

# Some properties of the Reaction-Diffusion Manifolds

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**Abstract**— The method of reaction-diffusion manifolds (REDIM) has been shown to be a very efficient tool for model reduction for reacting flows. The method constructs attracting low-dimensional manifolds in composition space accounting for the coupling of molecular transport with chemical reaction. The reduced kinetic mechanism is constructed as a table of a slow manifold mesh in the composition or state space. This work discusses an analysis of several properties of the REDIM method, namely, attractiveness and the role of the decomposition of motions, the REDIM existence and its dimension. The analysis is illustrated by study the influence of the source term eigenvalues and the local gradients on the REDIM manifold with the help of detailed system solutions. A premixed laminar free flame is considered to verify and illustrate the method.

## I. 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 known that the most complex part of this mathematical model is the chemical kinetic model (extremely large in terms of dimensions, non-linear and stiff) [1]. Typically, chemical kinetic mechanisms are developed, analyzed and reduced by using standalone homogeneous systems or within 1D spatial configurations (study of laminar flames).

The assumption about the existence of so-called attractive low dimensional manifolds takes a central role in developing modern model reduction schemes (see e.g. [2-10]). The main assumption of manifold based reduction schemes confines the detailed system during the evolution to a low-dimensional manifold embedded into the composition/state space of the detailed system. This brings a technical or formal meaning to the reduction procedure. At present, there are many approaches differing one from the other by the way of the manifold approximation, its description and its use.

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 however that not any invariant manifold can be applied, but it should be a good approximation for the system states during all stages of combustion process (i.e. is should be attractive and stable). In implementations, however, model reduction means reformulation of the system of governing equations on this low dimensional manifold [11].

The method of reaction-diffusion manifolds (REDIM) [12, 13] is an approach performing such type of model reduction [14]. This exploits the existence of differences in time scales of sub-processes in combustion process leading to a decomposition of the system dynamics and, as a consequence, to the manifold existence. The method constructs an attracting low-dimensional manifold 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 a discussion of several very important properties of the REDIM method: attractiveness, decomposition of motions, the REDIM existence and dimension. The analysis is illustrated by a premixed (syngas/air benchmark model) laminar free flame of relatively simple structure, which nevertheless contains main features of reacting flows.

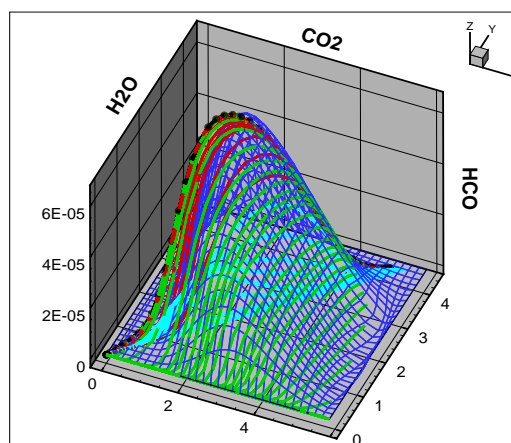


Fig. 1. The REDIM with the detailed system trajectories. Blue mesh is the REDIM given for a fixed gradient estimation, cyan, green and red lines are detailed system solutions. Black curve with symbols is the stationary system solution.

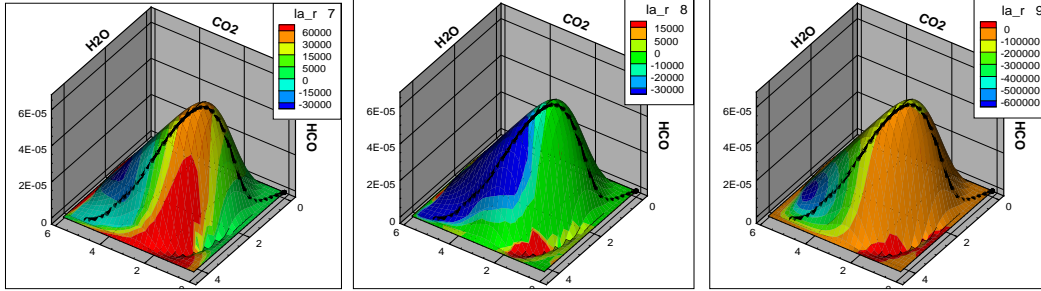


Fig 2. Contour lines represent real parts of three non-zero eigenvalues of the Jacobian of the reaction source term of the system calculated on the 2D REDIM (specific mole numbers are shown). The stationary solution of the detailed system (1) is shown by black line with symbols.

## II. REDIM

### A. REDIM – Invariance equation

In order to determine rigorously the low dimensional manifold taking into account both the molecular transport and chemical reaction one starts with the detailed model. It is shown below in general vector notations for low Mach number (pressure  $p=\text{const}$ , adiabatic – enthalpy  $h=\text{const}$ ) reacting flow which serves here as a reference case.

$$\frac{\partial \psi}{\partial t} = F(\psi) - \bar{v} \text{grad } \psi - \frac{1}{\rho} \text{div}(D \text{grad } \psi) \quad (1)$$

where  $\bar{v}$  represents the velocity field,  $\rho$  the density and  $D$  the  $(n \text{ by } n)$ -dimensional matrix of the transport/diffusion coefficients [15]. The state vector  $\psi$  is the  $(n = n_s + 2)$ -dimensional state space.  $F(\psi)$  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 to (1) with  $m_s \ll n_s$ :

$$M = \{\psi = \psi(\theta), \quad \theta \in R^{m_s}\}, \quad (2)$$

here  $\theta$  is a parameterization of the manifold. In principle, it can be any combination of the original variables, but during the REDIM construction process the coordinates are adapted locally to the form of the manifold in the composition space that makes the method flexible and independent from the parameterization. An approximation to the invariant manifold is obtained as the solution of (see Fig. 1) [10, 12]:

$$\begin{cases} \frac{\partial \psi(\theta, t)}{\partial t} = (I - \psi_{\theta}(\theta) \psi_{\theta}^+(\theta)) \cdot \{F(\psi(\theta)) - 1/\rho \cdot \\ \cdot [D \psi_{\theta} \text{div grad } \theta - (D \psi_{\theta})_{\theta} \circ \text{grad } \theta \circ \text{grad } \theta]\} \\ \psi(\theta, 0) = \psi_{\theta}(\theta) \end{cases} \quad (3)$$

for  $t \rightarrow \infty$ , where the subscript  $\theta$  denotes the partial derivatives with respect to  $\theta$  [12, 16].  $\psi_{\theta}^+(\theta)$  is the Moore-Penrose pseudo-inverse of  $\psi_{\theta}(\theta)$  [17]. Thus,  $M$  defines the states in the composition space where fastest chemical processes are relaxed similar to main assumption of the ILDM [3, 7, 9], moderate are strongly coupled with the transport terms (second and third terms in (3)) while slowest chemical modes are damped off by the relatively strong mixing processes. It is assumed whatever perturbations are the system relaxes fast towards  $M$  and the balance between diffusion and reaction established. This relaxation time can be roughly estimated by the smallest eigenvalue of the source term of the group of decoupled eigenvalues (see Fig. 2, right). 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  $\text{grad } \theta = \partial \theta / \partial x$ . It means higher dimensional manifolds account automatically for richer dynamical regimes.

### B. Spatial dependence

In the previous works [12, 13, 16] it has been shown that for the 1D case (spatial dimension, with Cartesian coordinate frame) the manifold depends weakly on the spatial coordinate, this dependence (see (3)) can be studied through the local parameter gradient  $\text{grad } \theta$ . An iterative procedure to handle this dependence on the spatial coordinate has been suggested in [13] 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 [16].

## III. ANALYSIS

### A. Source term eigenvalues

Let us consider the REDIM 2D manifold for a syngas/air system and the detailed system solutions. Figure 2 shows contours of eigenvalues of the Jacobian of the source term, which are calculated on the 2D REDIM manifold [12]. The stationary solution is shown to the stationary trajectory path in the composition space. These figures show by contours a typical spectrum of the Jacobian of the reaction source term for the chosen mechanism.

There are three groups of eigenvalues: zero eigenvalues (6 in total) correspond to conserved quantities as, for

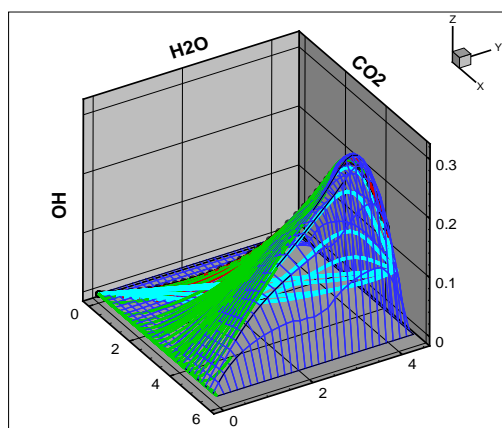


Fig. 3. 2D REDIM with non-stationary system solutions - color lines. Cyan lines show the evolution of the initial profile during first  $2 \times 10^{-5}$  seconds.

instance, elements conservations, the first non-zero eigenvalues are shown in Fig. 2. The first is positive (explosive) almost throughout the entire detailed system trajectory, the second is also small but negative (note, it can be positive as well for other set of system parameters etc.), while the real part of the rest of eigenvalues (see Fig. 2, right) are all negative and become very large in magnitude (not shown here).

#### B. Detailed system solution trajectories

Figures 1 and 3 illustrate additionally the composition space structure with 2D REDIM and detailed system solutions having extremely different initial profiles. Two artificial initial profiles have been chosen, which evolve during the system (1) integration. The green one represents the 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<sub>2</sub> (this corresponds to calculating of a mixture of CO<sub>2</sub>, N<sub>2</sub>, O<sub>2</sub> and H<sub>2</sub>.) While the cyan and red lines show 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  $2 \times 10^{-5}$  seconds of the system integration) indicates the fast initial transition, where the fast modes are relaxed and the solution reaches the slow invariant manifold. One can see that 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 and for a rough estimation of the system gradient, which is assumed to be constant throughout the whole domain, the manifold and the detailed system trajectory evolutions are very close.

#### IV. CONCLUSION

The REDIM method as an example of realization of the manifold based reduction methodology was discussed in this work. The role of the main assumption of decomposition of motions was investigated. The influence of the local gradients and manifold dimensions were

discussed. A premixed free flat flame of syngas/air mixture is considered as a reference benchmark model. For 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 only two eigenvalues 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. It allows us to overcome the problem of an infinite dimensional structure of the PDE system's slow manifold.

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