# Application of reaction-diffusion manifolds (REDIM) for the simulation of two-dimensional axisymmetric laminar diffusion flames

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**Abstract**

In this work, the Reaction Diffusion Manifolds method (REDIM), a method for the simplification of chemical kinetics, is applied to calculate two dimensional axisymmetric laminar diffusion flames. Since the REDIM identifies an $m_s$-dimensional slow invariant manifold, in its application only $m_s$ conservation equations in terms of generalized coordinates are solved for the scalar field and other thermo-chemical quantities (e.g. temperature, mass fractions) can be retrieved by interpolations from a look-up table. REDIMs are used to study a two-dimensional axisymmetric laminar counterflow diffusion flame in which one side is a premixed methane-air stream, and the other side is an air stream. The results based on detailed kinetics (GRI3.0) are compared with the results computed by using the 2D REDIM reduced chemistry.

## Introduction

The implementation of detailed chemical kinetics in the simulation of combustion processes introduces numerous species conservation equations with extremely high dimensions (the number of species equations *n* sometimes may exceed 1000) and nonlinear chemical source terms, which leads to a large stiffness of the governing equation system. Both the high dimensionality and the large stiffness result in extremely high computational costs. In order to minimize the computational effort, several methods, for instance, Intrinsic low-dimensional manifolds (ILDM) [1], Flamelet generated manifolds (FGM) [2], flame prolongation of ILDM (FPI) [5] or Reaction-diffusion manifolds (REDIM) [3] are used to simplify the chemical kinetics.

Counterflow flames [4] are widely used in numerical combustion to investigate the precision and accuracy of models. Gicquel et al. [5] investigate the response of a premixed flame to straining by computing a double-premixed counterflow flame, which demonstrates the suitability of flame prolongation of ILDM (FPI) for such calculations. In [6], two methods based on premixed flamelets (FPI and FGM) are extended to calculate the partially premixed and non-premixed counterflow flames, and the quality of the results in depends on whether the equivalence ratio exceeds the flammability limits. Yu et al. [7] performed the simulation of counterflow diffusion flames with oscillating strain rates computed based on a two-dimensional REDIM table, which showed that the REDIM is able to reproduce the response of both the steady and non-steady flame structures very well.

In our previous work, the results of the REDIM reduced model for non-premixed flames generated by considering simple 1-dimensional counterflow diffusion flame configurations covering different strain rates, show a very good agreement with detailed computations of counterflow flames. In this paper, we use the 2D REDIM to study a two-dimensional axisymmetric laminar counterflow diffusion flame in which one side is the inlet for a mixture of premixed methane-air, and the other side is an air stream. The first part of this paper introduces briefly the mathematical basics of the system describing the combustion with the detailed mechanism. The second part presents the mathematical background of the REDIM reduced chemistry. The third and fourth parts are the problem definition and the construction of REDIM table respectively. The last part is the implementation of REDIM and presentation of numerical results.

## Mathematical models based on detailed mechanisms

The combustion process based on detailed mechanisms (GRI 3.0 [8] used in the work) is simulated mathematically by solving the following governing equations, under an assumption of unity Lewis number, which may be written as (see [9]):

continuity

$$\frac{\partial \rho}{\partial t} + \nabla \cdot \left(\rho \vec{U}\right) = 0 \tag{1}$$

species mass fraction

$$\frac{\partial (\rho Y_k)}{\partial t} + \nabla \cdot \left(\rho Y_k \vec{U}\right) = \nabla \cdot (\rho D_k \nabla Y_k) + \dot{\omega}_k \tag{2}$$

momentum

$$\frac{\partial (\rho \vec{U})}{\partial t} = -\nabla \cdot \left(\rho \vec{U} \circ \vec{U}\right) - \nabla p + \nabla \cdot \tau + \rho \vec{g} \tag{3}$$

energy

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$$\frac{\partial(\rho h_s)}{\partial t} + \nabla \cdot \left(\rho \vec{U} h_s\right) + \frac{\partial(\rho K)}{\partial t} + \nabla \cdot \left(\rho \vec{U} K\right) - \frac{\partial p}{\partial t} - \nabla \cdot (\alpha \nabla h_s) = \dot{\omega}_T \quad (4)$$

equation of state

$$p - \frac{\rho R T}{\bar{M}} = 0 \quad (5)$$

where $\vec{U}$ = velocity vector, $\rho$ = density, $Y_k$ = mass fraction of species $k$, $D = \frac{\lambda}{\rho C_p} = D_k$ (Le =1), $\lambda$ = thermal conductivity, $C_p$ = heat capacity at constant pressure, $\dot{\omega}_k$ = reaction rate of species $k$, $p$ = pressure, $\nabla \cdot \tau$ = shear-rate tensor, $\vec{g}$ = gravitational acceleration, $h_s$ = sensible enthalpy, $K = \frac{1}{2}|U|^2$ specific kinetic energy, $\alpha$= thermal diffusivity, $\dot{\omega}_T$ = heat release rate, $R$ = universal gas constant, $\bar{M}$ = mean molecular weight and $t$ = time. In order to simulate the combustion process mathematically based on detailed mechanisms, we notice that the system of equation consisting of Eqn. (1)-(5) and $(n_s - 1)$ species equations is solved, where $n_s$ denotes the number of species.

The C++ toolbox OpenFOAM [10] in the work is used as the basic structure to calculate both the detail mechanism and the REDIM reduced chemistry because OpenFOAM has some advantages: high numerical accuracy and free availability. Therefore, the system of equation consisting of Eqn. (1)-(5) and $(n_s - 1)$ species equations used in the detailed mechanism is implemented to solve in OpenFOAM.

**Reaction-Diffusion Manifolds (REDIMs)**

The mathematical model based on REDIMs (details in reference [3]) can be described by the evolution equation of reacting flows with the state vector $\boldsymbol{\Psi} = (h, p, \frac{Y_1}{M_1}, \cdots, \frac{Y_{n_s}}{M_{n_s}})^T$, which is written as

$$\frac{\partial \boldsymbol{\Psi}}{\partial t} = F(\boldsymbol{\Psi}) - U \cdot \nabla \boldsymbol{\Psi} - \frac{1}{\rho} \nabla \cdot (\mathbf{D} \cdot \nabla \boldsymbol{\Psi}) \quad (6)$$

here $h$ is the specific enthalpy, $p$ is the pressure, the ratio of $\frac{Y_k}{M_k}$ denotes specific mole number consisting of mass fraction $Y_k$ and corresponding species molar mass $M_k$, $\mathbf{D}$ represents the $n \times n$ dimensional diffusion matrix given via [11], and $F(\boldsymbol{\Psi})$ is the source term.

The time scales of different chemical reactions span several orders of magnitude, which cover a range from $10^{-10}$ s to more than 1 s [4]. In terms of this, we can decompose the combustion system into fast and slow subprocesses. We suppose that the solution of Eqn. (6) belongs to an $m_s$-dimensional slow manifold and the low-dimensional invariant manifold can be defined as

$$M = \{\boldsymbol{\Psi}: \boldsymbol{\Psi} = \boldsymbol{\Psi}(\theta), \boldsymbol{\Psi}: R^{m_s} \rightarrow R^n\} \quad (7)$$

where $\boldsymbol{\Psi}(\theta)$ is an explicit function parameterized by the variable $\theta$ (an $m_s$-dimensional vector) and $M$ is the invariant $m_s$-dimensional system manifold. According to the reference [3], REDIM can be calculated by solving the following system of equations to its stationary solution:

$$\frac{\partial \boldsymbol{\Psi}(\theta)}{\partial t} = \left(\boldsymbol{I} - \boldsymbol{\Psi}_{\boldsymbol{\theta}}(\theta) \cdot \boldsymbol{\Psi}_{\boldsymbol{\theta}}^{+}(\theta)\right) \cdot \left\{\boldsymbol{F}\left(\boldsymbol{\Psi}(\theta)\right) - \frac{1}{\rho} \cdot [(\mathbf{D}\boldsymbol{\Psi}_{\boldsymbol{\theta}} \cdot \chi(\theta))_\theta \cdot \chi(\theta)]\right\} \quad (8)$$

where $\boldsymbol{\Psi}_{\boldsymbol{\theta}}^{+}$ is the Moore-Penrose pseudo-inverse of $\boldsymbol{\Psi}_{\boldsymbol{\theta}}$ (see [12]), and $\chi(\theta)$ is the gradient estimate. REDIMs use the concept of low-dimensional invariant manifold $M$ to project Eqn. (6) on the manifold:

$$\frac{\partial \theta}{\partial t} = \boldsymbol{\Psi}_{\boldsymbol{\theta}}^{+} \cdot \boldsymbol{F}(\boldsymbol{\Psi}(\theta)) - U \cdot \nabla \theta - \frac{1}{\rho} \boldsymbol{\Psi}_{\boldsymbol{\theta}}^{+} \cdot \nabla \cdot (\mathbf{D} \cdot \boldsymbol{\Psi}_{\boldsymbol{\theta}} \cdot \nabla \theta) \quad (9)$$

where $\boldsymbol{\Psi}_{\boldsymbol{\theta}}^{+}$ is given for a regular matrix $\boldsymbol{\Psi}_{\boldsymbol{\theta}}^{\boldsymbol{T}} \cdot \boldsymbol{\Psi}_{\boldsymbol{\theta}}$ by

$$\boldsymbol{\Psi}_{\boldsymbol{\theta}}^{+} = (\boldsymbol{\Psi}_{\boldsymbol{\theta}}^{\boldsymbol{T}} \cdot \boldsymbol{\Psi}_{\boldsymbol{\theta}})^{-1} \cdot \boldsymbol{\Psi}_{\boldsymbol{\theta}}^{\boldsymbol{T}}. \quad (10)$$

This pseudoinverse fulfills the condition:

$$\boldsymbol{\Psi}_{\boldsymbol{\theta}}^{+} \cdot \boldsymbol{\Psi}_{\boldsymbol{\theta}} = \boldsymbol{I}. \quad (11)$$

The terms like $\boldsymbol{\Psi}_{\boldsymbol{\theta}}^{+} \cdot \boldsymbol{F}(\boldsymbol{\Psi}(\theta))$, $\boldsymbol{\Psi}_{\boldsymbol{\theta}}^{+}$, $\mathbf{D} \cdot \boldsymbol{\Psi}_{\boldsymbol{\theta}}$ are computed by a modified and extended version of HOMREA [13] program and are stored in the REDIM table in advance. According to the above description, there are only (3+$m_s$) equations ($m_s \ll n_s$) solved in the REDIM approach, namely Eqn. (1), Eqn. (3), Eqn. (5), and other thermo-chemical quantities (e.g. temperature, mass fractions) can be retrieved by interpolation from a look-up table.

**Problem definition**

The flame studied in this paper is a two-dimensional axisymmetric laminar counterflow diffusion flame. A stream of methane mixed with air (25% $CH_4$ + 75% air in volume percent) is injected through one pipe in the left boundary while a stream of air (21% $O_2$ + 79% $N_2$ in volume percent) is injected from the right boundary. A brief schematic of the flame configuration is presented in Figure 1.

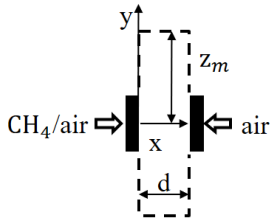


Figure 1. Schematic of the flame configuration and the axisymmetric computational domain.

The diameters of the nozzles for the fuel flow and the oxidizer flow are both 2 cm, and the distance $d$ between the two nozzles is 2 cm as well, in addition, the computational height is $z_m$ = 4 cm (measured from the centerline of the nozzle). The detailed boundary conditions considered in the work are listed in table 1.

The detailed mechanism GRI 3.0, which includes 53 species and 325 reactions is used. Moreover, the assumption of unity Lewis number is used in the paper, which has been shown to be a reasonable simplification in these kind of flame configurations, and furthermore the focus of this paper is not an analysis of the transport model, but a comparison between detailed and reduced chemistry.

Table 1. Boundary conditions.

| | $T$ | $p$ | $v$ |
|---|---|---|---|
| Left boundary | 293 K | zero-Gradient | 1 m/s |
| Right boundary | 293 K | zero-Gradient | 1 m/s |
| Top boundary | zero-Gradient | 1 bar | zero-Gradient |
| Bottom boundary | zero-Gradient | 1 bar | zero-Gradient |

**Construction of a 2D REDIM table**

In order to generate the REDIM tables, we need to compute the detailed solutions of different flame scenarios. The procedure of REDIM generation has been implemented in the INSFLA and HOMREA program [13]. As mentioned above, the REDIM table is obtained by solving Eqn. (8), which is formulated in terms of a partial differential equation (PDE). To solve this REDIM equation, one must specify the initial condition, boundary condition and, in addition, the gradient estimate:

- Initial condition: Since we are only interested in the steady solution of the Eqn. (8), any initial condition, which does not satisfy the invariant condition can be used. In the present work, the initial profile is determined from several detailed solutions, because it speeds up the integration of the REDIM evolution equation. More details can be found in [7].
- Boundary conditions: The boundary condition encloses the application range of the constructed REDIM table. In our considered example shown in Fig.1, the left boundary is defined by the fuel side ($CH_4$/air), and the right boundary by the oxidizer side (pure air). The boundaries of the manifold are specified as fixed boundary conditions from the detailed flame calculation [7].
- Gradient estimate: in the framework of the REDIM concept, the gradient estimate is only important for low dimension, and it becomes less and less important for higher dimension (usually higher than three-dimensional REDIM). In this work, we restrict ourselves to a two-dimensional REDIM, because it is shown to be enough for the considered system [7]. Following the reference [7], the gradient estimate is obtained from several detailed solutions, which represent reasonable physical scalar gradients for the considered system.

The remaining input to solve the REDIM evolution equation (8) is the choice of reduced coordinate $\theta$. As shown in [14], the REDIM equation (8) is invariant with respect to the reduced coordinate $\theta$. In other words, the generation of the REDIM reduced chemistry is independent on the choice of $\theta$. In this work, $(\phi_{N_2}, \phi_{CO_2})$ is selected to define the local coordinate.

The detailed construction of REDIM reduced chemistry can be found in [7]. Figure 2 shows the example of composition space of REDIM reduced chemistry in in $\phi_{N2}$ - $\phi_{CO2}$ - $\phi_{H2}$ projection, where the units of the variables listed in the corresponding axes in the figure is the specific mole number.

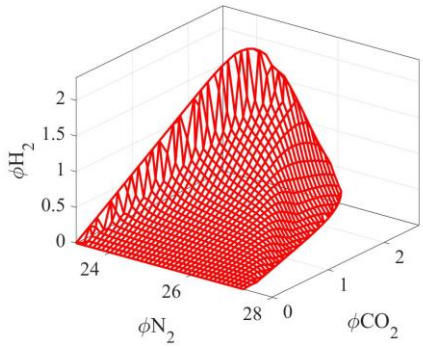


Figure 2. Example of composition space of REDIM reduced chemistry in $\phi_{N2}$ - $\phi_{CO2}$ - $\phi_{H2}$ projection.

**Numerical solution of the reacting flow equations**

In the present work, three kinds of mesh sizes (mesh 1, mesh 2 and mesh 3 listed below) are used to compute the two dimensional axisymmetric laminar diffusion flames with the detailed mechanism, respectively, in order to investigate the mesh dependence. In the computational domain between the two nozzles (2 cm × 2 cm), the mesh is equidistantly spaced along both x and y direction, but out of this domain, the mesh size increases proportionally in the y direction. The first mesh (mesh 1, coarse) has $\Delta x$ = 0.2 mm for $0 \le x \le 2$ cm, $\Delta y$ = 0.5 mm for $0 \le y \le 1$ cm, and increasing spacing starting from $\Delta y$ = 0.5 mm for $1 \le y \le 4$ cm. The second mesh (mesh 2, intermediate) has $\Delta x$ = 0.1 mm for $0 \le x \le 2$ cm, $\Delta y$ = 0.25 mm for $0 \le y \le 1$ cm, and increasing spacing starting from $\Delta y$ = 0.26 mm for $1 \le y \le 4$ cm. The third mesh (mesh 3, fine) has $\Delta x$ = 0.05 mm for $0 \le x \le 2$ cm, $\Delta y$ = 0.125 mm for $0 \le y \le 1$ cm, and increasing spacing starting from $\Delta y$ = 0.13 mm for $1 \le y \le 4$ cm.

The diffusion coefficient is calculated assuming a unity Lewis number (Le =1), $D = \frac{\lambda}{\rho C_p} = D_k$, and the thermal conductivity $\lambda$ is calculated by the following equation in the detailed mechanism based on OpenFOAM:

$$\lambda = \mu C_v (1.32 + \frac{1.77R}{C_v}) \quad (12)$$

where $\mu$ denotes the dynamic viscosity computed by Sutherland´s law [15] in OpenFOAM, $C_v$ heat capacity at

constant volume, universal gas constant R = 8314.5 J/(kmol·K). Sutherland´s law can be expressed as:

$$\mu = \frac{A_S\sqrt{T}}{1+T_S/T} \tag{13}$$

with the Sutherland coefficient $A_s$ and the Sutherland temperature $T_s$. Note, however, that the corresponding thermo-physical properties $\lambda$ and $\mu$ used in the HOMREA program for the calculation of the REDIM are based on a multi-component model for the thermal conductivity. The formulae of $\lambda$ and $\mu$ are written respectively as [16]:

$$\lambda_{mix} = \frac{1}{2}\left[\sum_i x_i\lambda_i + \left(\sum_i \frac{x_i}{\lambda_i}\right)^{-1}\right] \tag{14}$$

$$\mu_{mix} = \frac{1}{2}\left[\sum_i x_i\mu_i + \left(\sum_i \frac{x_i}{\mu_i}\right)^{-1}\right] \tag{15}$$

where $\lambda_{mix}$ and $\mu_{mix}$ are thermal conductivity and dynamic viscosity of the mixture and $x_i$, $\lambda_i$ and $\mu_i$ represent mole fraction, thermal conductivity and dynamic viscosity of the *i* th species, respectively. We notice the different approaches for the calculations of the thermo-physical properties may cause difference in the results of detailed mechanism and reduced mechanism calculations, and this discrepancy will be improved in our future work. Note that the transport model used to calculate the REDIMs is more accurate.

**Numerical results and discussion**

*Mesh dependence*

The computational results with the detailed mechanism (GRI3.0) are presented here in order to investigate the influence of flame structure caused by using the three mesh sizes. Figure 3 shows the structures of two dimensional axisymmetric laminar diffusion flames. Figures 4 and 5 display contours of temperature and profiles of selected species mass fractions along the centerline of the computational domain for three mesh sizes, respectively. In Figure 4, it is shown that the flame

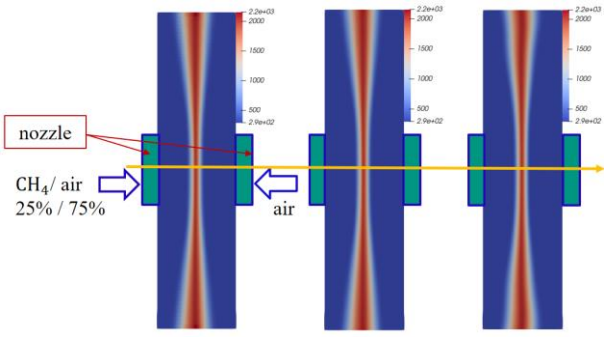


Figure 3. Temperature profiles on three mesh sizes, left figure: mesh 1; middle figure: mesh 2; right figure: mesh 3; the yellow line marks the centerline along the computational domain.

thicknesses computed by the three mesh sizes almost have the same value, and the error is less than 1% on the coarse mesh (mesh 1) compared with the thicknesses obtained by the fine mesh (mesh 2 and mesh 3). As can be observed, the peak temperatures (2002 K on mesh 1, 2013 K on mesh 2 and 2019 K on mesh 3) computed by the three mesh sizes have almost the same values, the error is less than 1% as well.

There are little differences between the minor species mass fractions in Figure 5, especially in the results of mesh 1 (coarse mesh), which means that the effect of mesh size in the calculations is negligible. Analyzing the above results, we think the accuracy of mesh 3 is fine enough to capture the flame structure, therefore, we will use the mesh size to calculate the flame configuration in detailed and reduced mechanism.

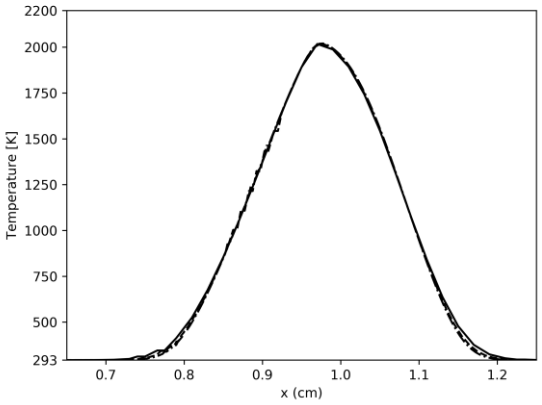


Figure 4. Comparison of results for temperature along the centerline of the 2D counter-flow flame on three mesh sizes, solid line: mesh 1, dashed line: mesh 2, dashed dotted line: mesh 3.

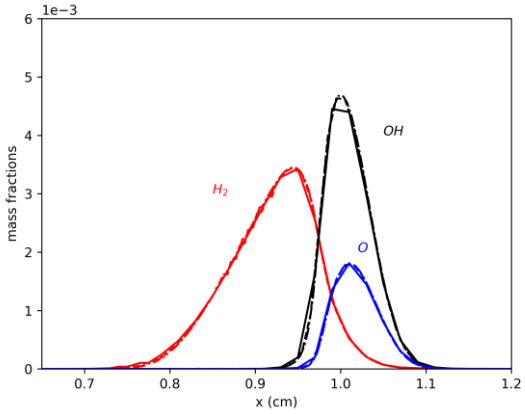


Figure 5. Comparison of results for minor species along the centerline of the 2D counter-flow flame on three mesh sizes, solid line: mesh 1, dashed line: mesh 2, dashed dotted line: mesh 3.

*Comparison of detailed and reduced models*

The computational results obtained by using the detailed mechanism (GRI 3.0) and REDIM reduced chemistry are compared here for mesh 3. Figure 6 shows the structures of two-dimensional axisymmetric laminar diffusion flames, in which the left part of each figure in Figure 6 shows the results obtained by using detailed

chemistry, while the right part shows results computed by the REDIM reduced model.

In the top part of Figure 7, it is shown that the flame thickness of detailed solution is slightly larger than the

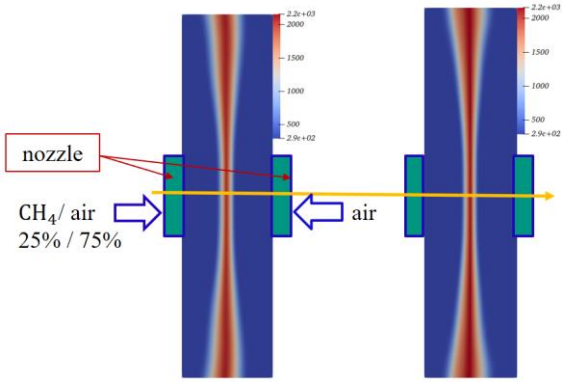


Figure 6. Temperature profiles on the fine mesh, left figure: detailed mechanism (GRI3.0); right figure: REDIM reduced mechanism; the yellow line marks the centerline along the computational domain.

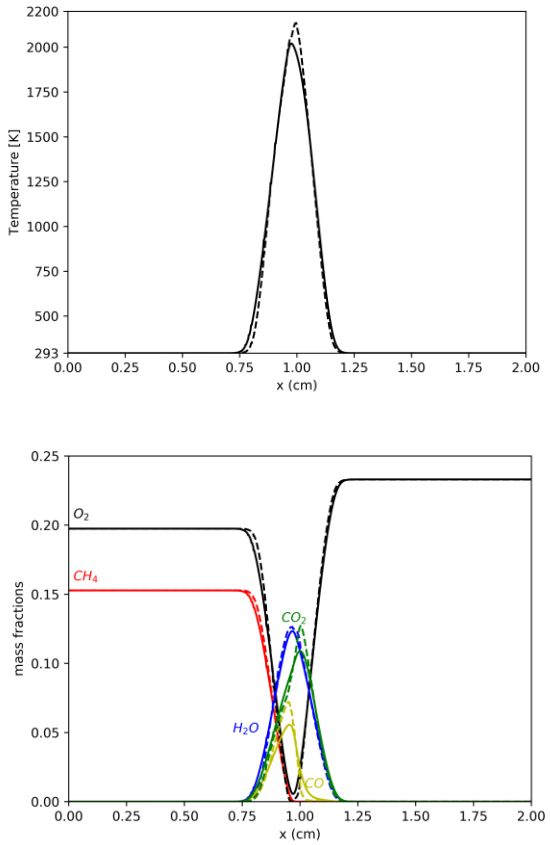


Figure 7. Comparison of results for temperature (top) and major species (bottom) along the centerline of the 2D counter-flow flame on the fine mesh, solid line: detailed mechanism (GRI3.0), dashed line: REDIM reduced mechanism.

one calculated by REDIM reduced chemistry, and the peak temperature (2127 K) obtained from REDIM reduced mechanism is higher than the peak temperature (2019 K) computed by the detailed solution, and the error is approximate 5%. However, this minor difference can not only be attributed to the reduced chemistry, but also to the fact to differences in the diffusion coefficient $D = \frac{\lambda}{\rho C_p}$, in which the definitions of heat conductivity $\lambda$ and dynamic viscosity $\mu$ terms in INSFLA program are different from the ones used in OpenFOAM (discussed above). Moreover, the REDIM table used in this work is generated by using gradient estimates from 1D flame configurations, which only take into account the one-dimensional molecular diffusion term. This could be improved by using multi-dimensional molecular diffusion terms [17] in the Eqn. (8) to generate the REDIM tables. Maxima of major species mass fractions ($CO_2$ and $CO$, in the bottom part of Figure 7) are overestimated by the REDIM reduced model, too, which may be also be caused by the different definitions of the heat conductivity $\lambda$ and dynamic viscosity $\mu$ terms, and this difference in transport models will be investigated in future work.

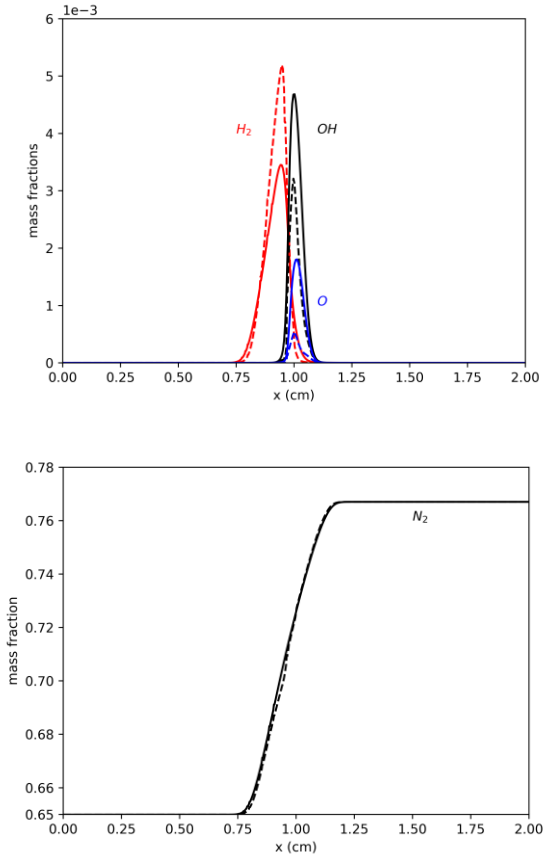


Figure 8. Comparison of results for minor species (top) and $N_2$ (bottom) along the centerline of the 2D counter-flow flame on the fine mesh, solid line: detailed mechanism (GRI3.0), dashed line: REDIM reduced mechanism.

There are differences between the minor species mass fractions calculated by the detailed mechanism and REDIM reduced chemistry respectively in the top part of Figure 8. Future work will analyze whether this is a result of the different transport coefficients or the accuracy of model reduction. If it is a result of the transport model,

then using the same definitions of heat conduction and dynamic viscosity in the detailed mechanism and REDIM reduced chemistry is reduces the differences. If it is the accuracy of the mechanism reduction, one can increase the dimension of REDIM (e.g. use a three-dimensional REDIM) to better capture the concentrations of minor species. Moreover, in the bottom part of Figure 8, the profile of $N_2$ calculated by REDIM reduced mechanism has a very good agreement with the values computed by the detailed mechanism (GRI3.0), which indicates that REDIM can well describe the $N_2$ mass fraction, which represents the mixing process.

**Conclusions**

In this work, the Reaction-diffusion Manifolds (REDIM) method is used as model reduction method to calculate a two-dimensional axisymmetric laminar diffusion flame. Computational results show that the REDIM approach can be well implemented for the simulation of combustion in OpenFOAM. Analyzing the profiles of temperature and major species mass fractions, it is shown that the REDIM can reproduce the flame structure very well. As for the minor species, we should further improve discrepancy of definitions of heat conduction and dynamic viscosity between the detailed mechanism and REDIM reduced chemistry, in order to describe their profiles well. Moreover, the computational cost of REDIM is only approximately 10 % of the CPU time [7] for calculation using the detailed chemical kinetics based on the same time step and mesh size, which means that REDIM can significantly reduce the computational effort.

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