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Large Eddy Simulation of the PRECCINSTA burner

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ABSTRACT

For the first time the Reaction–Diffusion Manifold (REDIM) technique is implemented together with a presumed Filtered Density Function (FDF) to carry out Large Eddy Simulation (LES) of lean premixed swirling flames in the well-known PRECCINSTA burner. The REDIM approach reduces detailed chemical kinetics based on low-dimensional reaction–diffusion manifolds in composition space, so that many species can be accurately estimated at a relatively low computational cost via a look-up table. In the present work, only one reduced coordinate, the CO_2 mass fraction, is considered in the REDIM look-up table. Implementation of the REDIM/FDF model is performed with two presumed FDF shapes, top-hat and clipped Gaussian. Two premixed flames are simulated, with equivalence ratios 0.75 and 0.83, respectively. Velocity, temperature and species concentration profiles are discussed and compared to the experimental data. The results are in good overall agreement with the corresponding experiment. It is also shown that the LES results obtained with the two presumed FDFs are very similar and the reason for this is analysed.

1. Introduction

Large Eddy Simulation (LES) has been gaining importance as a combustion simulation tool over the past few years due to its ability to predict instabilities, extinction, re-ignition and other unsteady phenomena with appropriate combustion models [1,2]. With the increase of computer power, LES will be used more and more often in combustion industry at the design stage [3]. However, there are still open challenges. In LES of turbulent combustion, a good model to account for the chemical dynamics is needed. Combustion of methane in air, for example, involves over 50 species and 300 reactions [4]. A straightforward utilization of such detailed chemical kinetics hence is prohibitive in a simulation using hundreds of millions of grid points and an unsteady turbulence-resolving approach in time, except in very particular cases of fundamental research. A model is required that is capable of using the essence of the detailed chemistry mechanism without the prohibitive cost of solving transport equations for numerous species.

Various mathematically motivated reduction schemes for combustion chemistry exist [5–7]. The Intrinsic Low-Dimensional Manifold (ILDM) [8] is an early one. The reaction process is described by means of an eigenvector analysis of the Jacobian matrix for the governing equations in composition space so that in the finally retained subspace (manifold) only slow scales are present. The Flame Prolongation of ILDM (FPI) [9] and the Flamelet Generated Manifold (FGM) [10,11] are two more recent approaches to downsize combustion chemistry by using trajectories in composition space obtained from the calculation of laminar flames. Recent review articles provide a detailed description of these techniques and discuss their respective properties [5–7].

Based on its predecessor ILDM, Bykov and Maas [12,13] recently developed a new technique called the Reaction–Diffusion Manifold (REDIM) to reduce detailed chemistry mechanisms while at the same time accounting for molecular diffusion. REDIM overcomes many of the deficiencies of ILDM, because it takes into account the coupling of reaction and molecular transport processes, and therefore is applicable in regions where chemical kinetics are slow and diffusion governs the overall process. With REDIM, the detailed chemistry mechanism is reduced, with the possibility to choose a distinct number of reduced coordinates. These reduced coordinates are used together with a look-up table to determine other variables, including the reaction rates. The equations for the reaction rates are highly non-linear and stiff. It is hence advantageous to be able to determine the reaction rates through a table, with no need to solve the equations.

Reduced chemistry can be utilized in combination with a Filtered Density Function (FDF), where filtering refers to the LES filter in space, compared to the unaltered Probability Density Function (PDF) of a Direct Numerical Simulation. This approach has the

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advantage of treating chemical reactions exactly without any further modeling. FDFs have been used with different chemistry look-up tables, such as ILDM [8] and a Flamelet library [14] to determine the distribution of a variable at the sub-grid scale (SGS). Generally, two methods can be used to calculate the FDF – transported FDF and presumed FDF. In the former case, the exact FDF is calculated by solving further transport equations. This method is more general, and copes better with the fact that variables are not statistically independent. On the other hand, this approach is very costly and at present too expensive for routine LES calculations [15,16]. In the RANS context the transported PDF method has already been successfully implemented with the REDIM technique [17,18]. With the presumed FDF method, the general shape of the FDF is devised *a priori*, and parameterised in terms of low moments, usually the mean and the variance. This method is cheaper and quicker, and still provides satisfactory results [19,20]. There are a number of well-established FDF shapes including the top-hat, the clipped Gaussian, the beta function, and so on. The top-hat is considered to be the simplest presumed FDF shape, applicable in a wide range of cases [19,20]. The clipped Gaussian shape is widely used in a range of applications, often with joint FDFs [21]. For turbulent combustion, the beta function is often used for a mixture fraction in a diffusion flame while it is rarely used when a reactive scalar is considered, such as the reaction progress variable in premixed combustion [22,23].

In the present paper, a new turbulent premixed combustion model for LES is described based on a combination of the REDIM technique and a presumed FDF. The new model is then validated by simulating two premixed methane/air flames in a well-known premixed combustor.

2. Turbulent premixed combustion modeling

REDIM is based on the solution of an evolution equation for a low-dimensional manifold in the thermo-kinetic space [12,13]:

$$\frac{\partial \boldsymbol{\Psi}}{\partial t} = \left(I - \boldsymbol{\Psi}_{\boldsymbol{\theta}} \boldsymbol{\Psi}_{\boldsymbol{\theta}}^{+}\right)\left\{F(\boldsymbol{\Psi}) + \frac{d}{\rho}\boldsymbol{\chi} \circ \boldsymbol{\Psi}_{\boldsymbol{\theta}\boldsymbol{\theta}} \circ \boldsymbol{\chi}\right\} \tag{1}$$

Here, the thermo-kinetic space is described by a vector $\boldsymbol{\Psi}$. This vector is a function of one or multiple reduced coordinates, given by the vector $\boldsymbol{\theta}$. In the present work, equal diffusivities of species and $Le = 1$ are assumed. The variable $\boldsymbol{\rho}$ is the density, $\boldsymbol{\chi}$ is the vector of spatial gradient estimates for $\boldsymbol{\theta}$, $\boldsymbol{F}(\boldsymbol{\Psi})$ is the vector of the chemical source terms, $\boldsymbol{\Psi}_{\boldsymbol{\theta}}$ the matrix of partial derivatives of $\boldsymbol{\Psi}$ with respect to $\boldsymbol{\theta}$ and $\boldsymbol{\Psi}_{\boldsymbol{\theta}}^{+}$ its Moore–Penrose pseudo-inverse, $\boldsymbol{\Psi}_{\boldsymbol{\theta}\boldsymbol{\theta}}$ is the Hessian matrix. The symbol '$\circ$' in Eq. (1) is an abbreviation for the multiplication of two vectors with a tensor of third order [12].

The method to obtain spatial gradients, $\boldsymbol{\chi}$, for the generation of the REDIM table is described in detail in the reference [12,13]. For the one-dimensional REDIM table, the initial spatial gradients can be obtained from a simulation of a laminar one-dimensional flame simulation with detailed chemistry. Of course an iterative procedure to re-new and minimize the influence of initial estimation of gradient could be used as discussed in [13]. In the present work the gradient estimations were obtained by a laminar flame calculation.

Any number of reduced coordinates can be used with REDIM. The flame considered here is a fully premixed methane/air flame, with constant equivalence ratio and without local extinction phenomenon, so that a single reduced coordinate is sufficient. In the present case the mass fraction of CO_2 is used. The other species (CH_4, CO, O_2, H_2O, N_2, and OH) as well as the density and the production rate of CO_2 are determined as a function of that coordinate via the look-up table. Fig. 1 shows the data from one of the employed one-dimensional REDIM tables for the density and the production rate of CO_2 employed in the simulations below for illustration.

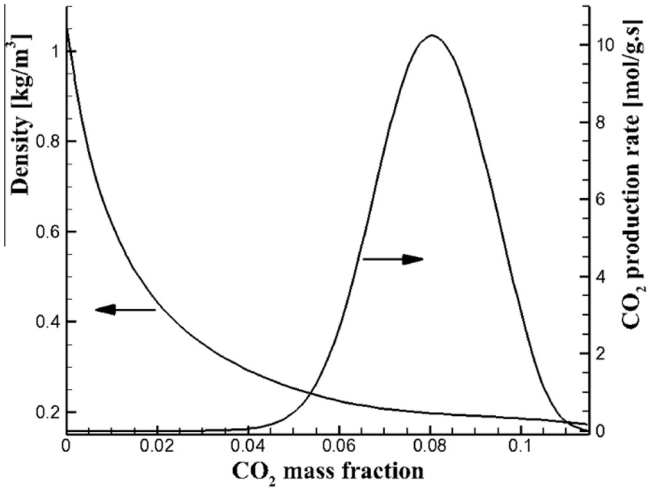

Fig. 1. The one-dimensional REDIM table for the density and the production rate of CO_2, for equivalence ratio $\phi = 0.75$. The temperature of the unburnt mixture is 320 K.

The transport equations solved are those for continuity, momentum and CO_2 mass fraction. The Favre filtered transport equation for the CO_2 mass fraction is:

$$\frac{\partial \bar{\rho}\widetilde{Y}_{CO_2}}{\partial t} + \frac{\partial}{\partial x_i}(\bar{\rho}\tilde{u}_i\widetilde{Y}_{CO_2}) + \frac{\partial}{\partial x_i}\left(\rho u_i \overline{Y}_{CO_2} - \bar{\rho}\tilde{u}_i\widetilde{Y}_{CO_2}\right) = \frac{\partial}{\partial x_i}\left(\bar{\rho}\overline{D}_{CO_2}\frac{\partial \widetilde{Y}_{CO_2}}{\partial x_i}\right) + \bar{\rho}\tilde{\dot{\omega}}_{CO_2} \tag{2}$$

The Favre filtered production rate, $\tilde{\dot{\omega}}_{CO_2}$, is determined from a pre-calculated REDIM/FDF table. This table is a short cut to convert the first and second moment of Y_{CO_2} by means of the REDIM table and the presumed FDF function into the required reaction rate in the following way. The filtered value and the variance of the CO_2 mass fraction are used to determine the shape of the Favre FDF, $\tilde{p}(\varphi; \widetilde{Y}_{CO_2}, \widetilde{Y}''^2_{CO_2})$. Here, φ is the chosen reduced coordinate of the REDIM table, i.e. the mass fraction of CO_2 in the present case. The mean value is obtained from Eq. (2), while the variance is modeled algebraically as proposed in [19]:

$$\widetilde{Y}''^2_{CO_2} \approx \frac{C}{4}\left[\left(\widetilde{Y}_{CO_2,n} - \widetilde{Y}_{CO_2,s}\right)^2 + \left(\widetilde{Y}_{CO_2,w} - \widetilde{Y}_{CO_2,e}\right)^2 + \left(\widetilde{Y}_{CO_2,u} - \widetilde{Y}_{CO_2,l}\right)^2\right] \tag{3}$$

where subscripts n, s, e, w, u, l denote the six adjacent computational cells in north, south, east, west, upper, and lower direction of the Finite Volume Method employed for spatial discretization, respectively. In (3), C is a model constant for which different values have been used in previous studies [19,23–25]. In the present work, the value of C is taken to be 0.2 according to [25].

For a general scalar variable f, depending on φ, its Favre filtered quantity at given $\widetilde{Y}_{CO_2}$ and $\widetilde{Y}''^2_{CO_2}$ is found with the Favre FDF integration via

$$\tilde{f} = \int_{\varphi_{\min}}^{\varphi_{\max}} f(\varphi)\tilde{p}(\varphi; \widetilde{Y}_{CO_2}, \widetilde{Y}''^2_{CO_2})d\varphi, \tag{4}$$

while the Reynolds-filtered density is calculated via

$$\bar{\rho} = \left[\int_{\varphi_{\min}}^{\varphi_{\max}} \frac{\tilde{p}(\varphi; \widetilde{Y}_{CO_2}, \widetilde{Y}''^2_{CO_2})}{\rho(\varphi)}d\varphi\right]^{-1}, \tag{5}$$

In the present work, the values of $\tilde{f}(\widetilde{Y}_{CO_2}, \widetilde{Y}''^2_{CO_2})$ and $\bar{\rho}(\widetilde{Y}_{CO_2}, \widetilde{Y}''^2_{CO_2})$ are tabulated using 100 $\widetilde{Y}_{CO_2}$ times 50 $\widetilde{Y}''^2_{CO_2}$ values.