

REDIM based reduced modeling of transient premixed combustion regimes

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1 Introduction

The correct description of turbulent combustion processes is a challenging problem in the development of combustion models. This holds especially in the case when model reduction methodologies are applied to reduce computational costs. Turbulent convective processes initiate considerable mixing and therefore increase diffusive transport processes. In the presence of high turbulence these convective mixing and diffusive transport processes perturb chemical processes significantly. In the case of free premixed flames very strong mixing pushes the flame profile in state space towards the so called mixing line. The mixing line is characterized by theoretically accessible states in the case of infinitely large mixing rate. Here, molecular transport processes are dominant and much faster than chemical processes [1].

In the present work the characteristics of transient regimes of flame propagation which have as initial profiles states situated along the mixing line in state space is investigated in the context of the Reaction Diffusion Manifold (REDIM) model reduction methodology. Mixing line states are only of theoretical nature, since they are associated to an infinitely high mixing rate. Nevertheless such scenarios represent a useful base for model testing. It is studied whether the application of the manifold based model reduction concept incorporates the properties of the transient combustion processes towards stationary state. The exact reproduction of such transient processes represents a key challenge for model reduction methodologies [2].

The transient behavior of detailed and reduced calculations is compared with regard to the time scales during transition to stationary state. Models are also compared regarding the induction time dependent on initial conditions. A suitable parameter is defined to enable a thorough time scale and induction time examination. The influence of the reduced model dimension on time scale of transition, induction time and the profile relaxation in state and physical space is examined by means of a 1D and a 2D reduced model. By the undertaken investigations the performance of REDIM model reduction method in such important transient scenarios is validated. A stoichiometric syngas-air system whose behavior is studied very well is considered for illustration of the methodology developed.

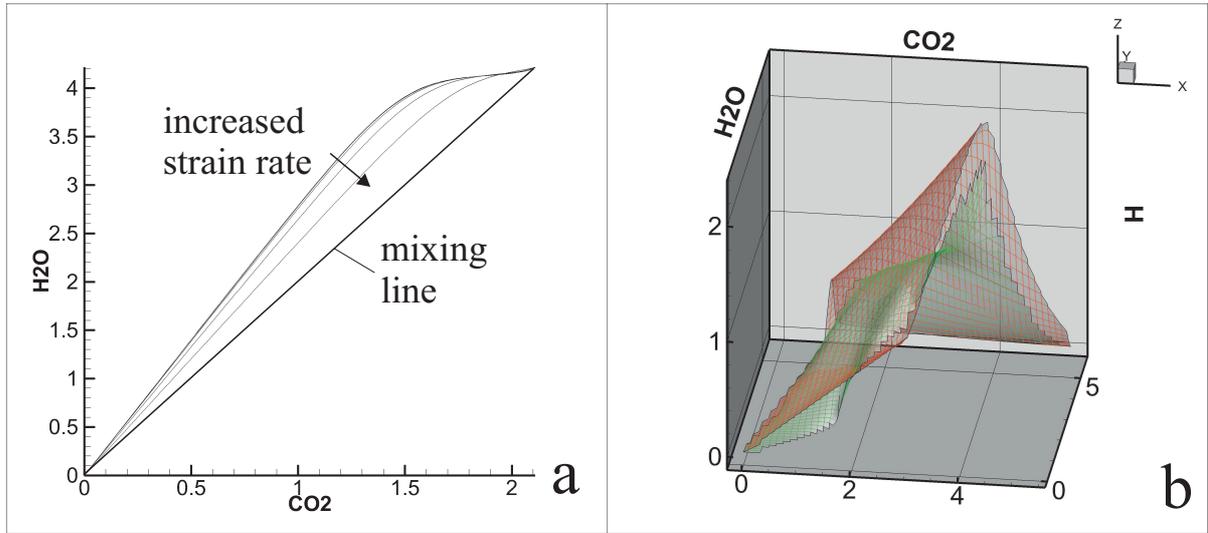


Figure 1: (a): Example showing the influence of mixing on flame structure: Increased strain rate in a non-premixed counterflow syngas-air diffusion flame [3]. (b): REDIM initial solution (red) and converged solution (green) in three dimensional state space representation.

2 The REDIM model reduction concept

The main assumption within the REDIM model reduction concept is the invariance condition. It states that relaxation processes as well as the stationary solution are confined to a REDIM of certain dimension at any time and location. The REDIM therefore captures the coupling between reaction and diffusion.

In order to describe the REDIM a suitable parametrization must be defined. The states Ψ on the manifold M can then be assigned to the coordinates of the parametrization

$$M = \{ \Psi = \Psi(\theta) | \Psi : \mathbb{R}^m \rightarrow \mathbb{R}^n, m \ll n \}, \quad (1)$$

where Ψ is the $(n = n_s + 2)$ -dimensional system state vector, M is the manifold of dimension m , $\theta = (\theta_1, \dots, \theta_m)$ is the vector of the local coordinates and n is the dimension of the complete thermochemical system state space. The assumption of confinement of transient processes and steady states to the REDIM is expressed by the so-called invariance condition statement [4, 5]. Reformulating the invariance condition into a PDE system enables an iterative solution procedure [6].

The solution procedure starts from an initial guess, which in the case of a free premixed flame corresponds to an extended ILDM [5]. Figure 1 (b) shows the initial guess for a 2D REDIM and the converged manifold for a syngas-air system. The manifold is parametrized based on its initial guess. That is, at the beginning of the REDIM solution procedure θ_1 and θ_2 represent linear functions of H_2O and CO_2 .

Once the manifold is found based on the iteration procedure its properties can be tabulated as functions of θ and used within the actual reduced model integration. For this purpose the PDE system of governing equations for reacting flows [7] is transformed into the reduced PDE system for the local coordinates θ [4]

$$\frac{\partial \theta}{\partial t} = \Psi_{\theta}^{+} \left(F(\Psi(\theta)) - v \Psi_{\theta} \text{grad}(\theta) + \frac{1}{\rho} \text{div}(D \cdot \Psi_{\theta} \text{grad}(\theta)) \right). \quad (2)$$

The number of PDEs in Eq. (2) corresponds to the dimension of the REDIM and is much lower than the number of detailed PDEs or the dimension of the entire thermochemical state space ($m \ll n$). Moreover, the tabulated manifold properties $\Psi_{\theta}(\theta)$, $\Psi_{\theta}^{+}(\theta)$, and $(D \cdot \Psi_{\theta})(\theta)$ simplify the solution procedure

of Eq. (2). Solving Eq. (2) yields the solution for the local coordinates $\theta(x, t)$ to which the states $\Psi(\theta)$ on the manifold can now be assigned.

3 Numerical experiments

A free laminar premixed syngas-air system is considered in the current study. The premixed composition consists of 1 mole CO, 1 mole H₂, 1 mole O₂ and 3.762 mole N₂. That is, a stoichiometric mixture configuration is considered.

In the present work the transition processes of flame configurations which initially are situated along the mixing line in state space are examined. According to this initial conditions in physical space must be generated for the numerical calculations. Initial conditions $\Psi(x, 0)$ for detailed calculations are defined through the left boundary condition $\Psi(0, t)$ and the initial condition on the right boundary $\Psi(x_{max}, 0)$

$$\Psi(x, 0) = \Psi(0, t) + \exp\left(-\left(\frac{x - x_{max}}{\sigma}\right)^8\right) \cdot (\Psi(x_{max}, 0) - \Psi(0, t)). \quad (3)$$

Through the initial condition on the right boundary the position of the initial profile in state space is determined. Right boundary states result from a linear interpolation between the premixed state, Ψ_{pre} , and the equilibrium state, Ψ_{eq} . Being exponential in physical space (Eq. 3) initial conditions lead to a linear profile in state space which is situated along the mixing line.

Initial conditions $\theta(x, 0)$ for both 1D and 2D reduced calculations are generated based on the initial conditions $\Psi(x, 0)$ for detailed calculations. First, the states $\Psi(x, 0)$ are projected onto the manifold, yielding corresponding states $\Psi(\theta(x, 0))_M$ on the manifold. $\theta(x, 0)$ is then calculated through $\theta(x, 0) = \Psi_\theta^+ \cdot \Psi(\theta(x, 0))_M$. Note that the direction of projection is chosen according to the initial parametrization of the manifold. In the present study CO₂ for the 1D and (CO₂, H₂O) for the 2D manifold were chosen as initial parametrization. Thus, the projection of detailed initial conditions $\Psi(x, 0)$ onto M is performed such that the values for CO₂ or (CO₂, H₂O) are kept constant.

Starting from several states along the mixing line the transition process of detailed and reduced calculations is investigated. Locations on the mixing line can be characterized by the associated specific mole number of CO₂ which is compared to the specific mole number CO_{2,eq} at equilibrium, e.g. an initial condition which is located in the center of the mixing line is characterized by $0.5 \cdot \text{CO}_{2,eq}$.

The time scale of the transition process is investigated based on the mean quadratic distance between transient profiles and a reference profile which corresponds to the stationary solution. By the means of the defined parameter it is also possible to represent elapsed time until transition processes begin, which is defined as the induction time. The mean quadratic distance ϵ_i for the i -th variable is defined as

$$\epsilon_i(t) = \frac{1}{N} \sum_{j=1}^N \frac{\sqrt{(\Psi_{i,j}(t) - \Psi_{i,j}^{ref})^2}}{\Psi_{i,max}^{ref}}, \quad (4)$$

where N corresponds to the number of profile gridpoints, $\Psi_{i,j}(t)$ is the considered i -th variable (species specific mole numbers, temperature etc.) of the transient profile at gridpoint j , $\Psi_{i,j}^{ref}$ is the corresponding i -th variable of the reference profile and $\Psi_{i,max}^{ref}$ is the maximum reference value of the i -th variable. Note that during the transient dynamics profiles are shifted in physical space and have to be aligned in order to enable the mean quadratic distance calculation.

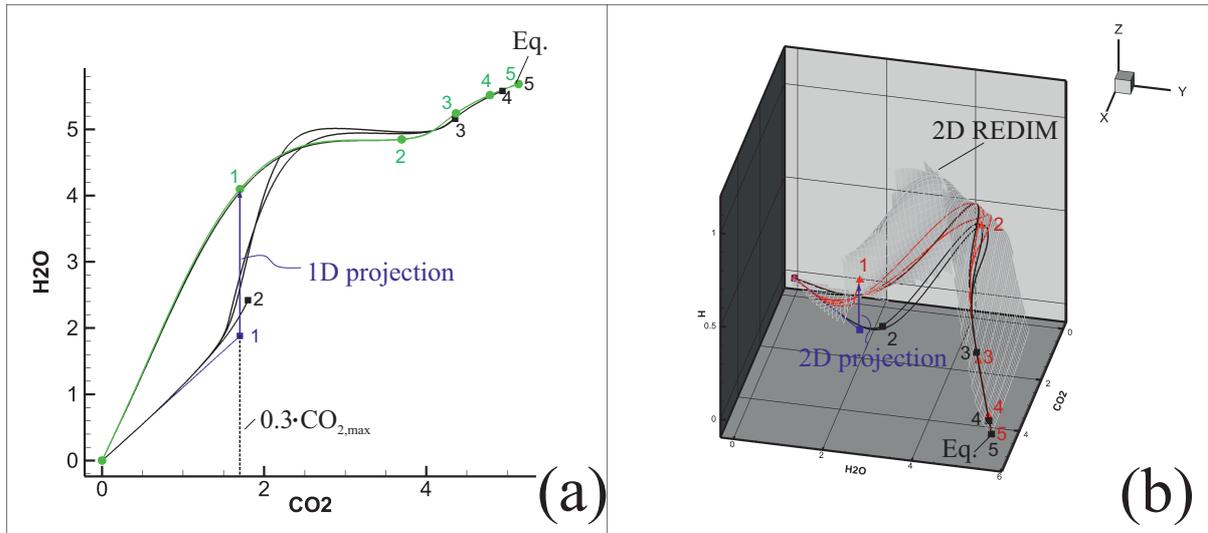


Figure 2: Transition towards the stationary state in state space representation. System solution profiles of detailed and reduced calculations at $0s$ (1), $4 \cdot 10^{-5}s$ (2), $2 \cdot 10^{-4}s$ (3), $8.5 \cdot 10^{-4}s$ (4) and $1s$ (5). (a): 1D reduced (green) are compared to detailed (black) profiles in CO_2 - H_2O -projection. (b): 2D reduced profiles (red) are compared to detailed (black) profiles in CO_2 - H_2O - H -projection.

4 Results

Transient processes of the stoichiometric syngas-air-system are investigated in the state space as well as in the physical space. At first, an initial solution characterized by a specific mole number of $0.3 \cdot \text{CO}_{2,\text{eq}}$ is considered. In Fig. 2 the transition processes of detailed and reduced calculations are compared in state space for different time steps. It can be observed in CO_2 - H_2O projection (see Fig. 2 (a)) how the initial solution is achieved for 1D reduced calculations. The states primarily situated along the mixing line are projected in direction of constant CO_2 values onto the 1D REDIM. Necessarily, specific mole numbers of other species, such as H_2O , experience a shift after projection is applied.

During the relaxation process the 1D reduced system solution profiles remain confined to the 1D REDIM. The 1D reduced profile progression is illustrated by the green dots, which represent the right flame boundary at different time steps. The right boundary position of 1D reduced profiles in state space in terms of CO_2 specific mole numbers is comparable to the right boundary position of the detailed profiles (black squares) after $2 \cdot 10^{-4}s$. From here the detailed profiles progress along the 1D REDIM and the 1D reduced model is able to capture the detailed relaxation towards the equilibrium in CO_2 direction. 1D reduced relaxation processes in H_2O direction are characterized by the initial shift due to the applied projection and the following relatively fast approximation between 1D reduced and detailed profiles.

The starting solution for the 2D reduced calculation is achieved by projection in direction of constant CO_2 - H_2O values onto the 2D REDIM (Fig. 2 (b)). In analogy to the 1D reduced calculations the relaxation of the 2D reduced system solution profiles remains confined to the 2D REDIM. Comparing reduced calculations to detailed calculations for the syngas-air system in CO_2 - H_2O projection (Fig. 2 (a)) shows that the 2D model is able to capture the relaxation process towards the stationary solution in CO_2 - H_2O direction due to its additional dimension. In CO_2 - H_2O - H projection (Fig. 2 (b)) we see that the projection onto the 2D REDIM leads to a shift in the specific mole numbers of H . Moreover it can be seen that the detailed profile first relaxes parallel to the 2D REDIM in a certain distance before proceeding along the 2D REDIM towards the equilibrium point. This shows that the 2D REDIM is an approximation for in general higher dimensional relaxation processes in transport

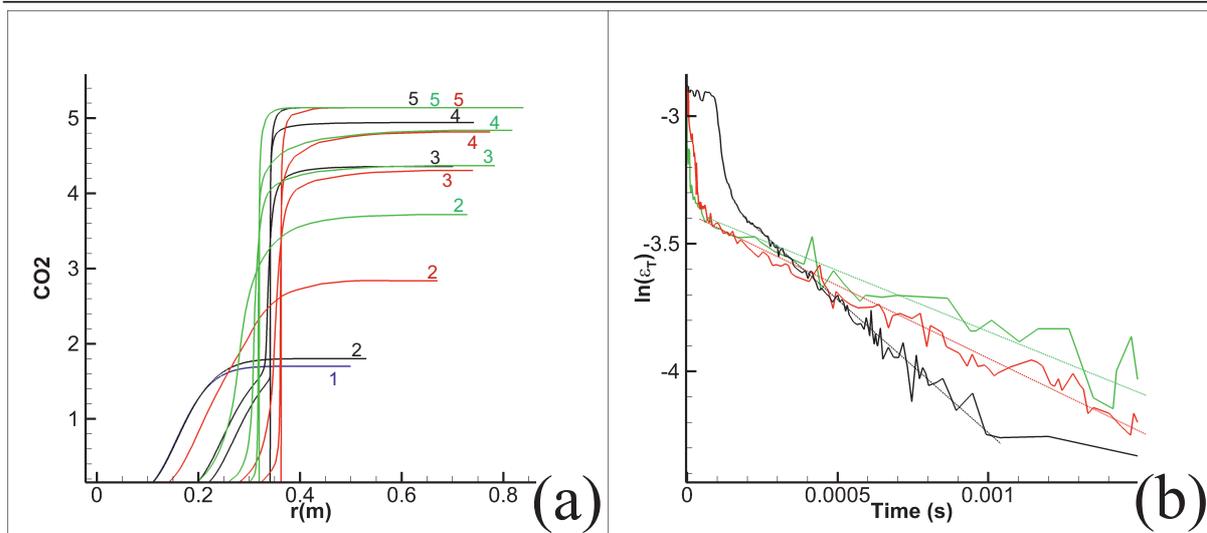


Figure 3: (a): Transition towards the stationary state in physical space representation. System solution profiles of detailed (black) and reduced (1D:green, 2D:red) calculations at $0s$ (1), $4 \cdot 10^{-5}s$ (2), $2 \cdot 10^{-4}s$ (3), $8.5 \cdot 10^{-4}s$ (4) and $1s$ (5). (b): Time dependent change of the logarithmic mean quadratic distance of temperature profiles of detailed (black) and reduced (1D: green, 2D: red) calculations.

dominated regimes. Here, the detailed profiles do not relax along the 2D REDIM until achieving the one dimensional stationary solution. Whereas in source term dominated regimes the relaxation process remains confined to the 2D REDIM once it has been reached by the profile.

The time dependent transient change of CO_2 in physical space is shown in Fig. 3 (a). Again it can be seen, that reduced calculations initially lead to a faster increase in CO_2 . However, reduced profiles are overtaken by the detailed profiles after $2 \cdot 10^{-4}s$ and the detailed calculation achieve the equilibrium point faster than the reduced calculations. During the transition process the 2D reduced model is able to reproduce the characteristic processes of increase in CO_2 specific mole numbers to a higher extend compared to the 1D model. Both reduced solution profiles however show good agreement with the detailed profiles after $8.5 \cdot 10^{-4}s$ (see Figure 2 (a) and (b), Fig. 3 (a)). After this time period dominant fast chemical processes are relaxed and the time scales of transition of reduced and detailed calculation are in the same order of magnitude. Moreover, Fig. 2 and Fig. 3 show that the stationary solutions of both reduced models correspond to the detailed stationary solution.

Fig 3 (b) depicts the time dependent change of the logarithmic mean quadratic distance of temperature profiles for the initial condition shown in (a). It can be seen that the detailed calculation leads to an induction time of about $1 \cdot 10^{-4}s$, depicted by the constant value of $\ln(\epsilon_T)(t)$. In contrast to that reduced calculations show an immediate decrease in $\ln(\epsilon_T)(t)$, indicating no induction time for the transitional process towards the stationary state. An examination of the slope of $\ln(\epsilon_T)(t)$ over a time period of $0.015s$ allows to interpret the time scales of transition. It is visible that the slope of $\ln(\epsilon_T)(t)$ for detailed calculation is steeper than the the slope of both reduced calculations after the induction time period. According to this, the transition process of the detailed solution profile towards the equilibrium elapses faster than both reduced transition processes. Comparing $\ln(\epsilon_T)(t)$ for both reduced calculations reveals that the 2D model leads to a faster transition process than the 1D model.

For the stoichiometric syngas-air system significant differences between detailed and reduced calculations referring to the induction time become visible only for initial solutions situated in the vicinity of the mixing point. Here, detailed calculations lead to extinction processes and no change of $\ln(\epsilon_T)(t)$

can be observed. However, such scenarios represent extreme test cases which are not interesting for investigation. Investigations for higher initial CO_2 specific mole numbers show that induction times for both detailed and reduced calculations vanish. Moreover, transition time scales of both detailed and reduced calculations are almost independent of the initial condition if initial CO_2 specific mole numbers higher than $0.5 \cdot \text{CO}_{2,\text{eq}}$ are considered.

5 Conclusion

In the present work properties of mixing line scenarios regarding the transition towards the stationary state is investigated in the context of the REDIM model reduction concept. A stoichiometric free premixed syngas-air flame is considered for this purpose. Results of 1D and 2D reduced calculations are validated by a comparison with detailed 1D calculations.

The study shows that 1D as well as 2D reduced calculations agree with detailed calculation after a time period of $8.5 \cdot 10^{-5} \text{s}$, i.e. after fast chemical processes can be considered as relaxed. Moreover, stationary solutions of both reduced models correspond to the detailed stationary solution. Thus, both reduced models are able to capture characteristic transitions which are dominated by relatively slow processes. In detail, the 2D reduced model is able to reproduce the time scale of the detailed transient processes to a higher extent compared to the 1D model. This holds for a wide range of initial conditions along the mixing line. A state space and physical space analysis also reveals that the 2D model captures the properties of the detailed transition process in more detail compared to the 1D model.

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