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A simplified CMC approach based on tabulated reaction rates applied to a lifted methane–air jet flame

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Abstract

This paper explores the possibility to close the conditional reaction rate in the Conditional Moment Closure (CMC) turbulent combustion model using tabulated chemistry. This combination, called TCMC (Tabulated CMC), is based on the resolution of transport equations for the conditional mean and variance of the progress variable mass fraction $Y_c = Y_{CO} + Y_{CO_2}$ in which chemical source terms are taken from a look-up table built with homogeneous reactor calculations. First and second order TCMC closures (respectively TCMCI and TCMCII) are proposed and are compared on the lifted methane–air flame experiment of Cabra et al. (2005) [2]. In this configuration, it is shown that the first order model is unable to predict a lifted flame, whereas TCMCII gives correct results in terms of mean composition and temperature. These results are found comparable to those obtained by Michel et al. (2009) [7] with the ADF-PCM (Approximated Diffusion Flame Presumed Conditional Moment) flamelet model based on the same progress variable and tabulated kinetics. On the contrary, conditional flame profiles are different in the lift-off zone, and lift-off height predictions are improved with TCMCII. Finally, the CPU time of TCMCII is found less than ten times that of ADF-PCM, using a unique mesh for all transport equations, which makes TCMC a realistic alternative to tabulated flamelet models.

Keywords: CMC; Tabulated chemistry; Flamelet; Autoignition

1. Introduction

In the context of increasingly stringent requirements for the energetic efficiency and pollutant emissions of combustion devices such as internal combustion engines and gas turbines, computational fluid dynamics (CFD) plays a key role in designing and optimizing new concepts. In many industrial applications (gas turbines, furnaces, Diesel engines) a lifted flame is observed. Controlling this height is crucial for the burner integrity, for flame stability (especially for low heating value fuels) and for resulting pollutants formation. Despite numerous studies on the subject, the stabilization mechanism is still not fully understood yet. It could be explained by flame extinction, flame propagation and in the case of dilution by a hot coflow, by autoignition like in the laboratory

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methane/air flame of Cabra et al. considered here [1].

In past studies, various combustion models have been tested on such flames. Transported pdf [2] allowed to recover correct lift-off heights, showing a stabilization of the flame by autoignition. To account for laminar diffusive effects, other models rely on Peters flamelet equation [3]. In the representative interactive flamelet (RIF) model [4], only a limited number of flamelets are accounted for, which results in a less accurate description of spatial diffusion, essential for flame stabilization. To account for micro-scale diffusive effects and keeping a low CPU time, various tabulated flamelet models were proposed based on the same equation. Among them, the ADF-PCM (Approximated Diffusion Flame PCM) model [5] was developed with the aim of including complex chemistry effects thanks to a tabulation technique similar to FPI [6] but based on autoigniting homogeneous reactor (HR) calculations. While in ADF-PCM only the mean local strain rate is considered, in [7], a presumed log-normal distribution of scalar dissipation was introduced in the look-up table generation to account for scalar dissipation fluctuations which are known to control the autoignition location [8]. The resulting model, ADF-PCM$_\chi$, led to improved lift-off heights compared to ADF-PCM in RANS (Reynolds Averaged Navier Stokes) on the same experiment.

Despite these encouraging results, tabulated flamelet models rely on the strong assumption that the flame structure can be approximated by a constant strain laminar diffusion flame. The Conditional Moment Closure (CMC) [9] is a general mathematical formalism which does not imply any assumptions on the topology of the reaction zone, which is very attractive for describing the stabilization of lifted flames. As noted in [10], CMC modeling for autoigniting jets was up to recently limited either to higher order closure (CMCII) with very simple kinetics [11] or to more complex mechanisms using first-order (CMCI) closure [12]. The difficulty is that complex chemistry is required for accurate autoignition description but at the same time, first-order modeling does not always allow to account for the high level of fluctuations observed in the stabilization region. Recently, De Paola et al. [10] performed first and second-order CMC with complex chemistry on their H2/air jet experiment, and found similar results for both models. Patwardhan et al. performed similar CMCI calculations on the H2/air jet flame [13] and found that for low coflow temperature, lift-off is controlled by premixed flame propagation while for higher temperature, autoignition becomes preponderant. In [14], detailed chemistry CMCI LES gave good results for the methane/air lifted flame and allowed to recover the periodic fluctuations of the leading point.

Despite the use of two distinct meshes (a fine one for the flow field and a coarser one for CMC equations) which allows CMCI to be used in several industrial applications (see e.g. [15]), its CPU cost remains high. For CMCII, the number of transport equations increases even more rapidly with the size of the mechanism. Besides, modeling the conditional reaction rate using Taylor expansions or presumed single scalar pdf becomes questionable for high levels of fluctuations and for large mechanisms [10]. The objective of this paper is to propose and evaluate an alternative conditional reaction rate model for CMC allowing to substantially reduce the CPU time. The idea is to apply the tabulated chemistry approach developed in ADF-PCM [5] to CMC equations: a single reactive scalar Y_c is considered, its reaction rate being given by a HR table. In other words, it consists in adding physical space contributions given by CMC to the ADF-PCM flamelet equation.

Section 2 presents briefly first and second order CMC equations applied to the progress variable Y_c. Section 3 presents the experiment, numerical set-up and the main results obtained with the twin flamelet and CMC models, highlighting the major differences between them.

2. Mathematical formulation

2.1. First and second order CMC equations

In the present model, first and second order CMC equations [9] are applied to a unique progress variable defined following the FPI tabulated chemistry approach [7,6]: $Y_c = Y_{CO} + Y_{CO_2}$. The instantaneous and local mass fraction Y_c is decomposed into its Favre conditional mean and fluctuations as: $Y_c(x,t) = Q(\eta,x,t) + Y_c''(\eta,x,t)$ with the conditional mean being defined as $Q(\eta,x,t) = \langle Y_c(x,t)|\xi(x,t) = \eta\rangle$. Here ξ is the mixture fraction and η is the sample space variable for ξ; angular brackets denote ensemble averaging subject to the condition $\xi(x,t) = \eta$. The conservation equation for Q then reads:

$$\frac{\partial Q}{\partial t} = \underbrace{-\langle \mathbf{u}|\eta\rangle.\nabla \mathbf{Q}}_{S_q^1} \underbrace{- \frac{\nabla.(\langle u'' Y_c''|\eta\rangle \bar{\rho}\widetilde{P}(\eta))}{\bar{\rho}\widetilde{P}(\eta)}}_{S_q^2} + \underbrace{\langle N|\eta\rangle \frac{\partial^2 Q}{\partial \eta^2}}_{S_q^3} + \underbrace{\langle \dot{\omega}_{Y_c}|\eta\rangle}_{S_q^4} \quad (1)$$

In the above equation term S_q^1 represents the conditional mean velocity. It is modeled neglecting conditional fluctuations around the Favre average (the linear approximation [9] was tested without significant impact on results): $S_q^1 = \tilde{\mathbf{u}}$. Term S_q^2 represents the turbulent diffusion and is classically