Analysis of transient processes in the context of REDIM

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***Abstract*— The method of reaction-diffusion manifolds (REDIM) has been shown to be a very efficient model reduction tool for reacting flows. The method is based on attracting low-dimensional manifolds defined in the composition space of a reacting flow system. The reduced kinetic mechanism is constructed as a table of a slow manifold mesh in the system composition space. This work discusses the ability of the method to describe transient behavior of a combustion system. In order to access this property of the reduced model two types of system dynamics are investigated with respect to the tangential and normal subspaces of the system slow manifold. This is accomplished by a local analysis of the eigenvalues of the chemical source term (projecting the Jacobian onto the tangential and normal subspace of the manifold) and by comparison of the detailed and reduced system behavior. Counter-flow diffusion flames of nitrogen-diluted Hydrogen-Air are used to illustrate the results.**

I. INTRODUCTION

In order to fully describe reacting flows mathematically a set of conservation equations for the ($n = n_s + 2$)-dimensional state vector $\psi = \left(h, p, w_1 / M_1, ..., w_{n_s} / M_{n_s}\right)$ has to be considered [1]. However, accurate models of chemical kinetics become not treatable in a reasonable time even by up to date soft- and hardware facilities due to the models complexity. Thus, the interest in automatic approaches that reduce the dimension and complexity of the system without quantitative loss of the accuracy has increased over the last decade. The assumption about the existence of so-called attractive low dimensional manifolds takes a central role in developing modern model reduction schemes [2-7].

The method of reaction-diffusion manifolds (REDIM) [7-11] is one of such approaches that allow us both to obtain a simplified description (model) of the chemical kinetics and to account for the influence of the molecular transport onto the reduced model. Similarly to other approaches, the main idea behind the REDIM is that the states of the detailed systems solution profiles $\psi = \psi(x,t)$ during the transient motion of the system are completely confined to a low(m_s)-dimensional subset of the state space. Thus, to describe the transient evolution, whenever the subset is known, less parameters would be needed - $m_s << n$. The manifold accounts for the fact that the reacting system states are tend to the states in the composition space where the fastest chemical processes are relaxed (similar to the main assumption of the ILDM method [2, 7]), moderate ones are strongly coupled with the transport, while relatively slow chemical processes are governed by strong molecular transport processes [8].

It has been shown in previous works that the REDIM approach is able to represent stationary solutions of 1D laminar and turbulent flames [8-11]. This work represents a discussion of properties of the method which describe its ability to capture transient motions such as extinction or re-ignition [11].

II. REDIM

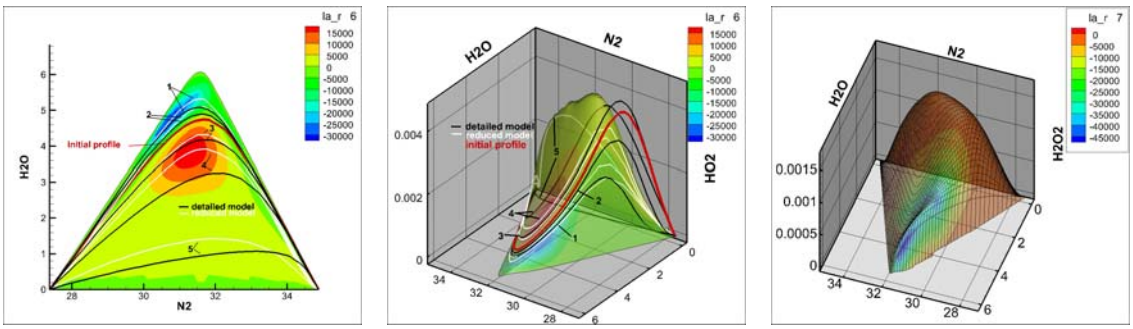
The method is searching for an approximate of an invariant manifold of relatively slow system motions $M = \left\{\psi = \psi(\theta), \quad \theta \in R^{m_s}\right\}$. Here θ is a parameterization of the manifold. An approximation to the invariant manifold is obtained as the stationary solution of a multi-dimensional parabolic system of partial differential equations [7]. In this way the system itself adapts to the states which optimally suits to capture the above mentioned structure of the decomposition of motions. In order to make use of it, the REDIM is tabulated in the form $\psi = \psi(\theta)$. Solving the conservation equations for the parameters θ yields the time dependent states within the manifold [7, 10, 11].

III. ANALYSIS

In order to verify the REDIM method and to address the transient system behavior a state space analysis of a 1D counter-flow diffusion flame has to be considered at first. Then, after a local analysis of the systems source term a comparison of the stationary and non-stationary system solution profiles of the detailed and reduced systems is carried out.

A. Tangential motions

The invariance condition of the REDIM postulates that the dynamics of the detailed system will at any time be tangential to the REDIM. However, if the system solution profile is perturbed and the system states leave the manifold it has to be addressed for a secure use of the reduced model. In this case the time scales of physical transport coupled with the time scales of chemical reaction lie beyond the band width of time scales covered by the two parameters θ. Suppose that there is a detailed stationary solution attached to the REDIM. In case of strong perturbations the transport processes will cause the detailed profile to leave the REDIM while moving to another stationary state where it is attached again to the REDIM. If the perturbations are strong enough



(a) (b) (c)

Fig 1. Contour lines represent real parts of the eigenvalues of the Jacobian of the transformed reaction source term of the system calculated on the 2D REDIM (all projections are in specific mole numbers). The transient solution of the detailed system is shown by black lines, solutions of the reduced model are white lines shown on the 2D REDIM, the red line shows a perturbed initial solution [11].

they can lead to extinction (or to another quasi-stable regime).

The question is how accurately the REDIM can capture the tangential part (i.e. the projection onto the tangential subspace) of these transient motions as well as the conditions which lead to extinction. In order to investigate the stability properties of the reduced model the local Jacobian $\frac{\partial F}{\partial \Psi}$ of the chemical source term is reformulated in terms of a basis of the composition space containing the vectors Ψ_θ [11]. The magnitude of the eigenvalues of the transformed Jacobian gives information about the transient behavior (see Fig. 1 (a), (b)).

B. Motions normal to the manifold

The attractiveness of the REDIM is justified by the decoupling of the fast chemical processes. It is assumed that whatever perturbations are the system relaxes fast towards *M* and the balance between diffusion and reaction is established. To confirm this assumption the local Jacobian of the chemical source term is reformulated in terms of a basis of the composition space containing the vectors $\Psi_\theta{}^\perp$ where the vector $\Psi_\theta{}^\perp$ is transversal to the tangential subspace of the manifold. As illustrated by the contour plot in Fig. 1 (c), where the real parts of the smallest in magnitude eigenvalue is shown, the eigenvalues of the transformed Jacobian are strictly negative and large in magnitude. Therefore, if perturbations cause the profile to leave the REDIM, the chemical processes will force the profile to move back onto the manifold. The relaxation time can be roughly estimated by the smallest eigenvalue of the projected source term.

IV. Conclusions

The ability to describe the transient (non-stationary) behavior of a reacting flow system by the REDIM method of model reduction was discussed. By analyzing the eigenvalues of the reformulated local Jacobian of the chemical source term in terms of a new basis of the tangential bundle it could be shown that the REDIM can capture both stable and unstable chemical modes that are coupled to the transport. Moreover, it could be shown, that strong negative eigenvalues of the Jacobian in terms of a basis containing vectors transversal to the tangential subspace substantiate the invariance assumption. It was shown how this procedure can be used to prove that the REDIM adequately captures the decomposition and the coupling of physical transport with chemical reaction for the case of transient dynamics.

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