

Sub-grid scale modeling of the equation of state for fully compressible combustion LES

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1 Introduction

Modern computing facilities allowing for well resolved flow simulations imply to revisit some of the classic modeling assumptions, in order to secure the accuracy of the description of the flow physics. In the simulations of turbulent flames, the modeling of the interactions between flow turbulence, thermodynamics and chemistry is a very sensitive point. Neglecting the effects induced by unresolved fluctuations of the species concentrations and of the temperature cannot be an option in the context of high-fidelity simulations. Along these lines, the treatment of the equation of state (EoS) in fully compressible Large-Eddy Simulation (LES) has not been addressed in detail so far. The filtering of the equation of state provides the filtered pressure in a fully compressible LES. Correlations between species, mass fractions and temperature are usually neglected to simply express the filtered pressure directly from the knowledge of the density-weighted filtered species mass fractions and temperature. A formulation that may be valid in the case of a strongly diluted mixture, but which fails in the particular case of oxy-combustion [1]. Even in the case of a binary mixture, it was illustrated in [8] how the error, brought by the simple linearisation of the filtered equation of state, grows with the filter size.

The equation of state for an ideal, or non-ideal gas, composed of n chemical species may be written in a generic form as a function of the partial densities, ρ_k , and temperature, T : $P = P(\rho_1, \dots, \rho_n, T)$. In the case of an ideal gas:

$$P = R \left(\sum_{i=1}^n \frac{\rho_i}{W_i} \right) T = \rho R \left(\sum_{i=1}^n \frac{Y_i}{W_i} \right) T = \rho r_{\text{Mix}} T, \quad (1)$$

where Y_i is the mass fraction and W_i is the molar weight of the i -th species. R is the universal gas constant and $r_{\text{Mix}} = (\sum_{i=1}^n Y_i/W_i) R = R/W$ the gas constant of the mixture and $W = (\sum_{i=1}^n Y_i/W_i)^{-1}$ the species averaged molar weight. Filtering this equation of state leads to:

$$\bar{P} = R \left(\frac{\overline{\rho T Y_1}}{W_1} + \dots + \frac{\overline{\rho T Y_n}}{W_n} \right). \quad (2)$$

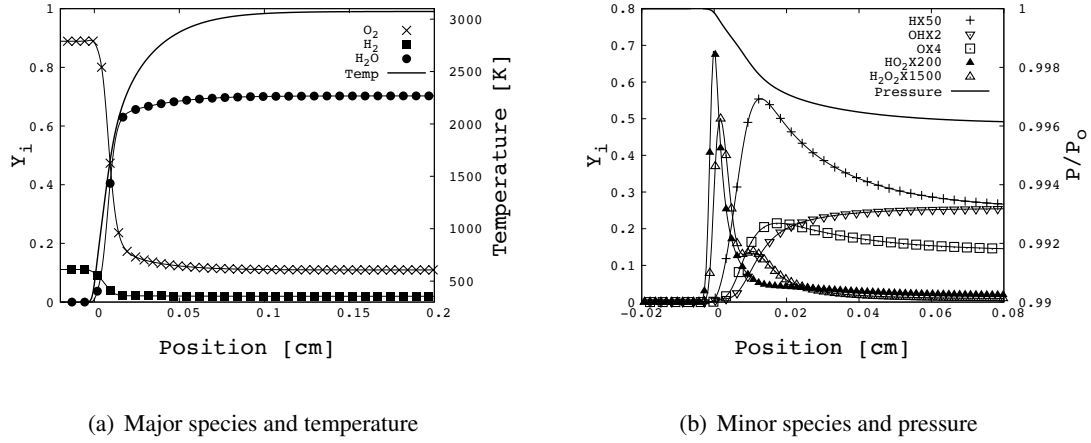


Figure 1: One-dimensional H_2/O_2 stoichiometric freely propagating premixed flame.

Today, in most fully compressible flow solvers, it is assumed that correlations between species concentrations and temperature can be neglected when filtering the equation of state $\overline{\rho Y_i T} = \overline{\rho} \widetilde{Y_i} \widetilde{T} \approx \overline{\rho} \widetilde{Y_i} \widetilde{T}$, where usual Favre (density weighted) filtering is introduced ($\widetilde{T} = \overline{\rho T} / \overline{\rho}$ and $\widetilde{Y_i} = \overline{\rho Y_i} / \overline{\rho}$). This assumption of weak variations of the mean molar weight may not be valid and this point is studied thereafter in the case of oxy-flames.

2 Canonical flames studied

Two canonical flows are examined to study space filtering of the equation of state. The fully compressible SiTCom-B¹ flow solver is used in which the convective terms are computed resorting to a fourth-order centered skew-symmetric-like scheme, the diffusive terms are discretized with a fourth-order centered scheme, time is advanced with a third-order Runge-Kutta method and the boundary conditions are prescribed with NSCBC. The first reacting flow is a one-dimensional premixed flame freely propagating in a stoichiometric mixture of H_2/O_2 . The chemistry is described with eight species O_2 , H_2 , H_2O , H , OH , O , HO_2 , H_2O_2 involved in 21 elementary reactions [9]. The transport coefficients are expressed with a mixture-average formulation [3]. For a resolution of $5\mu m$, Figure 1 shows distribution of major and minor species and temperature across the flame. The flame speed is $S_L = 10 m \cdot s^{-1}$ and the thermal flame thickness based on the temperature gradient is of the order of $200\mu m$.

The second reacting flow is a three-dimensional turbulent premixed flame developing downstream of a slot burner (Figure 2). The bulk velocity of the premixed jet is $70 m \cdot s^{-1}$ and its temperature is 300K. The temperature of the coflowing burnt gases is 3080K and the bulk velocity of this stream is $15 m \cdot s^{-1}$. Velocity fluctuations are added to the injected mean flow, according to a synthetic homogeneous turbulence with $u'/S_L = 2.1$. The structured mesh is composed of 200M cells with a resolution of $6.25\mu m$. A wrinkled premixed flame surface is observed, with eventually the formation of isolated pockets of burnt gases at the turbulent flame tip.

¹<https://www.coria-cfd.fr/index.php/SiTCom-B>

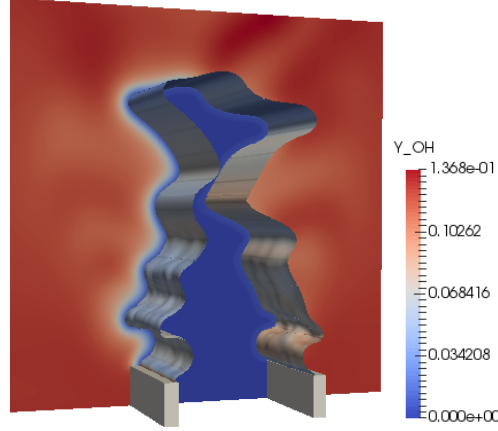


Figure 2: Snapshot of the stoichiometric H_2/O_2 slot-burner turbulent premixed flame.

3 Analysis of EoS filtering and SGS modeling

Expressing the equation of state in the linearized form, as usually done,

$$\bar{P} = R \left(\frac{\bar{\rho} \tilde{T} \tilde{Y}_1}{W_1} + \dots + \frac{\bar{\rho} \tilde{T} \tilde{Y}_n}{W_n} \right), \quad (3)$$

implies that SGS contribution $R \sum_{i=1}^n \frac{1}{W_i} (\bar{\rho} \tilde{T} \tilde{Y}_i - \bar{\rho} \tilde{T} \tilde{Y}_i)$, stays small compared to the filtered pressure. Filtered quantities are obtained in the one-dimensional flame and the three-dimensional DNS applying an approximate and discretized form of a Gaussian filter [5, 7]:

$$\bar{Y}_i = Y_i + \frac{\Delta^2}{24} \nabla^2 \bar{Y}_i, \quad (4)$$

in which an implicit formulation is chosen to secure stability and facilitate deconvolution discussed below. Figure 3 shows the distribution through the one-dimensional flame of $R(\bar{\rho} \tilde{T} \tilde{Y}_i - \bar{\rho} \tilde{T} \tilde{Y}_i)/(W_i \bar{P})$, for every species and its sum over all the chemical species. A filter size $\Delta = 300 \mu\text{m}$ is used. H_2O , H , OH and O have a positive contribution to the SGS term, up to 12% for H_2O while other species of this group contribute for less than 5%. The SGS term of HO_2 and H_2O_2 is of the order of a few % with a change of sign across the reaction zone. O_2 and H_2 have a negative SGS contribution, reaching -7% and -15%, respectively. The sum over all species is of the order of -4%.

The pressure variation expected through the laminar flame may be scaled from the conservation of momentum ($P + \rho u^2$), leading to

$$\frac{\Delta P}{P_o} = \frac{\rho_o}{P_o} \left(\frac{T_b}{T_o} - 1 \right) S_L^2, \quad (5)$$

where the subscripts ‘o’ and ‘b’ denote fresh and burnt gases respectively. In accordance with the one-dimensional flame simulation, a variation of the pressure of 0.494% is expected through the H_2/O_2 stoichiometric flame (Figure 1(b)). Therefore, the error brought by the linearization of the EoS is of the order of 8 times the flame pressure jump, which would significantly alter the quality of a simulation. Figure 4(a) shows a snapshot of $(\bar{P} - \bar{\rho} R \tilde{T} \sum_i (\tilde{Y}_i/W_i))/\bar{P}$ in a transverse plane of the slot burner three-dimensional

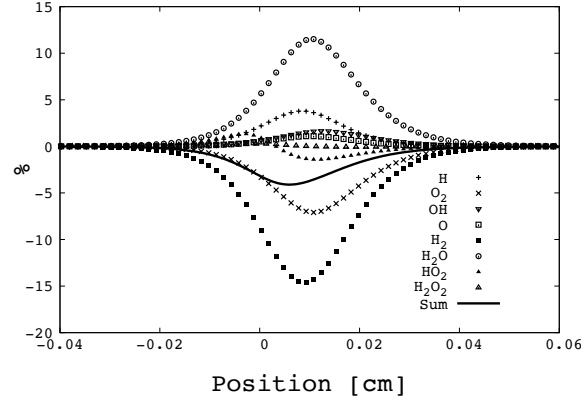


Figure 3: Distribution of $R(\overline{\rho T Y_i} - \tilde{\rho T Y_i})/(W_i \bar{P})$ (%) in 1D-Flame. *A priori* filtering $\Delta = 300 \mu\text{m}$.

flame for $\Delta = 300 \mu\text{m}$. As in the one-dimensional flame, the normalised SGS contribution peaks at -4%. The amplitude of this SGS part does not seem to be strongly correlated with flame curvature.

The relation $\overline{\rho Y_i T} = \overline{\rho Y_i} \overline{T} \approx \tilde{\rho Y_i} \tilde{T}$ assumes that correlations between temperature and species stay moderate and also that density weighted averaging could be applied to both Y_i and T , even though the density appears only once in the filtered expression. A new formulation may be proposed relaxing the later hypothesis:

$$\bar{P} = R \left(\frac{\overline{\rho T Y_1}}{W_1} + \dots + \frac{\overline{\rho T Y_n}}{W_n} \right), \quad (6)$$

where \bar{Y}_i has replaced \tilde{Y}_i . The corresponding normalized SGS term is $R(\overline{\rho T Y_i} - \tilde{\rho T Y_i})/(W_i \bar{P})$. The formulation (6) is examined in the three-dimensional flame. Figure 4(b) shows a snapshot of the departure between the filtered pressure and its estimation from Eq. (6). Compared to Figure 4(a), featuring the usual expression for the pressure, the SGS term that would be neglected is reduced by an order of magnitude. The mean of this term conditioned on the density weighted progress variable exhibits the same trend for the reduction of the part that would be left unresolved in a simulation. The relation (6), which appears as a valuable expression for the filtered pressure in the case of multicomponent and fully compressible flows, requires the calculation of \bar{Y}_i , which is not a transported information since density weighted quantities are usually considered in LES. Approximate deconvolution has been introduced under various circumstances to estimate unresolved terms from the knowledge of the information available on the mesh nodes [2, 4–6]. Reversing the approximate Gaussian filtering operation of relation (4) and applying it to the mesh size $\Delta = \delta_x$, brings an approximate deconvolution operator

$$\rho Y_i = \mathcal{L}_{\Delta}^{-1}[\tilde{\rho Y_i}] = \tilde{\rho Y_i} - \frac{\delta_x^2}{24} \nabla^2(\tilde{\rho Y_i}), \quad (7)$$

then, the Reynolds filtered mass fraction reads

$$\bar{Y}_i = \frac{\mathcal{L}_{\Delta}^{-1}[\tilde{\rho Y_i}]}{\mathcal{L}_{\Delta}^{-1}[\tilde{\rho}]} + \frac{\delta_x^2}{24} \nabla^2 \bar{Y}_i. \quad (8)$$

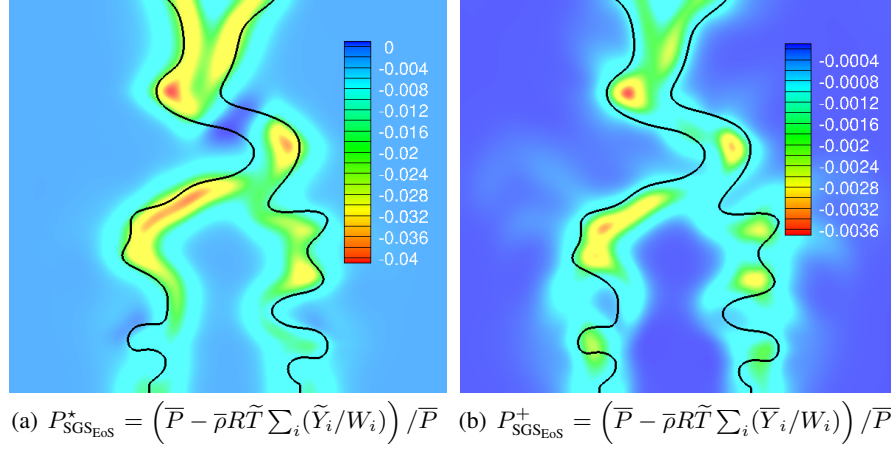
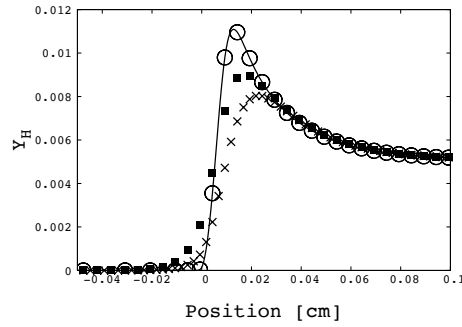


Figure 4: Snapshot in a transverse plane.

Figure 5: (—): Y_H ; \times : \tilde{Y}_H ; circle: Y_H from deconvolution; solid square: \bar{Y}_H ; 1D-Flame *a priori* filtering $\Delta = 300 \mu\text{m}$.

With this combination of an explicit formulation for deconvolution (7), and an implicit one for filtering (8), only derivatives of quantities resolved over the LES mesh are computed, thus avoiding the application of discretisation operators to the deconvoluted signals, which may not be fully resolved by the coarse mesh. This procedure is applied to the one-dimensional flame at first. Figure 5 shows the distribution of the mass fractions (original, density weighed filtered, deconvoluted and Reynolds filtered) for the H radical and $\Delta = 300 \mu\text{m}$. The deconvolution at Δ perfectly recovers the original profiles from the density weighted one and thus allows for computing the Reynolds filtered signal, which strongly differs from the density weighted one in the flame zone. Applied to the three-dimensional flame, the approximate deconvolution/filtering of the density filtered quantities provides an estimation of the filtered pressure with an error of the order of -0.55%.

4 Conclusion

The filtering of the equation of state, which provides the pressure in fully compressible simulations, has been discussed in the context of oxy-flames for which there is no species dominating the mean molar weight. Two H_2/O_2 reacting flows have been examined, a one-dimensional freely propagating premixed flame and a three-dimensional slot burner turbulent flame. In both of these flows, *a priori* LES filtering has revealed that the filtered pressure was better approximated using the Reynolds filtered mass fractions of the species to compute the molecular weight of the mixture. A deconvolution procedure has then been set up and evaluated to estimate the Reynolds filtered mass fractions from the density weighted transported ones.

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