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Turbulent combustion modelling of a confined premixed methane/air jet flame using tabulated chemistry

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Abstract

The present work addresses the coupling of a flamelet database that can accurately represent the flame structure in composition space with a low-Mach approximation of the Navier-Stokes equations. An advancement of the CFI combustion model, which is currently based on laminar premixed flamelets, is used for chemistry tabulation. This model can be applied to different combustion regimes from premixed to non-premixed combustion, although this work is concentrated on turbulent premixed flames for Reynolds-averaged Navier-Stokes (RANS) and large-eddy simulations (LES). A premixed confined jet flame, which has been investigated experimentally at the German Aerospace Center (DLR) is used for validation in adiabatic conditions showing satisfactory agreement.

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Keywords: turbulent combustion modelling, premixed flames, tabulated chemistry, RANS, LES

1. Introduction

Turbulent combustion models based on tabulated chemistry are becoming a fundamental approach to investigate the dynamics of flames at reduced computational cost. Instead of solving transport equations for all chemical species involved in the reacting process, one or several scalars are used to represent the combustion chemistry in composition space [1]. In the current work, an advancement of the CFI combustion model [2] for RANS and LES is presented and validated against the experimental data from Lammel et al. [3]. The conditions under investigation correspond to a confined lean premixed methane/air flame with equivalence ratio of 0.71. The test case is operated at ambient pressure with a mixture preheated up to 573 K. The chemical database is created based on laminar premixed one-dimensional flamelets, which take into account the full chemical kinetics and detailed transport phenomena. This flamelet library is then projected onto a scalar that describes the progress of reaction referred here as reaction progress variable (RPV). Turbulence-chemistry interaction is modelled by introducing the variance of the RPV (VRPV) in combination with a presumed beta probability density function (β-PDF). Closures for the variance are presented in RANS and LES framework. The combustion model is coupled to a low-Mach formulation of the Navier-Stokes equations and the Alya multiphysics code [4] is used as the framework of numerical analysis.

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2. Mathematical modelling

This section describes the governing equations as well as the chemistry tabulation employed in the numerical simulations to obtain the solution fields for RANS and LES.

2.1 Governing equations

The equations governing the reacting flow field are the continuity, momentum and temperature equations, which can be found elsewhere [5]. The RPV and VRPV transport equations are:

$$\frac{\partial \overline{\rho}\tilde{c}}{\partial t} + \nabla \cdot (\overline{\rho}\tilde{\boldsymbol{u}}\tilde{c}) = \nabla \cdot \left[(D + D_t)\nabla \tilde{c}\right] + \overline{S}_k$$

$$\frac{\partial \overline{\rho}\widetilde{c''^2}}{\partial t} + \nabla \cdot (\overline{\rho}\tilde{\boldsymbol{u}}\widetilde{c''^2}) = \nabla \cdot \left[(D + D_t)\nabla \widetilde{c''^2}\right] + \overline{P}_k + \overline{D}_k + \overline{Q}_k$$

where S_k, P_k, D_k and Q_k represent the source, production, dissipation and burning rate terms, respectively. The source term S_k is tabulated after integration over the β-PDF. The modelling of the production and dissipation terms is essentially different for RANS or LES. These terms have the following form in RANS [2]:

$$\overline{P}_k = 2\frac{\mu_t}{Sc_t}\left(\nabla \tilde{c}\right)^2, \quad \overline{D}_k = -\overline{\rho} C_\chi \frac{\epsilon}{k}\widetilde{c''^2}, \quad \overline{Q}_k = 2\rho\left(\widetilde{\dot{S}_k c} - \tilde{\dot{S}}_k \tilde{c}\right)$$

while for LES, those terms are of the form:

$$\overline{P}_k = 2\frac{\mu_t}{Sc_t}\left(\nabla \tilde{c}\right)^2, \quad \overline{D}_k = -2\overline{\rho}\frac{\mu_t}{\Delta^2 Sc_t}\widetilde{c''^2}, \quad \overline{Q}_k = 2\rho\left(\widetilde{\dot{S}_k c} - \tilde{\dot{S}}_k \tilde{c}\right)$$

2.2 Chemistry tabulation

The CFI approach reduces the stiffness of the reacting simulation by using a thermo-chemical database obtained from tabulating the combustion process. A laminar premixed one-dimensional flame calculation is carried out using CHEMKIN-II [6]. The detailed GRI-Mech 3.0 [7] consisting of 325 elementary reactions and 53 species is employed. The chemistry simulation provides the dependent variables as function of the (one-dimensional) coordinate *x*. In a second step, the results are mapped onto the RPV ($\varphi(x) \rightarrow \varphi(c)$), which is defined as:

$$c = \frac{\eta_k - \eta_k^u}{\eta_k^{eq} - \eta_k^u} \qquad \text{with:} \quad \eta_k = \sum_{j=1}^{N} b_j y_j \ , \quad \eta_k^{eq} = \sum_{j=1}^{N} b_j y_j^{eq} \ , \quad \eta_k^u = \sum_{j=1}^{N} b_j y_j^u$$

In this equation, the superscripts *u* and *eq* refer to the unburnt and equilibrium composition. b_j describes the RPV composition and can be understood as a weight factor indicating the contribution of the mass fraction of species j to the composed mass fraction η_k. It is calculated using the Computational Singular Perturbation (CSP) method [8, 2]. A stochastic approach is used to account for turbulence-chemistry interaction and the RPV is averaged using a β-PDF. Thereby, another dimension is added to the thermo-chemical database ($\varphi(c,c''^2)$).

3. Results

This section addresses the comparison of the numerical simulations for RANS and LES using the extension of the CFI combustion model with the experimental data from Lammel et al. [3], along with the adiabatic RANS results from Donini at el. [9]. The results presented here correspond to the reacting flow field assuming adiabatic conditions in the combustor. Results including the heat losses will be included in the extended paper.