An analysis of the attractive properties of REDIM manifolds for model reduction

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1 Introduction

The mathematical model of reacting flows of a combustion process is represented by the system of partial differential equations as the closed set of the standard conservation equations. It is well known that the most complicated part of this mathematical model is the chemical kinetic (extremely large in terms of dimension, non-linear and stiff) [1]. Hence methods of reduction of dimension and stiffness of large detailed chemical kinetic models are very important and have been developed intensively in the last years [2–7]. Many reduction methodologies focus on the chemical source term, however, because of the strong coupling of diffusion and reaction in the combustion process many existing operator splitting methodologies (see e.g. [8, 9]), split reaction and transport terms) may fail. This means that chemical kinetic models have to be analyzed and reduced taking into account the coupling with the molecular transport. On the other hand, applying the same transport term for reduced model as for the detailed one, while replacing the source term by a reduced mechanism, can lead to inaccurate results as well [9].

One of basic concepts of model reduction, which is a widely accepted concept in the combustion community, is the so-called attractive invariant low dimensional manifolds embedded in the composition space of a reacting system [10–12]. According to this concept, the system states are assumed to be confined to these manifolds during combustion processes. This idea leads to straightforward implementation schemes based on tabulation and interpolation procedures of the manifold. Thus, model reduction means reformulation of the system of governing equations on this low dimensional manifold [13]. Theoretically, in order to reduce the system one should look for an invariant manifold (e.g. manifolds composed from system solutions) of significantly smaller dimension than that of the original system. Note that not any invariant manifold can be applied, it is important to have a good approximation for the system states during all stages of combustion process. In implementations methods of model reduction can be characterized by the properties of the invariant manifolds involved (i.e. slow, fast, attractive and stable etc.), by the methods of approximation the manifolds and by methods of applying the constructed manifold. For instance, consider a very transparent example - the method of Flamelet Generated Manifolds (FGM) [14]. It is based on detailed (e.g. automatically invariant) stationary system solutions. However, attractiveness and stability as well as the question of how good this set of trajectories (set of stationary system solutions) describe the process at hand is not fully understood. There are problems with the choice of the system parameters that define particular solutions (e.g. scalar dissipation rate,

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flame curvature, flame stretch etc.), with parameterization, which variables have to be used for parameterizing and implementing the FGM manifold. Nevertheless, this method is a very efficient tool in the range of applications when the main FGM assumptions are valid.

The method of reaction-diffusion manifolds (REDIM) [15, 16] is an alternative approach to implement such type of model reduction [17]. This exploits the existence of differences in time scales of subprocesses in combustion process leading to a decomposition of the system dynamics and as a consequence to the manifold existence. The method allows us to construct an attracting low-dimensional manifolds in composition space accounting for the coupling of molecular transport with chemical reaction. Inputs to the method are a detailed reaction mechanism, boundary conditions of the reacting flow, and an estimate of the local gradients of the scalars in the flow. 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 PDE governing equations on this low dimensional manifold.

This work presents the premixed free flat flame of syngas/air mixture as a reference benchmark model for study attracting properties of the REDIM. It is relatively simple example, but nevertheless, it contains main features of combustion systems. For stoichiometric mixture composition the 2D REDIM manifold is constructed on the basis of a constant gradient estimation. Decomposition of motions and attractiveness of the REDIM is investigated and verified by the source term eigenvalues analysis with the help of detailed system solutions.

2 REDIM

To take into account both the transport and thermo-chemical properties of the detailed system into the reduced one, one naturally starts with the best available detailed mathematical description. In the case of a reacting flow system it is the Navier-Stokes equations system for reacting flows. It is shown below in general vector notations for low Mach number, adiabatic (p=const., h=const.) reacting flow which is the reference case in the study.

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

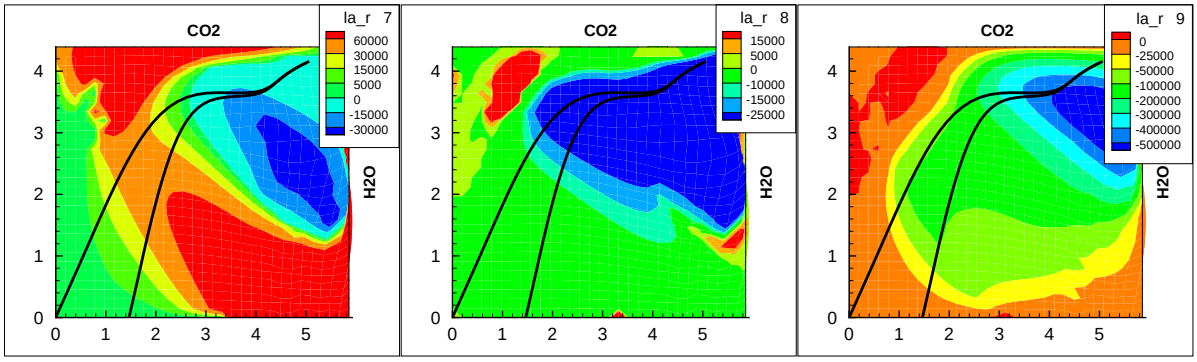
where v represents the velocity field, ρ the density and D the (n by n)-dimensional matrix of the transport/diffusion coefficients [1]. The state vector Ψ is the ($n = n_s + 2$)-dimensional state space vector $\Psi = (h, p, w_1/M_1, ..., w_{n_s}/M_{n_s})^T$, where h denotes the enthalpy, p the pressure, $w_1, ..., w_{n_s}$ 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.

The main purpose of the method is looking for an m_s-dimensional invariant manifold ($m_s << n_s$) to (1) $\Psi\left(\theta\right)$: $M = \{\Psi = \Psi\left(\theta\right), \Psi : R^{m_s} \rightarrow R^n\}$, where θ is a m_s-dimensional parameter on the manifold, e.g. in applications a fixed parameterization in terms of original variables can be used $\theta = (w_{H_2O}/M_{H_2O}, w_{CO_2}/M_{CO_2}, etc...)$ (as in figures shown below). However, in the construction process the coordinates are locally adapted to the shape of the manifold in the composition space, making the method flexible and independent from the parameterization.

The invariant manifold is obtained as the solution of

$$\frac{\partial \Psi\left(\theta\right)}{\partial t} = \left(I - \Psi_\theta \Psi_\theta^+\right) \cdot \left(F\left(\Psi\right) + \frac{1}{\rho}\,\left\{D\,\Psi_\theta\,\mathrm{div}\left(\mathrm{grad}\left(\theta\right)\right) + \left(D\Psi_\theta\right)_\theta \circ \mathrm{grad}\left(\theta\right) \circ \mathrm{grad}\left(\theta\right)\right\}\right) \tag{2}$$

for $t \rightarrow \infty$, where X_θ denotes the partial derivatives with respect to θ [15]. Ψ_θ^+ is the Moore-Penrose pseudo-inverse of Ψ_θ [19]. Thus, M defines the states in the composition space where fastest chemical



(a) Re(λ_7) (b) Re(λ_8) (c) Re(λ_9)

Figure 1: Contour lines represent real parts of three first 'smallest' non-zero eigenvalues of the Jacobian of the reaction source term of the system calculated on the 2D REDIM in projection onto $CO_2 - H_2O$ plane. Two stationary solutions of the detailed system (1) are shown by black lines.

processes are relaxed similar to the main assumption of the ILDM [6, 7, 11], moderating fast processes are strongly coupled with the transport terms (second and third terms in (2)) while the slowest chemical modes are dominated by the relatively strong mixing processes. It is assumed that the system relaxes fast towards M and the balance between diffusion and reaction establishes. This relaxation time can be roughly estimated by the smallest eigenvalue of the source term of the group of large decoupled eigenvalues. In this way, having the detailed solution one is able to estimate the manifold dimension by the number of chemical modes which are coupled with the diffusion time scales, roughly given by the local parameter gradients grad (θ).

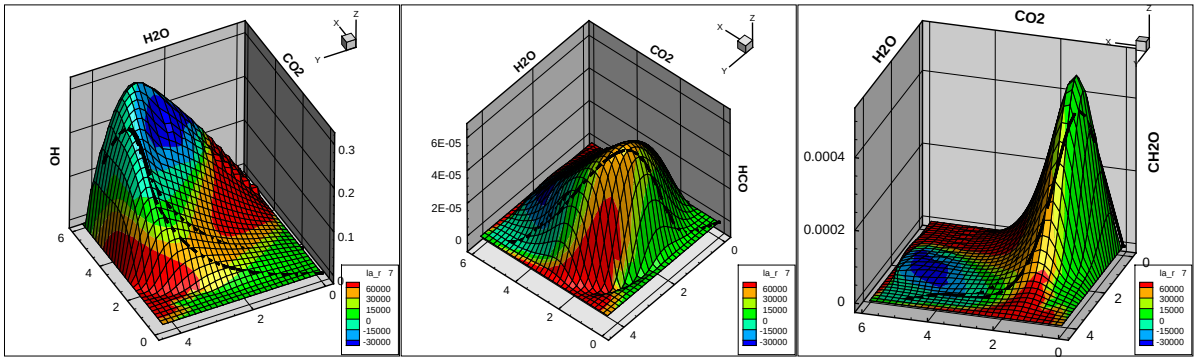
It means increasing the dimension of the reduced model accounts automatically for richer dynamical regimes. Because additional fast/slow chemical modes are allowed to couple with the mixing processes on the manifold that represents the reduced model.

3 Local gradients, eigenvalues

In order to illustrate the balance between reaction and diffusion, consider the REDIM 2D manifold for a syngas/air system and the dynamics of the detailed system solutions profiles. In our previous works [15, 16] it has been shown that for 1D case (spatial dimension, with Cartesian coordinate frame) the manifold depends weakly on the spatial coordinate. This dependence (see (2)) is due to the local parameter gradient grad $(\theta) = \partial\theta/\partial x$ and due to the second spatial derivative div $(\text{grad}\,(\theta)) = \partial^2\theta/\partial x^2$.

In this study, in order to construct the 2D REDIM a constant approximation of the parameter gradient has been implemented. An iterative procedure to handle this dependence on the spatial coordinate has been suggested in [16] for an equal diffusivity assumption (the second derivative cancels out from the manifold equation in this case) and further extended to the case of non-equal diffusivity case [18].

When the 2D REDIM has been tabulated, several detailed stationary and non-stationary system profiles are calculated with the source term eigenvalues evaluated on the REDIM manifold. Figure 1 illustrates the result of the eigenvalues analysis of the Jacobian of the source term. Two stationary solutions (same element composition and enthalpy to ensure the same equilibrium) are chosen to illustrate the system stationary profiles path in the composition space. Both trajectories end up at the same equilibrium corresponding to the composition past the free laminar plane flame, but have different initial mixture composition.



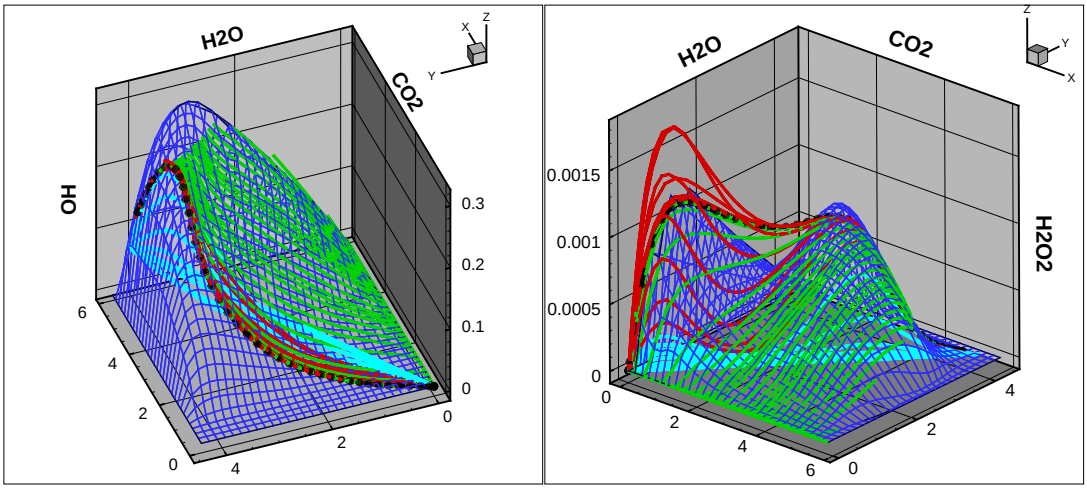
(a) OH (b) HCO (c) CH_2O

Figure 2: 2D REDIM in projections to major and minor species specific mole numbers. Contour lines show the values of the real part of the 'smallest' eigenvalue same as in Fig. 1a, solid lines are the detailed system stationary solutions.

This figure shows by contours a typical spectrum of the reaction source term for chosen mechanism. The mechanism contains $n_s = 13$ species [15], thus the overall system dimension is $n = 15$. There are $n_c = 6$ zero eigenvalues of the Jacobian of F correspond to conserved quantities: elements $(\mathrm{O},\ \mathrm{C},\ \mathrm{H},\ \mathrm{N})$, enthalpy and pressure. The first non-zero eigenvalue shown in Fig. 1a is positive (explosive) almost throughout the entire detailed system trajectory, the second 1b is also small (note, it can be positive as well for other sets of system parameters etc.) but negative while the real part of the rest of eigenvalues (see Fig. 1c, where the third is shown) are all negative and become very large in magnitude.

The second Fig. 2 illustrates that if one is interested in 2D slow invariant manifolds a rough approximations of the order of magnitude of the gradient is enough to obtain satisfactory approximation of the manifold. This is because the two moderate eigenvalues (sometime even positive) are accounted for and most unstable dynamics evolves within 2D REDIM. Moreover, one sees that the stiffness of the source term increases (there are only two eigenvalues are of moderate magnitude and the rest of the eigenvalues are extremely large and negative!). This removes further dependence of the reduced manifold on spatial gradients for higher dimensional manifolds embedded into the composition space.

Figure 3 illustrates additionally the composition space with the 2D REDIM and detailed system solutions. Two arbitrary initial profiles have been chosen, which evolve in time during the system (1) integration. The green one represents evolution of the initial profile joining the unburnt mixture with the mixture having the specific mole number corresponding to full conversion of CO into CO_2 (this corresponds to calculating of a mixture of CO_2, N_2, H_2 and O_2). While cyan and red lines shows the evolution of the system solution from the initial profile that joins the unburnt mixture with the chemical equilibrium. The cyan part (first 10 integration steps, until 2×10^{-5} seconds of the system integration) indicates the fast initial transition (see Fig. 3a) where the fast modes are relaxed and the solution reaches the slow invariant manifold. The trajectories approach the REDIM and finally converge to the same stationary solution shown by black curve with symbols. It can be seen that even for minor specie as HCO, CH_2O and H_2O_2 (see e.g. Figs. 2b, 2c and 3b) and for rough estimation of the system gradient, which is taken constant throughout the whole domain, the manifold and the detailed system trajectory evolutions are very close. It has to be noted that other radicals show an even better relaxation to the REDIM.



(a) OH (b) H_2O_2

Figure 3: 2D REDIM and the system detailed solutions in projections to specific mole numbers. Cyan, red and green lines show the detailed system solutions, blue mesh is the 2D REDIM, while black line with symbols is the stationary system solution.

4 Conclusions

The REDIM method was discussed in this paper within the framework of manifold based model reduction. The role of decomposition of motions and attractive properties of the REDIM were investigated. The influence of the local gradients on the manifold dimension is discussed. The premixed free flat flame of syngas/air mixture is considered as a reference benchmark model. For a stoichiometric mixture composition the 2D REDIM manifold was constructed on the basis of a constant gradient estimation. The Jacobian of the source term calculated on the 2D REDIM revealed that two eigenvalues only are coupled with the transport, while others are negative and very large. They can be decoupled which confirms the existence of the 2D attractive REDIM for chosen configuration. The analysis is illustrated and verified by comparison of the REDIM and the unsteady detailed system profiles in projection to some species mole numbers.

Acknowledgments

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