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REDIM reduced modeling of quenching at a cold wall including heterogeneous wall reactions

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ABSTRACT

In this work, the Reaction-Diffusion-Manifold (REDIM) is applied for Flame-Wall-Interactions with heterogeneous wall reactions. There are two major issues that have to be considered: A reduced description that text captures transient regimes like flame quenching has to be generated, and the boundary condition for the reduced system that accounts for heterogeneous wall reactions has to be specified.

Since the extinction at the wall is governed by at least two processes (chemical reactions and heat loss to the wall), a two-dimensional manifold is chosen for the reduced description to construct a REDIM which can handle heat loss and extinction.

For solving the issue of the boundary conditions, two different types of boundaries have to be defined. The boundary condition for the wall is specified via a gradient estimate which is given via the surface reaction rate. For those boundaries, which are not defined as boundaries in physical space, the gradient guess is projected onto the tangential space of the manifold's boundary. Before solving the REDIM evolution equation, a spatial gradient estimate and an initial guess for the manifold have to be defined. Both are obtained from detailed sample solutions of the transient system, which were performed with the in-house program INSFLA. Afterwards, the REDIM evolution equation is integrated to the stationary state and the necessary data for subsequent simulations are stored in REDIM-tables.

The problem of a head-on flame quenching at a cold wall is studied for premixed methane-air-flames at different pressures. In order to validate the reduced model, the generated REDIM-tables are used for computations with the same model configuration than the detailed computation, and species like CO are investigated as a function of the temperature T for different positions near the wall (such an investigation for experimental results was also carried out in Mann et al. for the pressure of 1 bar and the mass fraction of CO Mann et al., 2014). The reduced model reproduces the behavior of the extinction very well and both the detailed as well as the reduced simulations show a good agreement with the experimental results.

1. Introduction

Recent standards of pollutant mitigation and the need for further increase of efficiency of combustion facilities require additional detailed studies and modeling of combustion processes. One option to increase the efficiency with a significant reduction of pollutant formation is the operation of combustion facilities at higher pressures (Karata and Glder, 2012; Cavaliere and de Joannon, 2004; Zhu and Gore, 2005). This trend, e.g. in internal combustion engines (Golloch and Merker, 2005), leads to downsizing, and thus, the surface-to-volume ratio increases. As a result, the influence of the wall on the combustion process increases as well. This is, among other reasons, due to strong heat losses, viscous boundary layer and heterogeneous reactions on the wall. The presence of the wall causes perturbations of the flame propagation and among other reasons local quenching (Vena et al., 2012). In order to reduce pollutants and to increase the efficiency of combustion processes it is therefore important to focus today's research on the flame-wall-interaction (Gruber et al., 2010; Popp et al., 1996; Kedia et al., 2011; Dreizler and Bhm, 2015).

One important tool to study flame-wall-interactions is numerical modeling whereby the computation of detailed kinetics is very demanding. To decrease the computation time, reduced kinetic models are often introduced. These models have to provide reliable accuracy of the chemical kinetics without significant damage to the performance of reduced models. One methodology of model reduction, which has become very popular in recent years, is manifold-based model reduction concepts (Goussis and Maas, 2011).

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The low-dimensional manifolds representing the reduced model have to be constructed before the actual computation can be performed. The generated manifolds can then be used in subsequent numerical integration. In recent studies, there are several methods, which aim at construction of such manifolds but use different frameworks, e.g. the Flamelet Generated Manifold (FGM) (see e.g. Donini et al., 2015; Nguyen et al., 2010), which is a flamelet based method (Bykov et al., 2008a), the flame prolongation of ILDM (FPI) (Jha and Groth, 2012), the ILDM based method (Maas and Pope, 1992), and the Reaction-Diffusion-Manifold (REDIM) method (Bykov and Maas, 2007), which is based on the invariance condition (Gorban and Karlin, 2003) and on multiple time scales (Bykov et al., 2008b). The use of these techniques has become a routine nowadays, especially in modeling of turbulent flames (Wang et al., 2014). However, the treatment of very complex combustion systems with strong energy and mass transfer with the surrounding remains a very tricky and cumbersome task for these methods (Dinesh et al., 2012).

The REDIM method allows to generically construct an appropriate manifold accounting for detailed chemical kinetics as well as for molecular diffusion, where suitable initial/boundary conditions can be implemented to address the complex combustion system (Bykov et al., 2013; Steinhilber and Maas, 2013).

In this paper, the problem of a head-on flame quenching at a cold wall (Mann et al., 2014) is studied as a transparent and simple benchmark model to investigate the influence of the wall, whereby the wall, in contrast to previous work (Steinhilber et al., 2017), is considered as not inert. Therefore, boundary conditions to describe heterogeneous wall reactions are modified in the REDIM implementation. The molecular transport is considered by mixture averaged detailed diffusion model with the Soret effect included (de Charentenay and Ern, 2002). Thus, the approach presented here accounts for both, heterogeneous wall reactions and detailed molecular transport.

The REDIM is formulated with relevant boundary conditions and implemented for the considered combustion system. Namely, flame propagation and quenching at the wall for a stoichiometric, premixed methane/air combustion system. It is investigated both using the detailed chemical kinetic model (GRI 3.0 Smith et al., 1999) and the reduced one. In order to validate the resulting reduced model, detailed and reduced model computations are compared and discussed. The results show that the modified REDIM method fully accounts for heterogeneous reactions as well as for heat losses at the wall. It is demonstrated that the dynamics of the detailed combustion system is completely reproduced by the REDIM model both in physical space as well as in thermo-chemical system state spaces.

2. Model configuration for flame-wall-interaction

For the investigation of flame-wall-interactions a case of head-on-quenching is considered. This model system is comparable to corresponding experiments of Mann et al. (2014): A premixed laminar, stoichiometric methane/air flame moves towards a wall and extinguishes there. The wall temperature is $T_W = 300$ K and the pressure is considered to be constant at $p = 1$ bar. Moreover, the pressures $p = 0.2$ bar and $p = 10$ bar are studied in further computations to examine the impact of the wall reactions. It is assumed that the flow configuration is an infinite slab in y- and z-direction, and this enables the usage of the one-dimensional reacting flow solver INSFLA (Maas and Warnatz, 1988) to study the transient system behavior.

The initial conditions and the model configuration are illustrated in Fig. 1 by means of the temperature. The position $r = 0$ m represents the cold wall. On the left side of the domain there is unburnt gas of the temperature $T = 300$ K, on the right side of the domain there is hot burnt gas.

For the modeling of the chemical kinetics, the GRI 3.0 (Smith et al., 1999) mechanism with 53 species and 325 reactions is used. For the modeling of transport phenomena, a detailed transport mechanism with

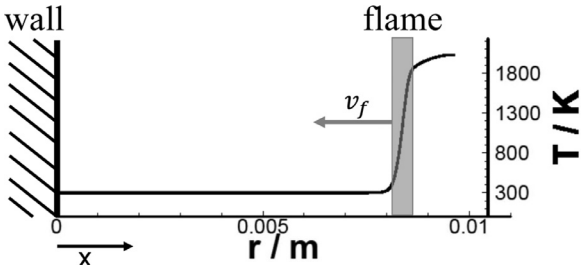

Fig. 1. Model configuration and initial condition of the flame extinction.

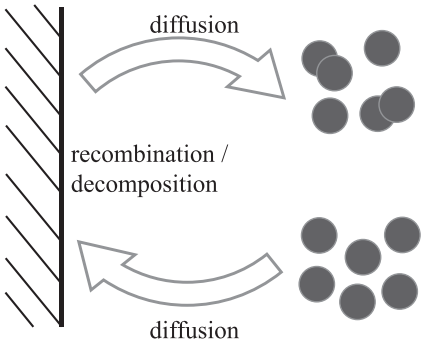

Fig. 2. Schematic illustration of the heterogeneous wall reactions.

thermal diffusion is accounted for based on the Curtiss–Hirschfelder approximation (de Charentenay and Ern, 2002).

The boundary conditions for the right part of the domain are assumed to be zero gradients for all variables. In contrast to the previous work, which assumed the wall to be inert, boundary conditions that account for heterogeneous wall reactions are applied for the species at the left part of the domain.

A schematic illustration of the heterogeneous wall reactions is shown in Fig. 2. If molecules, mainly radicals, impinge on the wall, they can either recombine or decompose with a certain probability to another molecule or they diffuse back to the gas phase without change. For this modeling, a reaction mechanism for the heterogeneous wall reactions is needed which is given in Table 1. Unstable radicals occurring at the cold wall react to more stable molecules and the reaction rate of species i in the surface reaction k is then given via (Maas and Warnatz, 1988)

$$\dot{\omega}_{i,k} = \frac{1}{\rho} \sum_{k=1}^{n} \gamma_k \cdot Z_l \cdot (\tilde{a}_{ik} - a_{ik}), \tag{1}$$

where γ_k is the probability of reaction (in this work assumed to be $\gamma_k = 10^{-2}$), $\tilde{a}_{ik}$ and a_{ik} are stoichiometric coefficients and the number of collisions with the surface is given with (Bird et al., 1960)

$$Z_l = \frac{1}{4} \cdot \sqrt{\frac{8RT}{\pi M_i}} \cdot c_i. \tag{2}$$

The complete rate of formation of the species i in all n_0 wall reactions is then given via

$$\dot{\omega}_i = \sum_{k=1}^{n_0} \dot{\omega}_{i,k}. \tag{3}$$

Table 1
Reaction mechanism for heterogeneous wall reactions.

1.00 HO_2	⟶	0.50 H_2O	+ 0.75 O_2
1.00 O	⟶	0.50 O_2	
1.00 H	⟶	0.50 H_2	
1.00 OH	⟶	0.50 H_2O	+ 0.25O_2