}(\tilde{Z}, S_Z) \approx \alpha_Z(S_Z) (\tilde{Z})^{\beta_Z(S_Z)} (1 - \tilde{Z})^{\gamma_Z(S_Z)} \quad (12)$$

where α_c, β_c and γ_c (respectively α_Z, β_Z and γ_Z) are three functions of the unmixedness S_c (respectively S_Z) to be specified. The chemical database is then reduced to few lines of code, a decisive advantage for implementation on massively parallel machines.

References

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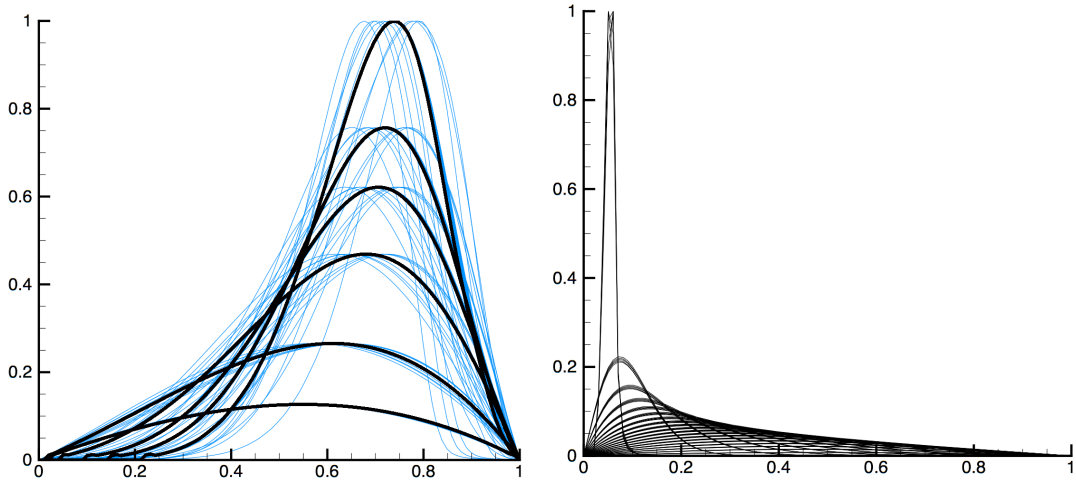


Figure 1: Functions $\mathcal{F}_c(\tilde{c}, S_c, \tilde{Z}, S_Z)$ and $\mathcal{G}_c(S_c, \tilde{Z}, S_Z)$ defined by Eq. (10). Left: $\mathcal{F}_c(\tilde{c}, S_c, \tilde{Z}, S_Z)$ is plotted as a function of \tilde{c} for six values of the unmixedness $S_c = 0.; 0.053; 0.105; 0.211; 0.474$ and 0.737 (thin blue lines). Bold lines correspond to conditional averages for a given value of the unmixedness (Eq. 11). Right: $\mathcal{G}_c(S_c, \tilde{Z}, S_Z)$ is plotted as a function of \tilde{Z} for 20 values of the unmixednesses S_c and S_Z regularly spaced from 0. to 1. Maximum values decrease and profiles evolve toward a parabolic shape for increasing unmixedness S_Z while the dependence with S_c is very weak.

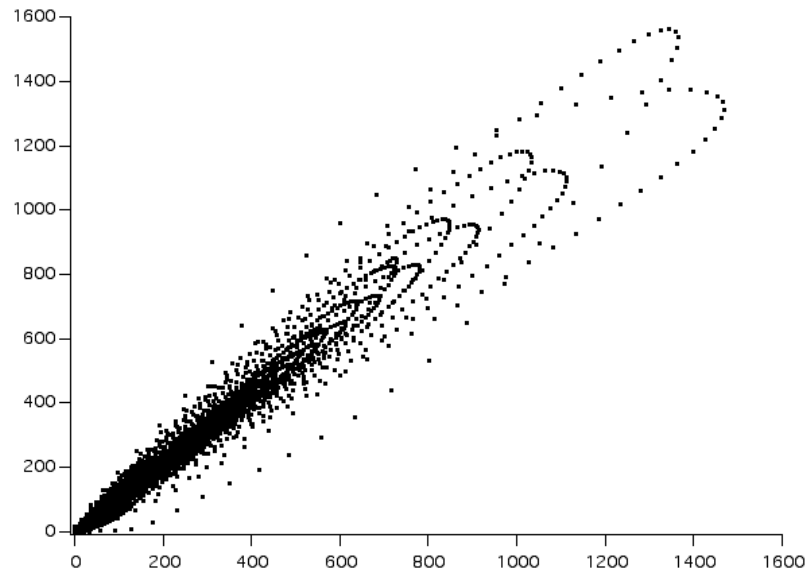


Figure 2: Scatter plot of the reaction rate $\bar{\omega}_c$ (s^{-1}) extracted from the chemical database as a function of its estimation from Eqs. (9) and (11). More than 380 000 samples corresponding to non-zero reaction rates are displayed. The correlation coefficient between actual and modeled reaction rates is 0.996.