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High-pressure methane-oxygen flames. Analysis of sub-grid scale contributions in filtered equations of state

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ABSTRACT

Turbulent combustion modelling under high-pressure conditions is a key issue for the design of future aero or rocket engines. In the context of large-eddy simulations, the exact filtered equation of state (EoS) is generally approximated by an EoS directly computed from the Favre filtered quantities for species mass fractions and temperature. The soundness of this approximation is presently addressed through the analysis of laminar CH_4-air and CH_4-O_2 high-pressure premixed and non-premixed flames. Their computations were performed either with the ideal gas equation of state (EoS) or with a high-pressure package that gather a cubic EoS along with additional pressure-dependent transport parameters and thermodynamic relations. Various kinetic schemes are used for the computation of laminar premixed flames and a comparison with available experimental data is provided for flame speed (S_L). Laminar premixed CH_4-O_2 flames exhibit micro metric flame thickness for pressures above 2.0 MPa as well as a high flame temperature (>3000 K). These flamelets were then filtered either with a Gaussian filter or through a β-pdf technique. The resulting filtered profiles were used to approximate the filtered pressure, $\overline{p}$. A negligible error is observed for CH_4-air flames when comparing $\overline{p}$ with the exact filtered pressure. However, significant errors were found for high-pressure CH_4-O_2 flames, that increase with the filter size. This behaviour is exacerbated for transcritical injections meaning that classical techniques that use tabulated thermochemistry methods in compressible codes must be revisited in that context. A correction to the tabulated chemistry approach coupled to a presumed subgrid pdf is finally proposed to comply with high-pressure considerations.

1. Introduction

Addressing the simulation of high-pressure flames is a numerical challenge that requires to combine a precise model for the flow description and an appropriated numerical strategy [1]. The framework of supercritical fluid flows simulation is well-known [2–4] but its use in a DNS (Direct Numerical Simulation) context is CPU demanding [5] and then limited to canonical problems. The use of LES (Large-Eddy Simulation) strategy requires models that are, most often, a direct use of low-pressure models without correction for high-pressure systems [6]. In particular, the coupling between the filtered equation of state (EoS), i.e. a function that link pressure (p), temperature (T) and density (ρ), and the equations that describe the flow motion, seems to be a key-point not so much addressed in the literature. If any EoS is written in a generic form as $p = p(\rho_k, T)$ with $\rho_k = \rho Y_k$, Y_k being the mass fraction of species k, the filtered EoS should be expressed as

$$\overline{p}(\rho_k, T) = p(\overline{\rho}_k, \tilde{T}) + p_{sgs}, \quad (1)$$

with p_{sgs} a subgrid scale contribution. The overbar denotes the spatial filtering operation and the tilde operator denotes the density weighted filtering defined for any variable $\mathcal{Q}$ as $\overline{\rho}\tilde{\mathcal{Q}} = \overline{\rho\mathcal{Q}}$. For ideal gas assumption p_{sgs} is commonly neglected [7]. For non-ideal gas, Selle et al. [8] showed that the validity of this approximation decreases with the increase of the filter size for binary mixtures at low Reynolds (Re) number. A model strategy is then required for the filtered pressure term appearing in the balance equations describing the flow motion as proposed in [9]. However, most of the current studies are based on low-Re DNS or experiments [10] which may be not representative of a real system where turbulence intensity is very strong. For instance, Petit et al. [6] showed that increasing the inlet velocity of Mayer's experiment [10] of one order of magnitude can lead to opposite results depending on the turbulence modelling used. Such a dependence on Reynolds number may be present when dealing with p_{sgs} in Eq. (1). Finally, real-gas

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cubic EoS have a strong non-linear behaviour that may be an issue when a filtering operation is employed [7]. In this paper, it is proposed to assess this issue by filtering 1D laminar premixed and non-premixed methane flames featuring ideal or real gas effects. Indeed, the structure of laminar flamelets is often viewed as the canonical structure of more complex turbulent flames. This strategy leads to store in a lookup table a set of conditioned flamelets [11], or alternatively, to store filtered flamelets [12–14].

In the past 10 years high-pressure non-premixed flamelets have been regularly studied numerically on counterflow flame configurations [15–18]. The impact of real gas effects has been found limited to the prediction of the dense stream, i.e. mainly cryogenic oxygen. Indeed, the heat coming from the flame increases the flame temperature and consequently reduces the impact of non-idealities: the compressibility factor stays close to unity in the flame [15] and insignificant impact has been observed on global quantities such as the heat release [17]. Cutrone et al. [19] then Kim et al. [20] showed that the non-premixed flamelet approach was able to simulate the LOx/methane combustion under their working conditions with a RANS formulation. No consequences on the mean pressure were noticed by the authors. Zong et al. [21] then Huo et al. [22,23] used this strategy to performed the LES of the high-pressure reactive CH_4-LOx combustion in the configuration of a shear coaxial injector. These simulations use compressible-flow equations with a preconditioned scheme to solve low-speed flows.

According to the authors, the only study dealing with supercritical freely premixed laminar flames was performed by Marchionni et al. [24] using the real-gas formulation of the Chemkin package [25]. Study's features are the introduction of the Redlich-Kwong EoS [26], the modification of the equilibrium reaction rate constants, which are used to compute reverse reaction rates in the kinetic scheme, and the consideration of pressure effects into thermodynamics calculations. The authors observe a low impact of real-gas models on methane-air mixtures for pressures below 4.0 MPa at ambient temperature (300 K). The predicted flame structures and flame speeds are thus essentially the same considering either ideal-gas or real-gas models. For pressures above 4.0 MPa, the decrease of the laminar flame speeds with a pressure increase is observed more rapidly when the real gas formulation is employed. A description of the structure of high-pressure CH_4/O_2 flames and its dependence on the chemical kinetic used is still lacking in the literature and it is addressed in this paper.

All these flamelets may be used in a RANS or LES solver through a tabulated chemistry approach [11,27]. The method to couple a fully compressible LES solver with a real-gas lookup table has been recently proposed by Lacaze and Oefelein [18] and Petit et al. [28]. Here again the proposed EoS was based on tabulated or filtered values without correction: $p_{sgs} = 0$.

To estimate the impact of the subgrid scale contributions in the equation of state, a set of laminar premixed and non-premixed CH_4-air and CH_4-O_2 flames featuring ideal and real gas EoS are first studied at low and high pressure (Section 2). These flames, as well as counterflow supercritical diffusion flames, are filtered with different various filter sizes to highlight the error made on the estimation of filtered pressure (Section 3). This behaviour is also assessed when constructing a lookup table to be used in LES for turbulent flows. A correction is then proposed. Conclusions are gathered in Section 4.

2. Supercritical premixed flamelets

2.1. Numerical solver

2.1.1. Governing equations

In the present study, the REGATH solver formerly used to compute supercritical counterflow flames [16,29] is adapted [30] to compute the structure of premixed flamelets. Using standard notations and considering the special case of stationary flames, the set of governing equations used for continuity, species and energy (h, total enthalpy) is given by, respectively:

$$\frac{\partial(\rho v)}{\partial y} = 0, \tag{2}$$

$$\rho v \frac{\partial Y_k}{\partial y} + \frac{\partial}{\partial y}(\rho Y_k V_k) - W_k \dot{\omega}_k = 0, \tag{3}$$

$$\rho v \frac{\partial h}{\partial y} - \frac{\partial}{\partial y}\left(\lambda \frac{\partial T}{\partial y}\right) + \frac{\partial}{\partial y}\left(\sum_{k=1}^{N_s} \rho Y_k h_k V_k\right) = 0, \tag{4}$$

the species diffusion velocity, V_k, follows the work of Pons et al. [16] for oxygen/methane flames where Soret and Dufour effects are neglected. W_k is the molecular weight of the kth species. The comparison of the flame speed computation with experimental data will be performed with variable and unity Lewis number (see Section 2.2). In Eq. (4), the determination of species enthalpy, h_k, may be found in [2]. Numerical technique is discussed in [31]. Finally, at the cold boundary, composition and temperature are prescribed; at the hot boundary, all gradients vanish.

2.1.2. Real-gas thermodynamics and transport

To address the computation of high-pressure flames, a pressure-dependent model for the description of thermodynamic and transport properties may be required. Following the recommendations of Poling et al. [26], thermodynamic properties, such as heat capacities, are evaluated based on fundamental thermodynamic theories. Each property is conveniently expressed as the sum of the ideal-gas formulation contribution and of a departure function that accounts for the dense-fluid effects. As in [15,16], the Soave-Redlich-Kwong (SRK) equation of state is chosen. As a consequence, pressure (p), density (ρ) and temperature (T) verify

$$p = \frac{\rho R_u T}{W - \rho b} - \frac{\rho^2 a\alpha(\omega)}{(W^2 + ubW\rho + wb^2\rho^2)}, \tag{5}$$

with $(u, w) = (1, 0)$ for SRK EoS [26]. R_u is the universal gas constant and W, the mean molar mass of the mixture. Using the Peng-Robinson (PR) EoS ($(u, w) = (2, -1)$ in Eq. (5)) instead of SRK EoS would not change the subsequent results as both equations give accurate results over the range of pressures, temperatures, and mixture states of interest for supercritical combustion [32,33]. For instance, Lacaze and Oefelein [18] recently performed the simulation of a supercritical H_2/O_2 counterflow flame with the PR EoS that compares very well with the reference simulation of Ribert et al. [15] who used the SRK EoS.

Considering the compressibility factor, $\mathcal{Z}$, defined as the deviation from ideal gas behaviour, Eq. (5) becomes

$$p = \mathcal{Z}\rho RT \quad \text{with} \quad R = \frac{R_u}{W}. \tag{6}$$

In Eq. (5), $a\alpha$ represents the attractive forces among molecules, b is the co-volume of molecules and ω is the acentric factor that quantifies the deviation from spherical symmetry in a molecule. These parameters are calculated with the Van der Waals mixing rules for a pool of N_s species:

$$a\alpha = \sum_{i=1}^{N_s}\sum_{j=1}^{N_s} X_i X_j \alpha_{ij} a_{ij}, \tag{7}$$

with $\alpha_{ij}a_{ij} = \sqrt{\alpha_i\alpha_j a_i a_j}(1 - \kappa_{ij})$ and,

$$b = \sum_{i=1}^{N_s} X_i b_i. \tag{8}$$