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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.

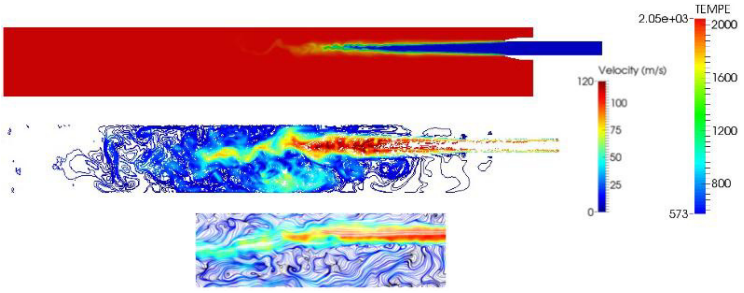

Figure 1: Cross-contours of temperature (top), streamwise velocity (middle) and experimental [3].

The main flow features can be identified from the instantaneous fields presented in Fig. 1. The flame is bent towards the far side of the burner due to the lateral recirculation zone created by the off-center positioning of the nozzle. The LES reproduces structures of the velocity field that are observed in the experiments, especially at downstream locations.

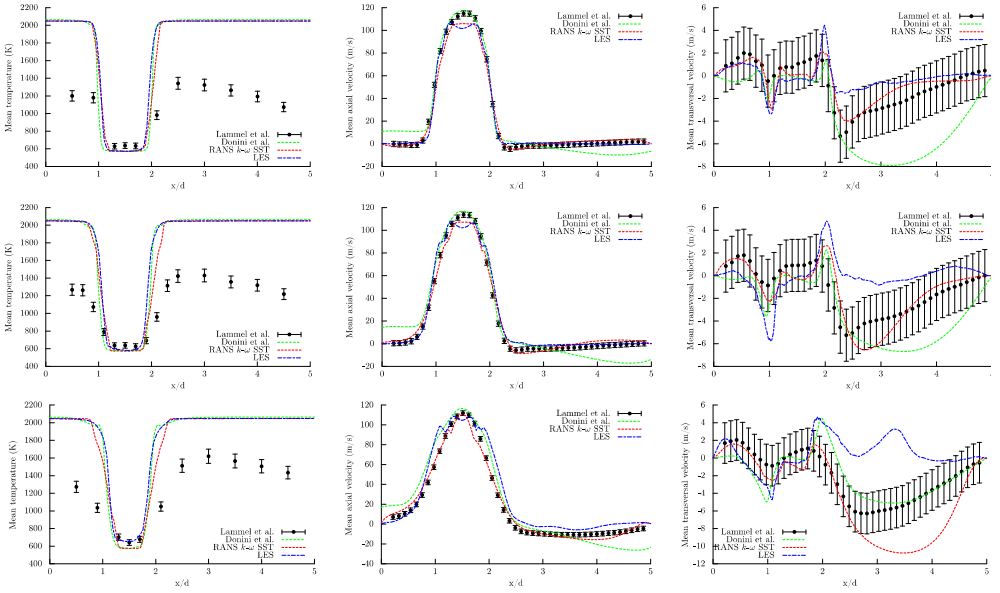

Figure 2: Comparison of numerical simulations and experimental data at three axial locations (top to bottom) for temperature, axial velocity and transversal velocity (left to right).

In Fig. 2, the simulation results are compared to the experimental data at three streamwise measurement positions, which are located at one, two and four nozzle diameters downstream of the jet exit. Temperature, axial and transversal velocities are shown for adiabatic conditions in RANS and LES framework. The temperature profiles evidence the strong effect of heat loss in this configuration that contributes to the reduction of the burning rates and peak temperatures. Both RANS and LES results show excellent agreement with the results from Donini at el. [9] for the temperature plots at all three locations. However, there are some discrepancies at predicting the jet spreading in the RANS model that will be further examined when the non-adiabatic cases are compared with the experiments. The axial velocity is well reproduced by the numerical simulations and correlates well with the experiments in most locations. At the most upstream location, both RANS and LES underpredict the peak value. In addition, the LES shows a small bump in the velocity profile caused by the density variation across the flame that

is currently being investigated. The underprediction of the peak value for the two models might be caused by a velocity profile at the nozzle exit that does not correctly predict the turbulence characteristics. Further downstream, the RANS and LES profiles show an excellent agreement with the experimental data. The peak values and the location of the recirculation zone are predicted satisfactorily, although it is slightly underpredicted by the LES. The plots of the transversal velocity also reveal a good agreement with the experimental data at most locations. While the RANS solution is well aligned with the experimental data for the upstream locations, the LES case underpredicts the transversal velocity along the recirculation zone.

4. Conclusions and future work

An advancement of the CFI combustion model is introduced to study turbulent combustion in adiabatic conditions with application for RANS and LES. Results are presented for a confined lean premixed jet flame. Due to the neglected heat losses to the walls, the temperature field in the simulation deviates significantly from the experimental data. This leads to an overprediction of the temperature in the entire domain. However, the temperature field is in excellent agreement with the adiabatic simulation of Danini et al. The predicted velocity fields are in good agreement with the experi- mental reference data. Only the location of the lateral recirculation zone is not captured exactly for both, RANS and LES. This can be explained by the neglected heat losses, which result in an underprediction of the flame length. The current work is focused on the adiabatic conditions. The extension to non-adiabatic flow will be included in the extended paper. The resulting changes in the solution procedure will be addressed and results for RANS and LES will be presented and compared to the experiments as well as the adiabatic results that are shown in this paper. As the current test case is characterized by high heat losses to the walls, a significant improvement, especially for the temperature field, is expected.

5. Acknoledgments

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