A filtered tabulated chemistry model for LES of partially-premixed flames

P. Auzillon, O. Gicquel, N. Darabiha, D. Veynante and B. Fiorina

EM2C - CNRS, Ecole Centrale Paris

Châtenay Malabry, France

1 Introduction

The turbulent combustion model F-TACLES (Filtered Tabulated Chemistry for LES) has recently been proposed to introduce detailed chemistry effects in Large Eddy Simulations [1]. The method, initially developed for turbulent premixed combustion, consists first in generating a chemical look-up table from filtered 1-D laminar premixed flames computed under detailed chemistry assumptions. Closure of the filtered progress variable balance equation is then carefully addressed from this filtered database. The model accounts for turbulent combustion by including sub-grid scale wrinkling effects in flame front propagation. This approach is well adapted to turbulent premixed flames [1] and reproduces accurately flame dynamics [2].

The objectives of the present work are to extend the F-TACLES model to turbulent partially-premixed flames. The modeling strategy is detailed in Section 2. Section 3 is dedicated to numerical tests of the model: 1-D flames submitted to equivalence ratio fluctuations are computed. Then preliminary simulations of a 3-D partially-premixed flame stabilized in a swirled burner [3] are shown.

2 Modeling filtered thermochemical quantities

2.1 Chemistry tabulation

The FPI approach [4, 5] assumes that the chemical subspaces accessed by a partially-premixed flame in a complex geometry configuration can be mapped by a collection of 1-D laminar premixed flames computed for various equivalence ratios using detailed chemistry. This assumption is relevant for premixed and partially-premixed flames [6]. One-dimensional laminar premixed flames are computed for equivalence ratios evolving within the flammability limits of a reactive mixture combustion under unity Lewis number assumption and using a detailed chemical mechanism. The tabulated chemistry technique is coupled to the LES compressible solver following the Tabulated Thermochemistry for Compressible formalism [7]. Thermo-chemical quantities are expressed in terms of two coordinates, the reaction progress variable c to measure the reaction progress [5] and the normalized mixture fraction z. For the

Correspondence to: pierre.auzillon@em2c.ecp.fr

combustion of methane/air mixture c is defined as $c = (Y_{CO} + Y_{CO_2})/(Y_{CO}^{eq} + Y_{CO_2}^{eq})$ that combines CO and CO_2 mass fractions. In a compressible solver, any thermo-chemical quantity φ is then expressed as $\varphi = \varphi[c, z]$ meaning that the variable φ is tabulated in a 2-D look-up table with coordinates c and z.

2.2 Filtered probability density function formalism

Homogenous and heterogenous mixtures are considered in this section. Sub-grid scale flame wrinkling is first not considered in the estimation of filtered quantities. It will be introduced in Section 3.2 in order to ensure that the flame propagates at a sub-grid scale turbulent flame speed.

Case a: homogenous mixture fraction at the sub-grid scale level

In F-TACLES approach, filtered thermo-chemical quantities are estimated from 1-D laminar premixed flame structure:

$$\overline{\varphi} = \int_{-\infty}^{+\infty} \varphi^*(x) G_\Delta(x - x') dx' \tag{1}$$

where G_Δ is a filter operator of size Δ and the * superscript denotes quantities issued from a 1-D laminar unstretched premixed flame computed for a given mixture fraction z. Filtered thermo-chemical quantities are then tabulated as a function of the Favre filtered progress variable $\widetilde{c}$ and the filter size Δ: $\overline{\varphi} = \overline{\varphi^*}[\widetilde{c}, \Delta]$.

$\overline{\varphi}$ can be rewritten also in c space with the introduction of the filtered density function $P_\Delta(c')$:

$$\overline{\varphi} = \int_0^1 \varphi^*(c') P_\Delta(c') dc' \tag{2}$$

where $P_\Delta(c')$ is the progress variable probability density function in a laminar flame filtered with a filter operator of size Δ.

Case b: heterogenous mixture fraction at the sub-grid scale level

To handle with mixture fraction heterogeneities at the sub-grid scale level, the joint filtered probability density function $P(z', c')$ is introduced:

$$\overline{\varphi} = \int_0^1 \int_0^1 \varphi^*(z', c') P(z', c') dc' dz' \tag{3}$$

Assuming that c and z are statistically independent:

$$\overline{\varphi} = \int_0^1 \int_0^1 \varphi^*(z', c') P(z') P_\Delta(c') dc' dz' = \int_0^1 \overline{(\varphi | z = z')} P(z') dz' \tag{4}$$

where $\overline{(\varphi | z = z')}$ is the conditional filtered value of φ:

$$\overline{(\varphi | z = z')} = \int_0^1 \varphi^*(z = z', c') P_\Delta(c') dc' = \int_{-\infty}^{+\infty} \varphi^*(z = z', x) G_\Delta(x - x') dx' \tag{5}$$

Favre filtered quantities $\widetilde{\varphi}$ are calculated using Favre formalism definition: $\overline{\rho}\widetilde{\varphi} = \overline{\rho\varphi}$.

The filtered chemical table is constructed as follows: a collection of 1-D laminar premixed flame is first computed for equivalence ratio evolving within flammability limits and using a detailed chemical mechanism under unity Lewis number assumption. The conditional filtered values $\overline{(\varphi|z=z')}$ are then obtained by filtering the whole set of 1-D premixed flames in x space accordingly to Eq. 5. Finally filtered variables are computed from Eq. 4, using the a β function to model $P(z')$, parametrized by the first and second order moments of the mixture fraction: $\widetilde{z}$ and $\widetilde{z''^2}$. Filtered thermo-chemical quantities $\overline{\varphi}$ are then stored in a look-up table, $\varphi = \overline{\varphi^*}[\widetilde{Y}_c, \Delta, \widetilde{z}, S_z]$ where $S_z = \widetilde{z''^2}/(\widetilde{z}(1-\widetilde{z}))$ is the unmixedness factor. $S_z = 0$ corresponds to a fully premixed mixture and $S_z = 1$ to a totally segregated mixture.

3 Closure of the filtered progress variable balance equation

3.1 No flame wrinkling at the sub-grid scale level

For LES, under unity Lewis number assumption, the filtered progress variable balance equation reads:

$$\frac{\partial \bar{\rho}\widetilde{Y_c}}{\partial t} + \nabla \cdot (\bar{\rho}\widetilde{\boldsymbol{u}}\widetilde{Y_c}) \quad = \quad \nabla \cdot \left(\overline{\rho D \nabla Y_c}\right) - \nabla \cdot \left(\bar{\rho}\widetilde{\boldsymbol{u}Y_c} - \bar{\rho}\widetilde{\boldsymbol{u}}\widetilde{Y_c}\right) + \bar{\rho}\widetilde{\dot{\omega}}_{Y_c} \tag{6}$$

where ρ is the density, $\boldsymbol{u}$ the velocity vector, D the diffusivity. $\dot{\omega}_{Y_c}$ is the progress variable reaction rate expressed in s^{-1}. Closure models have been proposed in [1] for the sub-grid-scale transport terms $-\nabla \cdot (\bar{\rho}\widetilde{\boldsymbol{u}\varphi} - \bar{\rho}\widetilde{\boldsymbol{u}}\widetilde{\varphi})$, the filtered laminar diffusion term $\overline{\rho D \nabla \varphi}$ and the filtered source term $\widetilde{\dot{\omega}}_{Y_c}$. This methodology is now extended to account for mixture fraction heterogeneities at the sub-grid scale. Wrinkling at the sub-grid scale is not first considered, it will be introduced in Section 3.2.

Filtered chemical reaction source term $\overline{\dot{\omega}}_{Y_c}$

The filtered source term for the filtered progress variable is estimated directly using Eq. 4:

$$\bar{\rho}\widetilde{\dot{\omega}}_{Y_c} = \int_0^1 \overline{(\rho\dot{\omega}_{Y_c}|z=z')} P(z') dz' \tag{7}$$

where $\overline{(\dot{\omega}_{Y_c}|z=z')}$ is estimated according to Eq. 5. In order to save CPU time during the LES, the filtered reaction rate is stored in a four-dimensional look-up table: $\widetilde{\dot{\omega}}_{Y_c} = \widetilde{\dot{\omega}}^*_{Y_c}[\widetilde{c}, \widetilde{z}, S_z, \Delta]$.

Filtered laminar diffusion terms

A model for the filtered molecular diffusion term has been discussed in [1] for premixed flames. The extension toward stratified combustion reads:

$$\nabla \cdot (\overline{\rho D \, \nabla Y_c}) \quad = \quad \nabla \cdot \left(\alpha_c \, \bar{\rho} D \, \nabla \widetilde{Y_c}\right) \tag{8}$$

where the correction factor α_c is estimated from 1-D filtered premixed flames :

$$\alpha_c[\widetilde{c}, \widetilde{z}, S_z, \Delta] = \frac{\overline{\rho D \frac{\partial Y_c^*}{\partial x^*}}}{\bar{\rho} D \frac{\partial \widetilde{Y_c}^*}{\partial x^*}} \tag{9}$$

In practice the following decomposition is required to compute $\frac{\partial \widetilde{Y_c}^*}{\partial x^*}$:

$$\frac{\partial \widetilde{Y_c}^*}{\partial x^*} = \frac{\partial}{\partial x^*}\left(\frac{\overline{\rho^* Y_c^*}}{\bar{\rho}^*}\right) = \frac{1}{\bar{\rho}}\left(\overline{\frac{\partial \rho^* Y_c^*}{\partial x^*}} - \widetilde{Y_c}^* \frac{\partial \bar{\rho}^*}{\partial x^*}\right) \tag{10}$$

As for the progress variable reaction rate, α_c is stored in a look-up table as $\alpha_c = \alpha_c[\widetilde{c}, \widetilde{z}, S_z, \Delta]$

sub-grid scale convection term

Assuming that the flame remains planar at the sub-grid scale level, the unresolved convection terms are directly estimated from the 1-D detailed chemistry laminar premixed flames [1] through the following relation:

$$\Omega_{Y_c}[\widetilde{c}, \widetilde{z}, S_z, \Delta] = \overline{\rho u}.\widetilde{Y_c} - \overline{\rho u.Y_c} \quad = \overline{\rho_0 S_l}\frac{\partial \widetilde{Y_c}^*}{\partial x^*} - \overline{\rho_0 S_l \frac{\partial Y_c{}^*}{\partial x^*}} \tag{11}$$

where $\rho_0 = \rho(c = 0, z)$ is the fresh gas density and S_l is the unstretched laminar flame speed and $\frac{\partial \widetilde{Y_c}^*}{\partial x^*}$ is computed accordingly to Eq. 10. The sub-grid scale convection term of the progress variable is then also stored in a 4-D look-up table: $\Omega_{Y_c} = \Omega_{Y_c}[\widetilde{c}, \widetilde{z}, S_z, \Delta]$.

Note that the flame front, submitted to mixture fraction heterogeneities across the flame front, propagates in the direction normal to the reaction zone and relatively toward the fresh gases at the speed $\widetilde{S_l}$ given by:

$$\bar{\rho}\widetilde{S_l} = \int_0^1 \rho S_l(z = z')P(z')dz' \tag{12}$$

3.2 Flame wrinkling at the sub-grid scale

To account for sub-grid scale wrinkling that occurs in practical LES of turbulent flames, the flame wrinkling factor $\Xi = S_T/\widetilde{S_l}$ is introduced, where S_T is the turbulent flame burning velocity. Ξ has to be modeled, for this article, the model given by Charlette *et al.* [8] has been chosen for the 3-D computation. The filtered balance equation of the progress variable reads :

$$\frac{\partial \bar{\rho}\widetilde{Y_c}}{\partial t} + \nabla \cdot (\bar{\rho}\widetilde{\boldsymbol{u}}\widetilde{Y_c}) = \nabla \cdot \left(\Xi\alpha_c[\widetilde{c}, \widetilde{z}, \widetilde{z''^2}, \Delta]\, \bar{\rho} D\, \nabla \widetilde{Y_c}\right) + \Xi\Omega_c[\widetilde{c}, \widetilde{z}, \widetilde{z''^2}, \Delta] + \Xi\bar{\dot{\omega}}_c[\widetilde{c}, \widetilde{z}, \widetilde{z''^2}, \Delta] \tag{13}$$

4 Numerical test cases

The model described above is implemented into the LES AVBP code (*www.cerfacs.fr/4-26334-The-AVBP-code.php*) following the TTC formalism [7]. Two validation test cases are presented in the following sections.

4.1 1-D flame computations

We consider a 1-D planar flame submitted to mixture fraction fluctuations. The propagation speed of this planar flame is affected by sub-grid scale mixture fraction variance. If the unmixedness factor S_z remains constant across the flame front, the flame burning velocity should verify Eq. 12. To check this property, a set of steady methane/air 1-D filtered flames has been computed for a filter size of $\Delta = 20\delta_r$ (δ_r is the full width at half maximum of the reaction rate) and for different values of S_z. The chemical look-up table is obtained using the GRI 3.0 detailed mechanism. A totally premixed flame at the stoechiometry without mixture fraction fluctuations at sub-grid scale is computed as a reference. Each "stratified 1-D flame" corresponds to a mean mixture fraction equal to the stoechiometry but with different mixture heterogeneities quantified by the value of S_z. Temperature profiles of these "stratified 1-D flames" are plotted in Fig. 1 (a) and the corresponding flame burning velocities are shown in Fig. 1 (b). A very good agreement is observed between the estimated (symbols) and the theoretical, Eq 12 (solid line), flame propagation speeds.

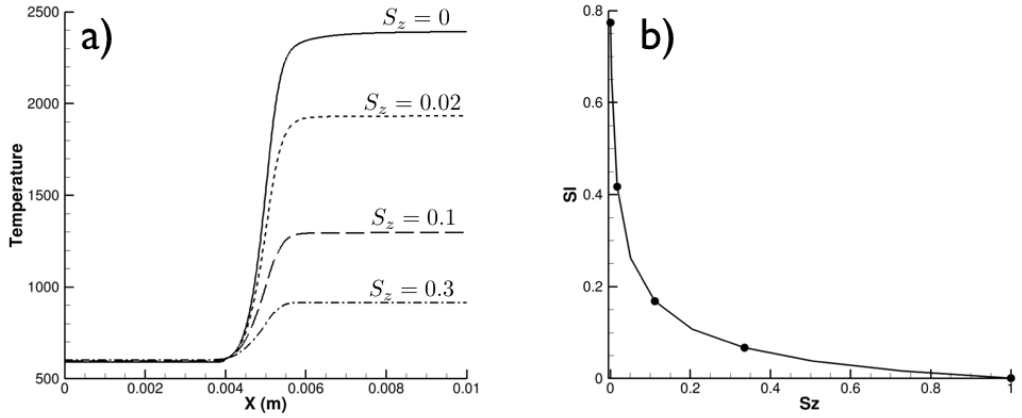

Figure 1: 1-D simulations of stratified flame with F-TACLES a) : Temperature profiles. b): Flame speed; ■: estimated propagation speed ; – : theoretical propagation speed given by Eq. 12

5.2 LES of a 3-D turbulent stratified swirled flame (in progress)

F-TACLES model is applied to study a complex partially-premixed configuration, MOLECULES, experimentally investigated by Janus *et al.* [3] and recently computed by RANS approach by Schneider *et al.* [9] . The geometry is representative of a gas turbine combustion chamber. It consists of a plenum, a swirl-injector and a combustion chamber. A methane jet is directly injected through the center of the swirler. The air is injected into the swirler with a mass flow rate of 30 g/s. The global equivalence ratio is 0.8. An unstructured mesh, composed of 40,2 millions tetratedras, has been designed. Preliminary result of the reactive case simulation is shown in Fig.2. Current work focuses on the LES of the reactive case and comparisons with experimental data.

6 Acknowledgment

We thank Prof Andreas Dreizler and Dr. Simone Schnfelder for providing us the burner geometry and the experimental data. This work was supported by the ANR-07-CIS7-008-04 Grant of the French Ministry of Research and accessed to the high performance computing resources of IDRIS and CINES under the allocation 2009-i2009020164 made by GENCI (Grand Equipement National de Calcul Intensif).

References

[1] B. Fiorina, R. Vicquelin, P. Auzillon, N. Darabiha, O. Gicquel, and D. Veynante, "A filtered tabulated chemistry model for LES of premixed combustion," *Combust. Flame*, vol. 157, no. 3, pp. 465–475, 2010.

[2] P. Auzillon, B. Fiorina, R. Vicquelin, N. Darabiha, O. Gicquel, and D. Veynante, "Modeling chemical flame structure and combustion dynamics in LES," *Proc. Combust. Inst. 33*, vol. In Press, Corrected Proof, 2011.

[3] B. Janus, A. Dreizler, and J. Janicka, "Experiments on swirl stabilized non-premixed natural gas flames in a model gas turbine combustor," *Proc. Combust. Inst. 31*, no. 2, pp. 3091 – 3098, 2007.

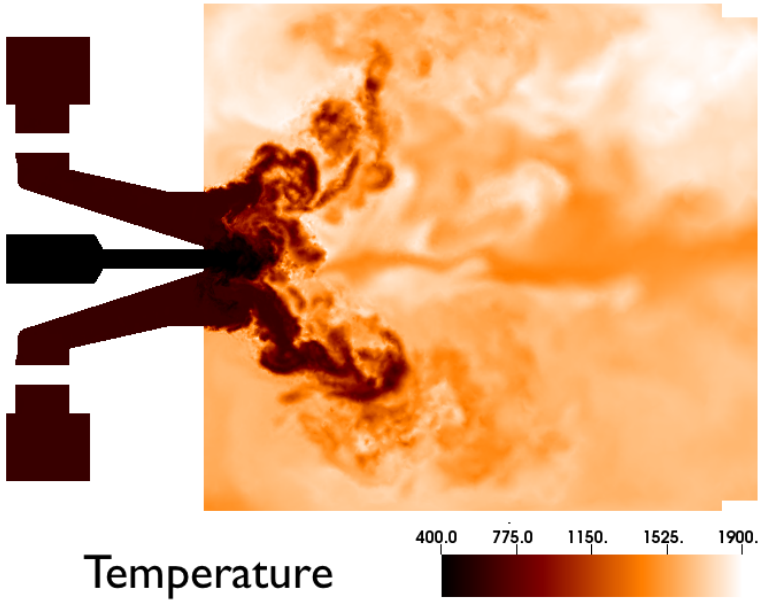

Figure 2: LES of the reactive case in the MOLECULES combustion chamber: iso-colours of the temperature field.

[4] O. Gicquel, N. Darabiha, and D. Thévenin, "Laminar premixed hydrogen / air counterflow flame simulations using flame prolongation of ildm with differential diffusion," in *Proc. Combust. Inst. 28*, 2000, pp. 1901–1908.

[5] B. Fiorina, R. Baron, O. Gicquel, D. Thévenin, S. Carpentier, and N. Darabiha, "Modeling non-adiabatic partially-premixed flames using flame prolongation of ILDM," *Combustion Theory and Modeling*, vol. 7, pp. 449–470, 2003.

[6] B. Fiorina, O. Gicquel, L. Vervisch, S. Carpentier, and N. Darabiha, "Approximating the chemical structure of partially-premixed and diffusion counterflow flames using FPI flamelet tabulation," *Combust. Flame*, vol. 140, no. 3, pp. 147–160, 2005.

[7] R. Vicquelin, B. Fiorina, S. Payet, N. Darabiha, and O. Gicquel, "Coupling tabulated chemistry with compressible CFD solvers," *Proc. Combust. Inst. 33*, vol. In Press, Corrected Proof, 2010.

[8] F. Charlette, C. Meneveau, and D. Veynante, "A power-law flame wrinkling model for les of premixed turbulent combustion, part i: non-dynamic formulation," *Combust. Flame*, vol. 131, no. 1/2, pp. 159–180, 2002.

[9] E. Schneider, A. Maltsev, A. Sadiki, and J. Janicka, "Study on the potential of BML-approach and G-equation concept-based models for predicting swirling partially-premixed combustion systems: URANS computations," *Combust. Flame*, vol. 152, no. 4, pp. 548 – 572, 2008.