Implementation of ILDMs Based on a Represenation in Generalized Coordinates

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Introduction

The simulation of reacting flows using detailed chemistry introduces a large number of species (sometimes more than 1000) and reactions. Therefore, detailed chemical kinetics is usually computationally prohibitive for turbulent reactive flows and it is necessary to devise methods to reduce chemical kinetics. The concept of ILDM (Intrinsic Low Dimensional Manifolds) [1,2] is one of these techniques. Based on an eigenvector analysis of the jacobian matrix of the chemical source terms, it generates automatically reduced mechanisms to describe the chemical dynamics by a small number of reaction progress variables. For the implementation of the ILDM method two sub-tasks arise: first, an efficient generation of the reduced mechanism, and, second, the projection of the governing equations in the CFD code to the reduced variables. There are several possibilities for the projection of the governing equation system. Whereas the ILDM can be generated using a locally adapted parametrization, in most CFD applications it is used in terms of a fixed parametrization. In this case, the governing equation system is projected to 2-4 major species concentrations characterizing the reaction progress (e.g. CO_2, H_2O). This methodologie is intuitive, because of the direct physical meaning of the reduced variables. However, the use of a fixed parametrization can cause problems in the numerical solution because this parametrization might be not unique or ill-conditioned. Another possibility is the implementation of the ILDM in terms of generalized coordinates. This corresponds to a projection of the governing equation sytem to grid coordinates of the ILDM. In this way the reduced coordinates are everywhere ideally adapted to the reaction progress and uniqueness is guaranteed. Furthermore, due to the orthogonal unit structure of the grid the interpolation during the CFD calculation turns out to be robust and efficient. In the following such an implementation in terms of generalized will be presented.

Mathematical Model

In chemically reacting systems the thermochemical state is completely determined by the $(n = n_s + 2)$-dimensional vector $\Psi = (h, p, w_i/M_i \ldots w_{ns}/M_{ns})^T$ where h denotes the enthalpy, p the pressure, w_i the species mass fractions of the n_s chemical species and M_i the molar masses, and the evolution of the thermokinetic state is governed by

$$\frac{\partial \Psi}{\partial t} = F(\psi) - v \cdot \mathrm{grad}\Psi - 1/\rho \cdot \mathrm{div}(D \cdot \mathrm{grad}\Psi) \tag{1}$$

where t denotes the time, $F(\Psi)$ the n-dimensional vector of chemical source terms, v the velocity, ρ the density, and D the (n by n)-dimensional matrix of the transport coefficients. According to the ILDM concept (see e.g. [1, 2]) the thermokinetic state is a function of a small number m of reduced variables ($\Psi = \Psi(\theta)$), and physical perturbations which tend to pull off the system from the ILDM have to be projected back onto the manifold using a projection operator P [2]. If the ILDM is calculated by a multidimensional continuation method [3] all information on the ILDM, the dynamics, and the transport properties is known as functions of the m_s-dimensional vector of mesh coordinates θ, and the use of grid coordinates θ is an ideal choice as reactive variables. It can be shown by simple calculus that the projected equations in terms of an arbitrary parametrization of the manifold read

$$\frac{\partial \theta}{\partial t} = \Psi_\theta^+ \cdot F\big(\psi\big) - v \cdot \mathrm{grad}\theta - 1/\rho \cdot \Psi_\theta^+ \mathrm{P} \cdot \mathrm{div}(D \cdot \Psi_\theta \cdot \mathrm{grad}\theta) \tag{2}$$

where Ψ_θ is the (n by m_s)-dimensional matrix of partial derivatives of Ψ with respect to θ and Ψ_θ^+ denotes its Moore-Penrose pseudo-inverse. All terms necessary for subsequent use in the CFD calculation with reduced chemistry can be pre-calculated and stored during the generation of the ILDM if they are only functions of Ψ and θ:

- the n by m_s-dimensional gradient Ψ_θ and its pseudo inverse Ψ_θ^+
- the chemical source term projected to the reduced variables
- the projection matrix for the transport term
- the transport matrix

The ILDM table is generated in a pre-processing step, and the state Ψ, the projected chemical source term $\Psi_\theta^+ F$, as well as the matrices $1/\rho \cdot \Psi_\theta^+ P$ and and $D\Psi_\theta$, which are needed for the solution of (2) are calculated and stored at each point of the ILDM table which is parameterized by its mesh indices which correspond to the generalized coordinates θ. Because the mesh is orthogonal and equidistant, it is ideally structured for an efficient interpolation during the table look-up.

Results

In order to verify our method presented above, we implemented the method in a laminar 1-D flame calculation [4] and performed simulations of laminar premixed syngas/air flames. The unburnt mixture composition is $X_{CO} = 0.150$, $X_{O2} = 0.131$, $X_{H2} = 0.112$ and $X_{N2} = 0.606$, the unburnt temperature is 298 K, and the pressure is 1 bar. Two- and three-dimensional ILDMs have been implemented. In the following figures results for free flame computation are presented. Figure (1) shows, that even the use of a 2-dimensional reduced mechanism yields accurate results for the major species. The accuracy is, however, increased if a 3-D ILDM is used. Figure (2) shows the profile of CH_2O over the spatial coordinate. It can be seen that a 3-D manifold can give an appropriate description of this minor species.

Figure (3) shows the profiles of the generalized coordinates over the spacial coordinate. It can be seen, that each additional reaction progress variable varies in a smaller range, therefore, only a small domain of the state space in the additional direction is

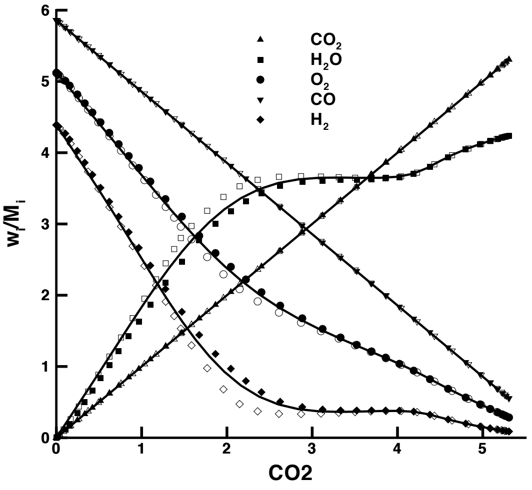

Figure 1: Major species concentrations of a unstrained flame versus CO_2

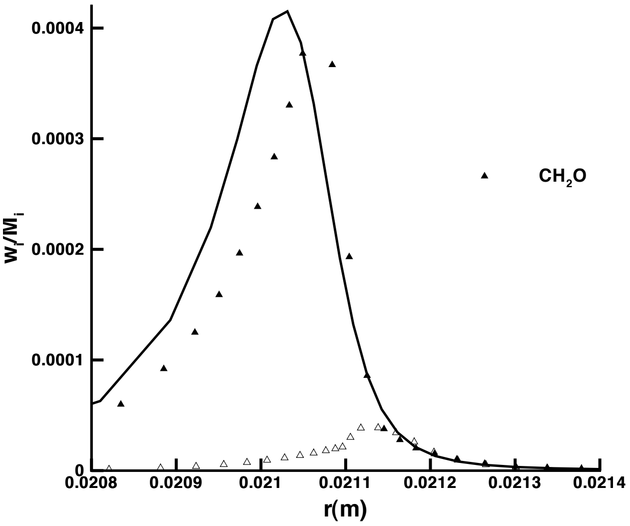

Figure 2: CH_2O versus the spatial coordinate

accessed by chemical reaction and has to be tabulated during generation of the ILDM. This is due to the fact, that the assumption of fast relaxation for the corresponding chemical processes is better and better fulfilled with increasing dimension. Furthermore, we investigated strained flames at various strain rates. For these flames a good agreement is obtained, too. Even the location of the flame is predicted quite well.

The results show that a representation of ILDMs in terms of generalized coordinates offers the advantage of a robust and efficient implementation. The reduced calculations yield good agreement with the results obtained from the detailed calculation. The use of generalized coordinates is very well suited for a on-demand generation of the ILDM

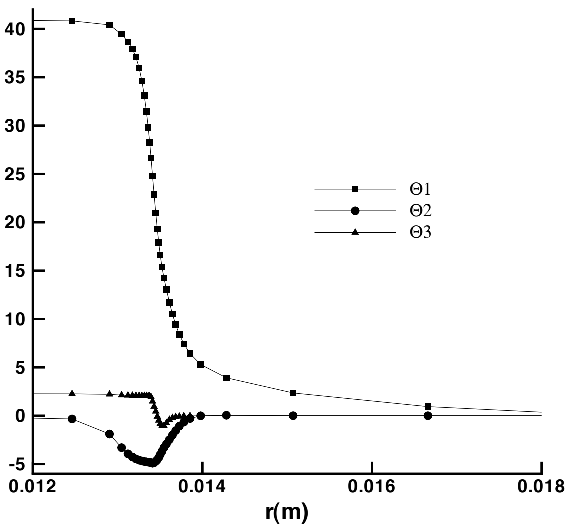

Figure 3: Generalized coordinates θ versus the spatial coordinate

simultaneously with the CFD calculation.

Acknowledgements

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