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Reduction of Reacting Flow Models by the Reaction-Diffusion Manifolds Method for Methane/Air Turbulent Jet Diffusion Flames

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Resumo. Combustion processes are usually described using detailed chemical kinetic mechanisms. Sometimes, in the modeling of the complex burner systems is necessary to use chemical reduction techniques to decrease the stiffness of the system of differential equations. The principal difference among the existing reduction methods appears in the tactics to distinguish between slow and fast processes. In the present work the Reaction-Diffusion Manifolds method is applied to the methane/air reaction mechanism, in order to reduce the chemical kinetic model, depending on transport properties. The approach allows incorporating the effect of the coupling of reaction and diffusion processes. The methodology applied, based on slow manifolds of low dimension, allows decreasing the computational time needed to obtain results for confined turbulent jet diffusion flame. The Large-Eddy Simulation is required to represent the turbulent flow. The numerical results compare favorably with the experimental data available in the literature.

Palavras-chave. Methane, Flames, Turbulence, REDIM

1 Introduction

A large variety of models describing several processes occurring in combustion, as chemistry and turbulence, and a variety of numerical tools needed to solve the underlying equation systems have been developed [9]. It is known that typical kinetic models used in reacting flows contain many elementary reactions, are stiff and non-linear. Hence methods of dimension reduction of large detailed chemical kinetic models are very important and have been developed intensively in the last years.

Chemically reacting flows are governed by a strong interaction of chemical kinetics with molecular transport properties. Therefore, the reduced models for such systems have to take into account both the chemical reaction and the diffusion processes. To deal with this problem, the developed reduction method, the so-called Reaction-Diffusion Manifolds (REDIM) method accounts for the transport properties [6].

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Most of the existing methods exploit the so-called natural multi-scale structure of the system of governing equations. It is assumed that there are some fast modes or processes which are relaxed quickly and that only the slow processes govern the overall system dynamics. As a result, the long term system evolution is represented primarily by the dynamics of the slow reactions along a stable geometrical attractor with invariant properties, while the fast processes are relaxed. Moreover, removing the fast modes and reducing the dimension decreases the stiffness of the system of differential equations. This in turn allows larger time steps during the integration and, therefore, solves one major problem of the numerical implementation.

The reduced kinetic mechanism is constructed as a table of a slow manifold mesh in the composition or state space. The manifold table contains all necessary information about the reduced kinetics as well as about the projection of the original system of governing equations on this low dimensional manifold. Thus, the actual reduction is realized by a reformulation of the system of governing equations on the lower dimensional manifold, that approximates the full system dynamics in the state space.

Note that the 1D REDIM method, fully corresponds to the flamelet method, because it reproduces the detailed stationary solution. However, it allows an extension to higher dimensions and, therefore, it solves problems where 1D flamelets cease to describe the complex chemistry-transport interaction in an accurate way.

Turbulent combustion modeling is a very broad subject. In recent years many studies have been devoted to applicability of combustion models in Large-Eddy Simulations (LES). The objective of Large-Eddy Simulations is to compute explicitly the largest structures of the flow, while the effects of the smaller one is modeled [4]. This is particularly interesting for simulations of chemically reacting flows, where chemical reactions in nonpremixed combustion occur only by molecular mixing of fuel and oxidizer, which in practical applications occur only on the dissipative turbulent scales, the combustion process occurs essentially at the smallest scales of the sub-filter.

The works from Boersma and Lele [2], Veynante and Vervisch [10] and Peters [8] help to understand multiscale modeling of combustion and the work from Barlow and Frank [1] presents experimental data to check/compare the results of methane/air turbulent jet diffusion flames, considered here.

2 Mathematical Description

In the following the mathematical concept of the REDIM method is presented. To simplify the presentation of the suggested technique let us first introduce a vector notation. The vector $\mathbf{\Psi} = (\Psi_1, ..., \Psi_n)$ will characterize the thermochemical state of the system. In this vector notation the system of governing equations for a reacting flow can be written as

$$\frac{\partial \mathbf{\Psi}}{\partial t} = \mathbf{F}(\Psi) - \mathbf{u} \cdot \nabla \mathbf{\Psi} + \frac{1}{\rho} \nabla \cdot (\mathbf{D} \nabla \mathbf{\Psi}) \equiv \mathbf{\Phi}(\mathbf{\Psi}), \tag{1}$$

where $\mathbf{\Psi}$ and $\mathbf{F}(\mathbf{\Psi})$ are $n = 1 + n_{sp}$-dimensional vectors, $\mathbf{\Psi} = (T, Y_1, ..., Y_{n_{sp}})^T$, $\mathbf{F}(\Psi) = (\dot{w}_T, \dot{w}_1, ..., \dot{w}_{n_{sp}})^T$ is the thermo-chemical source term and $\mathbf{D} = \lambda / c_p \cdot \mathbf{I}$ is a $n \times n$-

dimensional diffusion matrix, in the present work equal diffusivities are assumed.

Here, ρ is the density, $\mathbf{u}$ denotes the velocity field, T the temperature, Y_k the mass fraction of the k-th species, t the time, λ the thermal conductivity, c_p the heat capacity, $\dot{w}_T = Q\dot{w}_k$, Q the combustion heat and $\dot{w}_k$ the reaction rate of the k-th species. When multiple reactions are involved in a reactive process, the contribution of each is added to calculate the consumption/production of each species, i.e

$$\dot{w}_k = W_k \sum_{r=1}^{n_r} (\nu''_{kr} - \nu'_{kr}) \left[\dot{k}_{fr} \prod_{k=1}^{n_{sp}} \left[\frac{\rho}{W_k} Y_k \right]^{\nu'_{kr}} - \dot{k}_{br} \prod_{k=1}^{n_{sp}} \left[\frac{\rho}{W_k} Y_k \right]^{\nu''_{kr}} \right], \tag{2}$$

where W_k is the molecular weight, ν'_{kr} and ν''_{kr} are stoichiometric coefficients of the k-th species in r-reaction, $\dot{k}_{fr}$ and $\dot{k}_{br}$ are forward and backward rate constants.

According to our assumption, the system solution in the state space belongs to a m_s-dimensional invariant manifold defined by an explicit function $\mathbf{\Psi}(\theta) : M = \{\mathbf{\Psi} : \mathbf{\Psi} = \mathbf{\Psi}(\theta), \mathbf{\Psi} : R^{m_s} \to R^n\}$, $m_s \ll n$, where θ is a m_s-dimensional parameter on the manifold, which represents local coordinates. The slow manifold is defined by using a projection operator onto the normal space $(TM)^{\perp} : P_{(TM)^{\perp}} = (I - \mathbf{\Psi}_\theta \mathbf{\Psi}_\theta^+)$ of M and by the invariance condition

$$(I - \mathbf{\Psi}_\theta \mathbf{\Psi}_\theta^+) \cdot \mathbf{\Phi}(\Psi) = 0. \tag{3}$$

Here $\mathbf{\Psi}_\theta^+$ is the Moore-Penrose pseudo-inverse of $\mathbf{\Psi}_\theta$.

To solve the manifold equation (3), we need to solve the PDE system

$$\frac{\partial \mathbf{\Psi}(\theta)}{\partial t} = (I - \mathbf{\Psi}_\theta \mathbf{\Psi}_\theta^+) \cdot \mathbf{\Phi}(\Psi). \tag{4}$$

The stationary solution $\mathbf{\Psi}(\theta, \infty)$ defines the desired manifold. The equation (4) can be simplified by

$$\frac{\partial \mathbf{\Psi}(\theta)}{\partial t} = (I - \mathbf{\Psi}_\theta \mathbf{\Psi}_\theta^+) \cdot \left(\mathbf{F}(\theta) + \frac{\lambda}{\rho c_p} \mathbf{\Psi}_{\theta\theta} \circ \nabla(\theta) \circ \nabla(\theta) \right). \tag{5}$$

For more details about the REDIM method, you can consult the works of Bykov and Maas [3].

2.1 1D REDIM

In this paper, we develop a 1D REDIM for the methane/air reaction mechanism, considering the reaction set given by Peters [7]. This mechanism contains 35 reactions and 15 species.

Now, let us assume that the REDIM is parameterized by the progress variable $\theta = Z$, the mixture fraction. The mixture fraction is an extremely useful variable in combustion, in particular for diffusion flames. It is simply defined by $Z = Y_{N_2} - Y_{N_2^{OX}} / Y_{N_2^F} - Y_{N_2^{OX}}$, where $Y_{N_2^{OX}}$ and $Y_{N_2^F}$ are constant and represent the nitrogen mass fraction in the oxygen stream and fuel stream, respectively. Z is a conservative scalar ranging from 0 to 1, which relates the level of mixing between the oxygen and the fuel.

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The gradient vector $\mathbf{\Psi}_\theta$ is given by $\mathbf{\Psi}_\theta = \left(\frac{\partial T}{\partial Z}, \frac{\partial Y_1}{\partial Z}, ..., \frac{\partial Y_{n_{sp}}}{\partial Z}\right)^T$.

Assuming that $Y_1 = Y_{N_2}$, the system of equations (5) is now given by the stationary solution of

$$\rho\frac{\partial T}{\partial t} = \rho\frac{\chi}{2}\frac{\partial^2 T}{\partial Z^2} + \dot{w}_T, \tag{6}$$

$$\rho\frac{\partial Y_k}{\partial t} = \rho\frac{\chi}{2}\frac{\partial^2 Y_k}{\partial Z^2} + \dot{w}_k, \tag{7}$$

where $\chi = \frac{2\lambda}{\rho c_p}|\nabla Z|^2$. In equations (6) and (7) the Lewis numbers of all chemical species has been assumed to be unity. This assumption has been argued that in turbulent combustion only a thin region around the reaction zone is governed by molecular transport, whereas turbulent transport is predominant in the outer inert mixing region, implying unity Lewis numbers [9].

2.2 Frave Equation for Large Eddy Simulation

In this study, we consider the turbulent compressible flow to simulate a jet diffusion flame. Unfortunately, usually the full numerical solution of the instantaneous balance equations is limited to simplified cases, where the number of the time and length scales present in the flow is not too great. To overcome this difficulty, an alternative is to use large eddy simulation (LES). The largest turbulence scales are explicitly computed in the LES and only the smallest, low-energy modes, are modeled. The prediction of mean flow and mixing by LES is often found to be superior to classical steady RANS models, which frequently fails for highly turbulent flow analysis.

In most LES of compressible flows, the flow variables are Favre averaged or density weighted [2], $\widetilde{f} = \overline{\rho f}/\overline{\rho}$, where the bar denotes the standard LES filtering. Using the Favre average and after applying the standard LES filtering technique, we find the following governing equation for momentum/Navier-Stokes, mixture fraction, temperature and species mass fractions:

$$\frac{\partial(\bar{\rho}\widetilde{u}_i)}{\partial t} + \frac{\partial(\bar{\rho}\widetilde{u}_i\widetilde{u}_j)}{\partial x_j} = -\frac{1}{M^2}\frac{\partial \bar{p}}{\partial x_i} + \frac{\partial}{\partial x_j}\left(\frac{\bar{\mu}_t}{R_e}\widetilde{\sigma}_{ij}\right) \tag{8}$$

$$\frac{\partial(\bar{\rho}\widetilde{Z})}{\partial t} + \frac{\partial(\bar{\rho}\widetilde{u}_j\widetilde{Z})}{\partial x_j} = \frac{\partial}{\partial x_j}\left(\frac{\bar{\mu}_t}{S_c}\frac{\partial \widetilde{Z}}{\partial x_j}\right) \tag{9}$$

$$\frac{\partial(\bar{\rho}\widetilde{T})}{\partial t} - \frac{\widetilde{\chi}}{2}\frac{\partial^2(\bar{\rho}\widetilde{T})}{\partial \widetilde{Z}^2} = \widetilde{\dot{w}}_T \tag{10}$$

$$\frac{\partial(\bar{\rho}\widetilde{Y}_k)}{\partial t} - \frac{\widetilde{\chi}}{2}\frac{\partial^2(\bar{\rho}\widetilde{Y}_k)}{\partial \widetilde{Z}^2} = \widetilde{\dot{w}}_k \tag{11}$$

In these equations M is the Mach, R_e the Reynolds and $S_c \sim 0.4$ the Schmidt numbers. At low Mach numbers ($M < 0.01$) the spatial variations in pressure are small compared to the pressure itself and may be neglected in the equation of state, where the pressure may be approximated by a constant [5]. Therefore, the density is approximated using the

state relation $\bar{\rho} = (pW)/(R\widetilde{T})$, where R is the ideal gas constant. The pressure term is obtained by equation $\nabla^2\bar{p} = \Delta t\left(\frac{\partial\widetilde{u}_i}{\partial x_i} + \frac{\partial\bar{\rho}}{\partial t}\right)$.

The characteristic length and time-scales where combustion takes place are typically well below the resolved grid scales, and the combustion process has been modeled entirely at the subgrid level. Thus, most subgrid-scale stress models are based on an eddy viscosity assumption. In the most commonly used model, developed by Smagorinky, the eddy viscosity μ_t is obtained by assuming that the small scales are in equilibrium, so that energy production and dissipation are in balance. This yields an expression of the form $\mu_t = \bar{\rho}(C_s\Delta)^2|\widetilde{S}_{ij}|$, where $|\widetilde{S}_{ij}| = (2\widetilde{S}_{ij}\widetilde{S}_{ij})^{1/2}$, $C_s \simeq 0.2$ is the Smagorinsky coefficient and the filter size is set equal to $\Delta = (\Delta x\Delta y\Delta z)^{1/3}$ where Δx, Δy and Δz denote the grid spacings in the corresponding directions. Simulations are conducted on a three-dimensional Cartesian mesh with non-uniform spacings in each of the three directions.

3 Numerical Tests

Numerical tests were carried out using the central second order finite difference method in the space. Central schemes are preferred because they are not dissipative, this property is generally considered necessary to prevent damping of small scales of turbulence, which are important in reactive flows. The Runge-Kutta method was chosen to obtain numerical solutions of high accuracy and to extend the stability region.

The configuration used for the validation of the proposed models is a piloted methane/air jet diffusion flame (Sandia Flame D). Sandia Flame D consists of a main jet with a mixture of 25% methane and 75% air by volume. The nozzle is placed in a coflow of air and the flame is stabilized by a pilot with diameter $Dp = 18.2\ mm$, as shown the Figure 1 (a). The Reynolds number for the main jet is $R_e = 22400$ based on the nozzle diameter $d = 7.2\ mm$ and the bulk jet velocity $49.6\ m/s$. The burner has a proportional relationship $L = 11D$, where $D = 10d$. This figure (side right) shows the representation of the two-dimensional mesh of the burner used. It is structured and non-uniform mesh with geometric progression. Transient simulations of the mixing layer are performed with a mesh consisting of $149(L) \times 51(D)$. The mesh refinement is located at the nozzle exit and along the center line of the burner where the gradients of the dependent variables are high.

The validation of the REDIM modeling is performed by comparing of previous detailed computational and experimental results. To this flame, all details experimental are provided and regularly updated in the web site [1].

In the figures which follow, we have the projections of the stationary solutions of equation (10) and (11) for a jet turbulent diffusion flame configuration. The initial conditions are $Y_{O_2,i} = 0.23$, $Y_{CH_4,i} = 0.16$ and zero for all other species. All computations were performed with a time step of $\Delta t = 0.000001$.

The Figure 1 (b) shows numerical and experimental results for the H_2O and CO_2 mass fractions in the mixture fraction space (Z). Where $Z = 0$ and $Z = 1$ the mass fraction of products is zero, because these points has pure fuel ($Z = 1$) or pure oxygen ($Z = 0$). The mass fraction of the products grows along the fraction of the mixture until reaching its maximum value, where is the stoichiometries mixture, that is, ideal burning conditions.

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The Figure 1 (c) shows the profile of the H_2O and CO_2mass fractions along the central axis of the jet. Numerical solutions are compared with the experimental data, too. The results show that the mass fraction of these products increases as the jet develops, achieving its maximum value, near $x/d = 60$, that is the position of stoichiometries condition. After achieving this maximum value, the mass fraction decays. The numerical results are in reasonable agreement with the experimental data, through error bar is observed that most of the results are within the parameter. The differences might be inherent in the simplification process required to allow a problem more accessible.

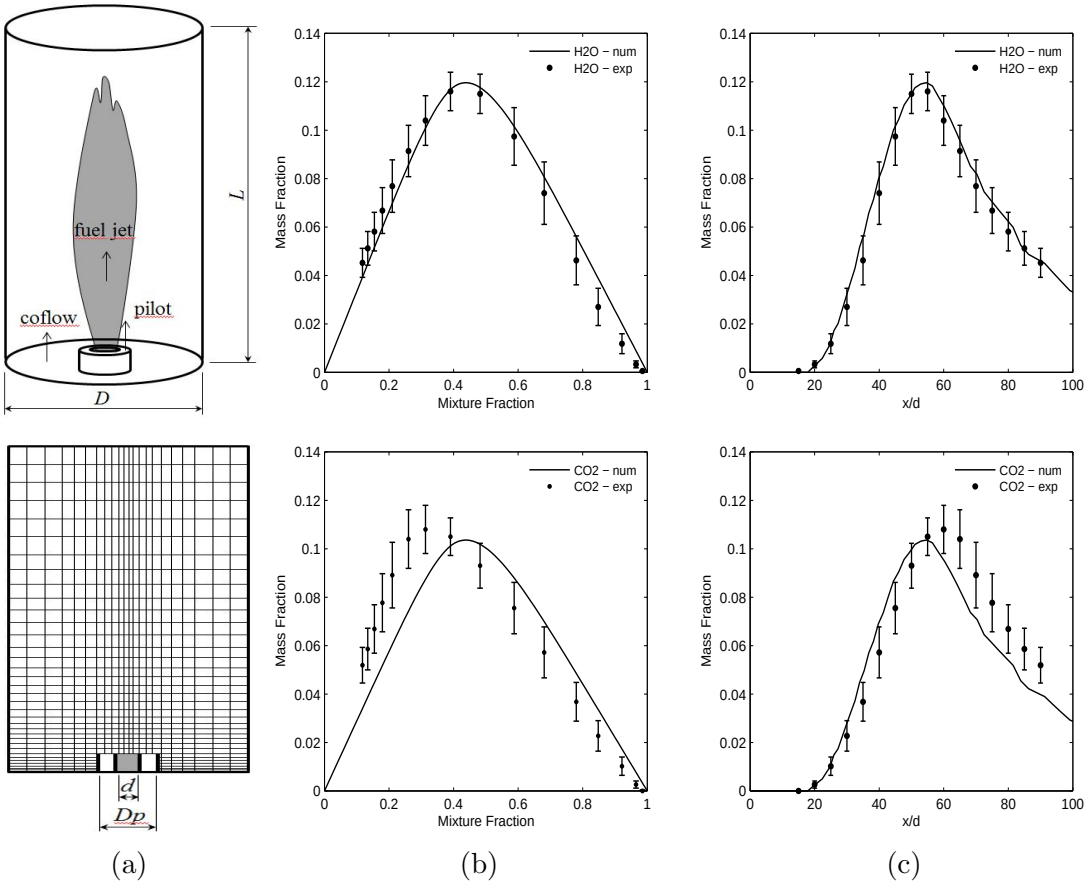

Figura 1: (a) Burner sketch with a structured and non-uniform mesh. (b) Numerical and experimental results for the H_2O and CO_2 mass fraction in the mixture fraction space. (c) Numerical and experimental results for the H_2O and CO_2 mass fraction along the central axis, considering a methane turbulent jet diffusion flame.

4 Conclusions

The studies presented here are concerned to the efficiency of REDIM method to simulate a methane/air turbulent jet diffusion flame. For the one dimensional case (1D-

REDIM), the thermo-chemical variables are related to the mixture fraction and the equations are solved by finite-difference method. The computational results for 1D-REDIM are in agreement with experimental data for all quantities. It was observed that the developed method is computationally cheap and efficient, which turns it appropriate to study similar problems, for future implementation in more complex calculations, and to use it hierarchically to produce initial conditions for detailed numerical simulations.

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