Reduction of reacting flow models by the REDIM method

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1   Introduction

It is known that typical kinetic models used in recting flows are extremely large, stiff and non-linear [1]. Hence methods of dimension reduction of large detailed chemical kinetic models are very important and have been developed intensively in the last years. Although significant progress is made in both theoretical [2, 3, 4] and numerical aspects (see [5, 6, 7, 8] for more references and details about existing methods of system reduction) there are fundamentally weak points in many existing methods [9]. A main problem of application of reduction methods or reduced kinetics models is the fact that the reduced chemistry modelling is very often based purely on the analysis of the source term, neglecting the potential impact of the transport processes on the so called 'slow manifold'. Additionally, applying the same transport term for reduced model as for the detailed one without a proper projection, while the source term is replaced by a reduced chemistry model, can lead to inaccurate results as well (see e.g. [9] for more details).

In the present work the method of Reaction Diffusion Manifolds (REDIM) for automatic reduction of chemical kinetics models depending on transport properties of the media and configuration of the reacting flow is discussed. The approach allows to incorporate the effect of coupling of reaction and diffusion processes. 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 low dimensional manifold that approximates the full system dynamics in the state space.

The proposed method follows the general framework of invariant system manifolds (see e.g. [10, 11]). The main assumption which allows application of this concept is the existence of differences in time scales of subprocesses in reacting flows leading to a decomposition of the system dynamics. This assumption is evidently valid for typical cases of dynamical systems describing recting flows where large differences in time scales stem from the natural properties of combustion kinetics.

The method is applied to a premixed laminar flame of relatively simple structure, but nevertheless containing main features of recting flows. The comparison of the full system behavior and reduced one shows the potential of the suggested approach to approximate the system dynamics even in regions of the state space far from the equilibrium point of the source term.

2   Mathematical background

We start with a formulation of a typical system of PDEs of a low Mach number reacting flow and use a detailed equation system in general symbolic vector notations (an extension to high Mach number flows is possible without any principal difficulties)

$$\frac{\partial \Psi}{\partial t} = F\left(\Psi\right) - v\,\mathrm{grad}\left(\Psi\right) - \frac{1}{\rho}\,\mathrm{div}\left(D \cdot \mathrm{grad}\left(\Psi\right)\right) \equiv \Phi\left(\Psi\right), \tag{1}$$

where v represents the velocity field, ρ the density and D the (n by n)-dimensional matrix of the transport/diffusion coefficients [1], in the present work equal diffusivities is assumed. The state vector Ψ is the ($n = n_s + 2$)-dimensional state space vector $\Psi = \left(h, p, \frac{w_1}{M_1}, ..., \frac{w_{n_s}}{M_{n_s}}\right)^T$, where h denotes the enthalpy, p the pressure, $w_1, ..., w_{n_s}$ the species mass fractions and $M_1, ..., M_{n_s}$ the molar masses. $F(\Psi)$ is the n-dimensional vector of the thermo-chemical source term and t denotes the time.

According to our assumption, the system solution in the state space is "close" or belongs to an m_s-dimensional invariant manifold defined by an explicit function $\Psi\left(\theta\right)$: $M = \{\Psi = \Psi\left(\theta\right), \Psi : R^{m_s} \rightarrow R^n\}$, 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 $(TM)^{\perp}$: $P_{(TM)^{\perp}} = I - \Psi_\theta \Psi_\theta^+$ of M and by the invariance condition [10])

$$\left(I - \Psi_\theta\,\Psi_\theta^+\right) \cdot \Phi\left(\Psi\right) = 0. \tag{2}$$

Here Ψ_θ^+ is the Moore-Penrose pseudo-inverse of Ψ_θ [12]. To solve the manifold equation (2) a reformulation in terms of a multi-dimensional parabolic PDEs system for $\Psi = \Psi\left(\theta, t\right)$ is suggested

$$\frac{\partial \Psi\left(\theta\right)}{\partial t} = \left(I - \Psi_\theta\left(\theta\right)\,\Psi_\theta^+\left(\theta\right)\right) \cdot \Phi\left(\Psi\left(\theta\right)\right), \tag{3}$$

such that the stationary solution $\Psi\left(\theta, \infty\right)$ defines the desired manifold. The system (3) is integrated starting from an initial guess for the invariant manifold given by the extended ILDM approach [13] until the solution converges. Thus, according to the basic assumption of the invariant manifolds method, the state vector Ψ of (1), in any point of the flow and at any time, belongs to the manifold i.e. the system dynamics in the state space is completely described as a movement within this manifold.

3   Reaction Diffusion Manifolds and implementation

Note that the assumption about the dependence of the stationary set of the system (3) on local coordinates only, namely $\Psi\left(t, x\right) = \Psi\left(\theta\left(t, x\right)\right)$, is not generally valid and used here as an approximation. There is also a problem with such formulation because the last term in the transport part of $\Phi\left(\Psi\right)$ (see (1) and (4) depends on the gradient of the local parameter [11]

$$\Phi\left(\Psi\left(\theta\right)\right) = F\left(\Psi\right) - v\,\Psi_\theta\,\mathrm{grad}\left(\theta\right) -$$
$$-\frac{1}{\rho}\left(D \cdot \Psi_\theta\,\mathrm{div}\left(\mathrm{grad}\left(\theta\right)\right) + \left(D \cdot \Psi_\theta\right)_\theta \circ \mathrm{grad}\left(\theta\right) \circ \mathrm{grad}\left(\theta\right)\right). \tag{4}$$

To remove the dependence on the gradient of local parameter (4) the following modification of the evolution equation (3) is suggested (see [11] for more details)

$$\frac{\partial \Psi\left(\theta\right)}{\partial t} = \left(I - \Psi_\theta \Psi_\theta^+\right) \cdot \left(F\left(\Psi\right) - \frac{1}{\rho}\,D\,\left\|\Psi_\theta^T\,\mathrm{grad}\left(\Psi\right)\right\|^2 \frac{1}{m_s}\mathrm{Tr}\left(A\right)\right), \tag{5}$$

where

$$\left(\mathrm{Tr}\left(A\right)\right)_i = \sum_j \Psi_{\theta_j \theta_j}^i \left(\Psi_{\theta_j}^T \Psi_{\theta_j}\right)^{-2}, \;\; \Psi_{\theta_j}^T \Psi_{\theta_j} = \sum_k \left(\frac{\partial \Psi_k}{\partial \theta_j}\right)^2.$$

The modified invariance equation (5) defines the REDIM and incorporates the impact of the diffusion through the modified diffusion term and the gradient of the local parameter $\mathrm{grad}\,(\theta)$, which is now approximated by the norm of the original system gradient - $\left\| \Psi_\theta^T \mathrm{grad}\,(\Psi) \right\|$. Therefore, if one knows roughly the norm of the gradient, then it is sufficient to approximate the reduced manifold with an acceptable level of accuracy.
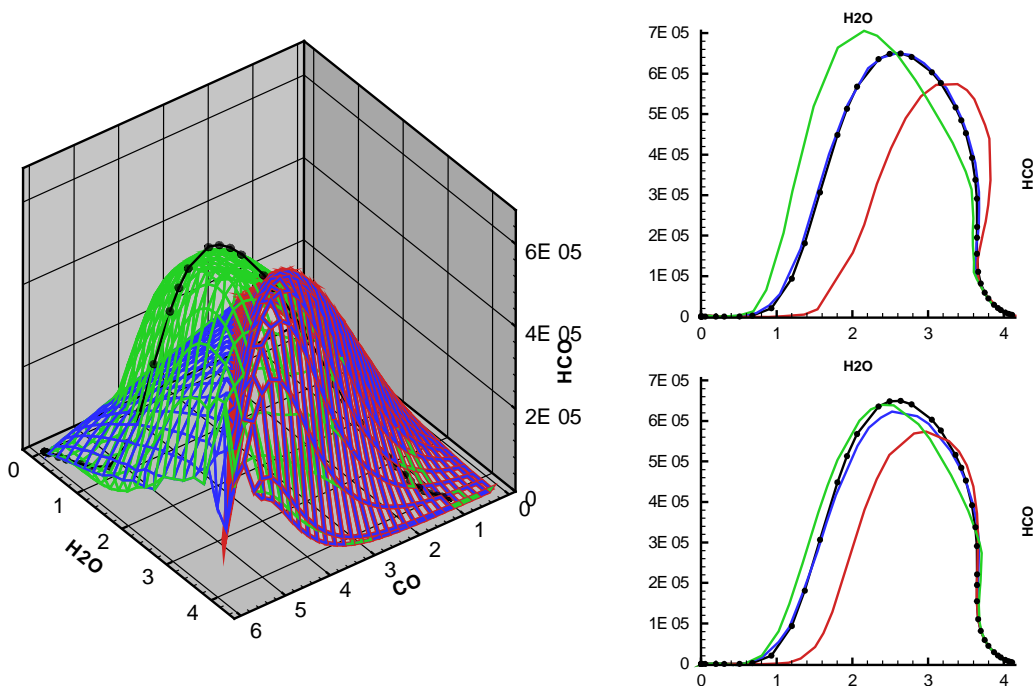

Figure 1: Projections of the state space. Left figure - 2D manifolds: red+blue is the extended ILDM used as an initial guess, green is the 2D REDIM; black curve with filled symbols is the full system stationary solution. Right figure - full (black) and reduced (colored) system stationary solutions for different approximations of the system gradient, the upper figure is based on a 1D model, the lower figure shows the result of a 2D reduced model.

Figure 1 (left) shows a 2D REDIM for a syngas/air system and the detailed system stationary solution in a projection onto the $H_2O - CO_2 - HCO$ subspace. One can see that the system solution deviates from the standard ILDM, which is used as an initial solution for (5), in the domain where the temperature is low (close to the origin), but the REDIM captures rather well the system solution.

The right figures illustrate how the stationary solution of the reduced model depends on the approximations of the system gradient of the syngas/air laminar flat flame example. In this case the system gradient approximations were varied within two orders of magnitude, but nevertheless the reduced model produces reasonable results even for minor species like HCO and in the so called low temperature domain. Moreover, increasing of the manifold dimension by one it becomes less sensitive to the estimation of the system gradient. Although two orders were used for the gradient estimation the deviation of the reduced solutions are in a small range of several percent.

4   Conclusions

A new approach for automatic mechanism reduction - the REDIM method is discussed in this work. The method is developed as an attempt to approximate the PDEs system behavior in the state space. The

REDIM manifold is defined as a stationary set of a multidimensional parabolic PDEs system defined in the state space. The dependence on the spatial coordinates is removed due to the suggested modification of the so called invariance condition, which overcomes the problem of an infinite dimensional structure of the PDE system's slow manifold.

The constructed manifold approximates well enough the stationary system solutions even in the low-temperature domain, which previously was a problematic point of several reduction methods. It allows a reasonable description of the minor species evolution through the laminar flame front. It was found that the sensitivity to the system gradient estimation decreases with the increase of the manifold dimension. Numerical simulations show that the reduced and detailed models are in a good agreement.

References

[1] Warnatz J et al. (2000). Combustion. Springer Verlag.

[2] Zagaris A et al. (2004). Fast and slow dynamics for the computational singular perturbation Method. Multiscale Modelling and Simulation. 2: 613-638.

[3] Bykov V et al. (2005). Novel numerical decomposition approaches for multiscale combustion and kinetic models. Journal of Physics: Conference Series. 22: 1-29.

[4] Davis MJ (2006). Low-dimensional manifolds in reaction-diffusion equations. 1. Fundamental Aspects & 2. Numerical Analysis and Method Development. Journal of Physical Chemistry A. 110: 5235-5272.

[5] Nafe J and Maas U (2003). Hierarchical Generation of ILDMs of Higher Hydrocarbons. Comb. Flame, 135:1726.

[6] Bykov V et al. (2006). On a modified version of ILDM approach: asymptotic analysis based on integral manifolds. IMA J. Applied Mathematics, 71:359382.

[7] Borok S et al. (2006). Model Reduction and Coarse-Graining Approaches for Multiscale Phenomena. Springer, BerlinHeidelbergNew York, 55-81.

[8] Valorani M et al. (2006). An automatic procedure for the simplification of chemical kinetic mechanisms based on CSP. Combustion and Flame. 146: 29-51.

[9] Lam SH (2006). Reduced chemistry-diffusion coupling, accepted to appear in Combustion Science and Technology.

[10] Gorban A et al. (2004). Constructive methods of invariant manifolds for kinetic problems. Physics Reports. 396:197-403.

[11] Bykov V and Maas U (2006). The extension of the ILDM concept to reaction-diffusion manifolds, Combustion Theory and Modelling, in print.

[12] Golub GH and C.F. van Loan (1989). Matrix Computation. The Hopkins University Press. Baltimore, London.

[13] Bykov V and Maas U (2007). Extension of the ILDM method to the domain of slow chemistry. Proc. Comb. Inst. 31, 465-472.