REDIM Reduced Modeling of Flame-Wall-Interactions of Premixed Natural Gas / Air Systems

Christina Strassacker, Ulrich Maas
Karlsruhe Institute of Technology, Institute of Technical Thermodynamics
Engelbert-Arndold-Strasse 4, Karlsruhe 76131, Germany

1 Introduction

There is an ongoing trend towards downsizing in the development of modern engines like internal combustion engines. This trend leads to an increased surfacetovolume ratio in the combustion chamber and the influence of the wall rises. Therefore, todays research focuses on so-called flame-wall-interactions (FWI) because combustion processes close to walls are strongly influenced by the interaction between the flame and the wall.
Numerical simulations of reacting flow systems have become a powerful tool to study combustion processes like FWI. Quantitative predictions of combustion processes can be obtained with detailed models of chemical kinetics and of molecular diffusion [1]. These detailed models result in a large CPU time, especially for transient or complex combustion regimes. In order to reduce the computational time needed for the calculation, reduced models are developed and applied (see e.g. [2–4]). One model reduction method is the Reaction Diffusion Manifold (REDIM) method [5]. In the last years, several REDIMs have been generated for different model configurations to describe FWI (e.g. Head-on Quenching - HOQ and Side-Wall Quenching - SWQ) and for different fuels. However, only REDIMs for FWI of fuels consisting of one component have been generated up to now. One important fuel which consists of several species and is incresingly used and investigated (e.g. in [6–8]) is natural gas. Therefore, contrary to previous works, a REDIM for a premixed natural-gas / air mixture is developed and generated in this work. The fact that natural gas consists of different species challenges the REDIM generation. Different components within the fuel lead to different behaviours of the chemical kinetics (see e.g. [9]) and different transport processes. This means e.g., that the diffusivity of methane is much higher than the one of the larger molecule propane. Within this work, a REDIM accounting for these different processes is generated. After the generation of the REDIM, it is validated by comparing the results of detailed kinetics with the results of the reduced kinetics. It is demonstrated, that the REDIM method can be applied for fuels which consist of different species.

2 Model configuration for flame-wall-interactions

For the construction and validation of the REDIM for FWI, a model confiuration that has been studied in a number of experimental and numerical investigations [10–12] is used. A laminar premixed flame

Correspondence to: christina.strassacker@kit.edu

propagates towards a cold wall and extinguishes there due to heat losses. The unburnt gas is a stoichiomedtric mixture of the natural gas surrogate which consists of $90\ \mathrm{mol\%}\ \mathrm{CH_4}$, $9\ \mathrm{mol\%}\ \mathrm{C_2H_6}$ and $1\ \mathrm{mol\%}\ \mathrm{C_3H_8}$. The fresh gas as well as the wall temperature are assumed to be constant at $T = 300\ \mathrm{K}$ and the pressure is assumed to be constant at $p = 1\ \mathrm{bar}$. Due to the symmetry, this system can be described by only one spatial coordinate and the one-dimensional reacting flow solver INSFLA [13] is used to study this problem numerically.
For the modeling of the molecular transport, a detailed transport model including thermal diffusion is accounted for based on the Curtiss-Hirschfelder approximation [14]. The detailed kinetics is described by the UCB Chen mechanism consisting of 49 species and 324 reactions [6].

3 Construction of the REDIM for flame-wall-interactions

The REDIM method is a reduced kinetic model that accounts for both chemical reaction and molecular transport. The generation of the reduced model is based on the assumption, that the time scales of the fast chemical processes can be assumed to be quasi-steady state because they are completed in a very short period of time. The slow chemical processes which overlap with the time scales of the diffusive processes need to be accounted for. These slow chemical time scales define the dimension of the reduced model [5].
In order to obtain the temporal evolution of a reacting system with detailed kinetics, partial differential equations for the state vector $\boldsymbol{\psi} = (h, p, \frac{w_1}{M_1}, ..., \frac{w_{n,s}}{M_{n,s}})$ have to be solved. Here, h represents the specific enthalpy, p the pressure and $\frac{w_i}{M_i}$ the specific mole number consisting of mass fraction w_i and the molar mass M_i of the species i. Due to the above mentioned assumption of the REDIM method, the state vector is parametrized by a low-dimensional vector of reduced coordinates ($m << n$, where m defines the dimension of the REDIM) and can therefore be expressed as $\boldsymbol{\psi} = \boldsymbol{\psi}(\boldsymbol{\theta})$. Here, $\boldsymbol{\theta} = (\theta_1, \theta_2, ..., \theta_m)$ defines the parametrization vector of the REDIM. This means that less partial differential equations need to be solved and the system is reduced from n to m dimensions.

Before solving the REDIM evolution equation, an initial guess of the manifold as well as a gradient estimate need to be specified [5]. Analogous to previous works [12, 15, 16], both are obtained via detailed sample solutions of the model configuration. For the generation of the two-dimensional initial guess, the states of the HOQ configuration are parametrized with the specific enthalpy h and the sum of the specific mole numbers of $\mathrm{CO_2}$ and $\mathrm{H_2O}$ to enable a unique parametrization. Within the REDIM method, the choice of parametrization is only important for the generation of the initial guess and not for the REDIM integration procedure.
As already mentioned, the gradient estimate for the generation of the REDIM is taken from detailed sample solutions of the HOQ configuration. The top left illustration of Fig. 2 shows the gradient estimate of the specific enthalpy as a function of the parametrization variables of the REDIM. Here, the region in the state space where the laminar flat flame and the wall occur are indicated. It can be seen, that the spatial gradient of the specific enthalpy is very high in regions where the wall is located in the physical space.
At the boundaries of the REDIM, Dirichlet boundary conditions are applied for simplicity. Note, that more sophisticated boundary conditions can be applied without any fundamental problems (see e.g. [12, 17, 18]).
The REDIM evolution equation [5] is solved until the stationary solution $\boldsymbol{\psi} = \boldsymbol{\psi}(\boldsymbol{\theta})$ is found for $t \to \infty$. Figure 2 shows the REDIM in the state space. Three of the figures show the REDIM illustrated as a function of the parametrization variables and one of the three different components of the fuel, $\mathrm{CH_4}$, $\mathrm{C_2H_6}$ and $\mathrm{C_3H_8}$. It can be observed that the consumption of the different fuels during the HOQ process differ quantitatively and qualitatively. On the one hand, $\mathrm{CH_4}$ is a relatively small molecule with a higher diffusivity than $\mathrm{C_2H_6}$ and $\mathrm{C_3H_8}$. Therefore, $\mathrm{CH_4}$ diffuses faster into the flame front which leads to a

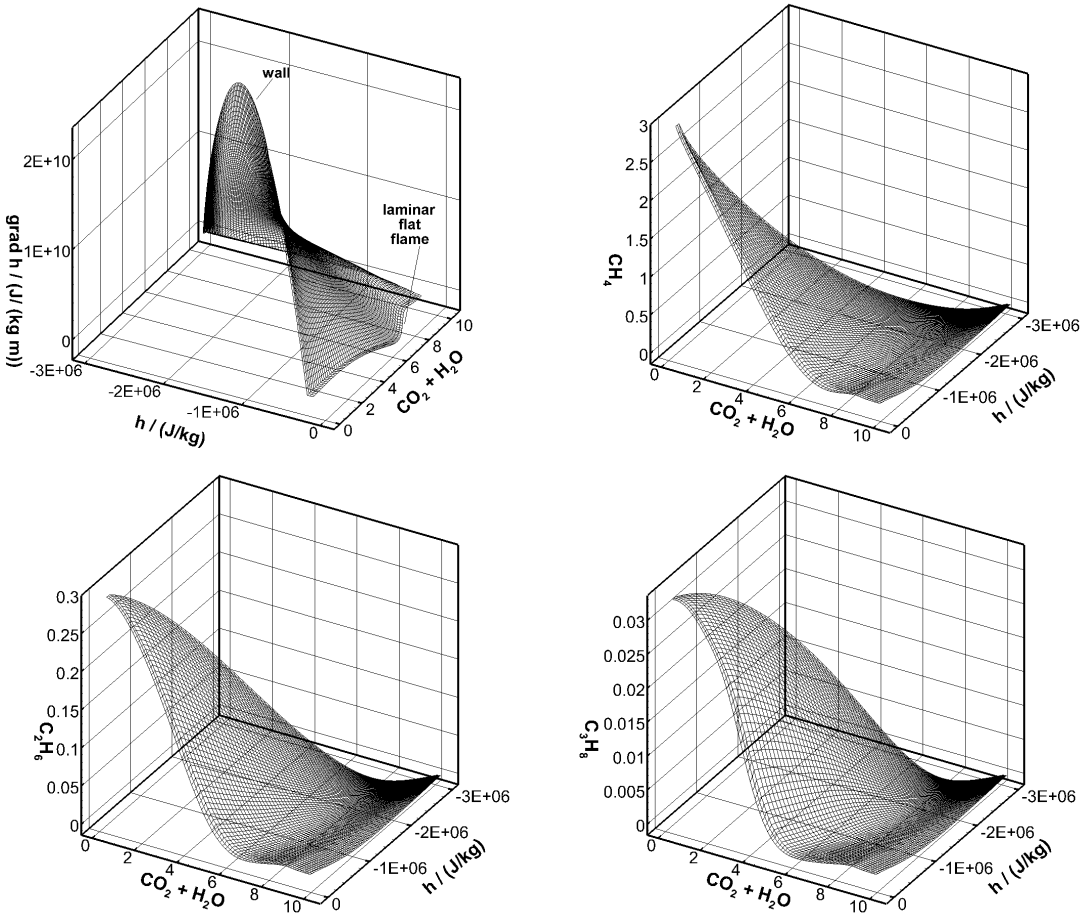

Figure 2: REDIM and gradient estimate of the specific enthalpy (top left illustration) in the state space. The REDIM is illustrated as a function of the specific enthalpy h and the sum of CO_2 and H_2O. The species are given in specific mole numbers (in $\mathrm{mol\ kg^{-1}}$).

faster decrease (higher slope) close to the unburned gas ($CO_2 + H_2O \approx 0$). On the other hand, C_2H_6 and C_3H_8 decompose very fast to intermediate species which leads to a high slope within the flame front of the laminar flat flame. These different processes need to be considered within the REDIM which challenges the REDIM generation.

4 Validation of the reduced model

For the validation of the reduced model, the REDIM is used in calculations with reduces kinetics of the model configuration. Afterwards, the results are compared to the results of the detailed kinetics. For the implementation of the REDIM, a reduced model equation in generalized coordinates is used. This reduced model equation is given by

$$\frac{\partial \boldsymbol{\theta}}{\partial t} = \boldsymbol{\psi}_{\boldsymbol{\theta}}^{+} \boldsymbol{F} - \boldsymbol{U} \cdot \mathrm{grad}\boldsymbol{\theta} + \frac{1}{\rho} \boldsymbol{\psi}_{\boldsymbol{\theta}}^{+} \mathrm{div}\left(\boldsymbol{D}\boldsymbol{\psi}_{\boldsymbol{\theta}} \mathrm{grad}\boldsymbol{\theta}\right) \tag{1}$$

and is implemented in INSFLA. The terms $\boldsymbol{\psi}_{\boldsymbol{\theta}}^{+}\boldsymbol{F}$, $\boldsymbol{\psi}_{\boldsymbol{\theta}}^{+}$ and $\boldsymbol{D}\boldsymbol{\psi}_{\boldsymbol{\theta}}$ are stored in the REDIM-table [5]. Due to the two-dimensional REDIM, only two conservation equations have to be computated. The

reduced calculations are performed with Eq. 1 starting from the same initial solution as the detailed kinetics. In order to compare the results of the detailed and reduced kinetics, an investigation in the state space which is very common in the investigation of FWI is used. Therefore, different species are investigated as a function of the temperature for different distances in front of the wall. Figure 3 shows this investigation for the specific mole numbers of CO, CH_4, C_2H_6, C_3H_8, CH_3 and CH_2OH at the positions $r_1 = 1.0\,\mathrm{mm}$, $r_2 = 0.2\,\mathrm{mm}$, $r_3 = 0.1\,\mathrm{mm}$ and $r_4 = 0.04\,\mathrm{mm}$ in front of the wall for the detailed kinetics (solid lines) and reduced kinetics (dashed lines). It can be observed, that the detailed kinetics are reproduced very well by the reduced kinetics. This holds for the different components of the fuel, the intermediates and even for very minor species like CH_2OH. The different consumption behaviors of the fuel components which has been shown in Fig. 2 can also be seen in Figure 3 and CH_4 is decomposed faster than the other two fuel components.

In order to further validate the reduced model, the heat flux densities $q_W = |-\lambda \mathrm{grad} T|$ towards the wall of the detailed and reduced calculations are compared. Both the time of the maximum heat flux density as well as the magnitude of the maximum heat flux density are important values for the characterization of FWI. Figure 4 shows the heat flux densities of the reduced and detailed kinetics as a function of the time. It can be observed, that the maximum heat flux density as well as the time of the maximum heat flux density are reproduced very accurately by the reduced kinetics.

The investigation in the state space as well as the investigation of the heat flux density towards the wall demonstrate, that the REDIM reduced kinetics reproduce the detailed kinetics very well. Therefore, the suggested reduced model can be used to accurately describe the FWI.

5 Summary and conclusions

In the current work the REDIM method was demonstrated for premixed natural gas-air system with Flame-Wall-Interactions (FWI). In this way it was shown that the REDIM method is not restricted to single-component fuels. For the modeling of the molecular diffusion, a detailed diffusion model including thermal diffusion was accounted for. The REDIM has been generated by solving the REDIM evolution equation. Aftewards, the REDIM was implemented in the reduced model equation in generalized coordinates. In order to validate the generated REDIM, the results of the reduced calculation are compared to the results of the detailed kinetics. This comparison showed, that there is a good agreement of the reduced and detailed kinetics and the transient system behavior of the model configuration is reproduced very well. This leads to the conclusion, that the suggested reduced model can be used to accurately describe the Flame-Wall-Interactions.

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References

[1] Warnatz J, Maas U, Dibble RW. (2001). Combustion (Vol. 3). Berlin: Springer.

[2] Fiorina B, Baron R, Gicquel O, Thevenin D, Carpentier S, Darabiha N. (2003). Modelling non-adiabatic partially premixed flames using flame-prolongation of ILDM. Combustion Theory and Modelling, 7(3), 449.

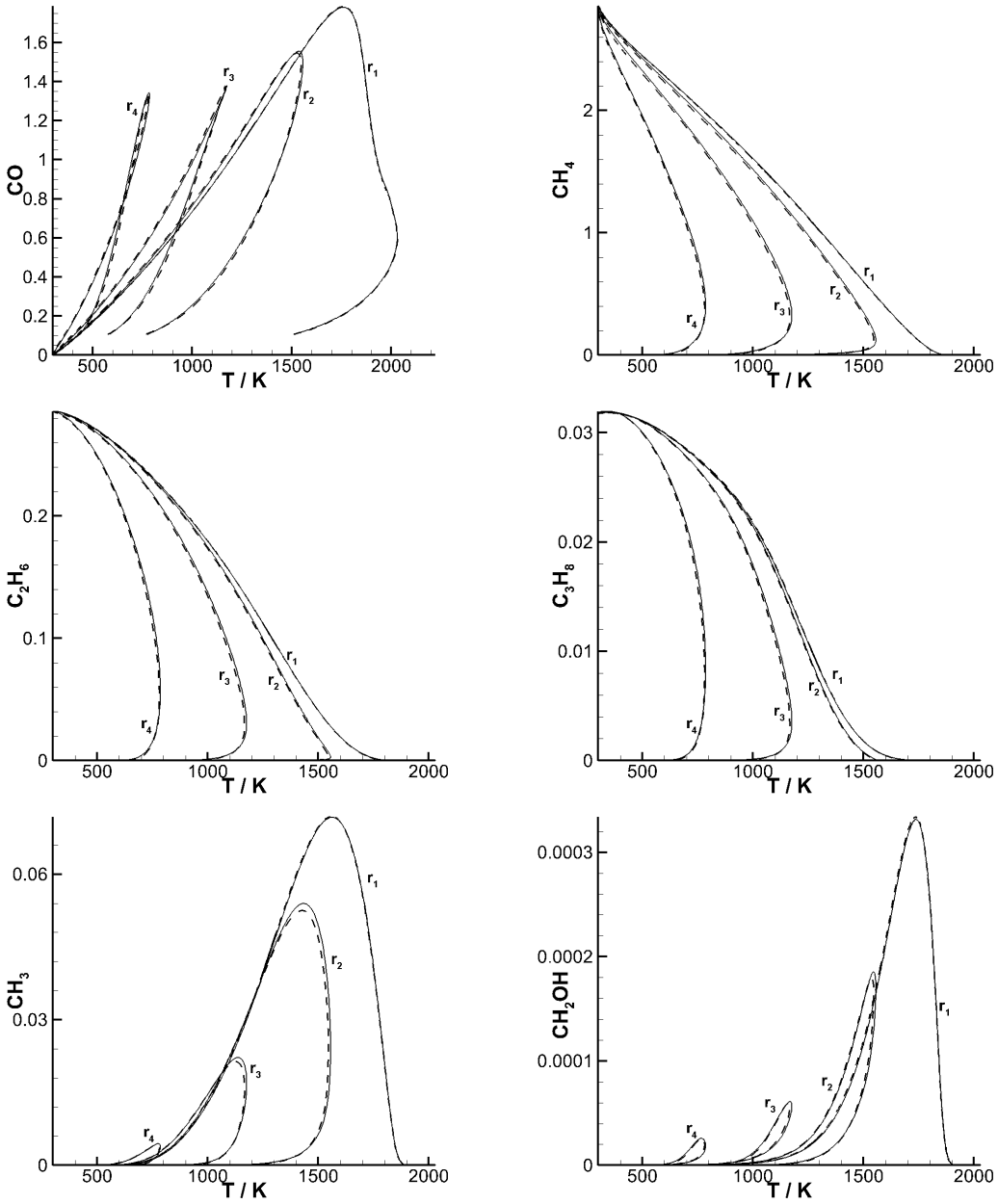

Figure 3: Values of the specific mole number of different species (in $\mathrm{mol\,kg^{-1}}$) over temperature T that occur at the positions $r_1 = 1.0\,\mathrm{mm}$, $r_2 = 0.2\,\mathrm{mm}$, $r_3 = 0.1\,\mathrm{mm}$ and $r_4 = 0.04\,\mathrm{mm}$ for the detailed kinetics (solid lines) and reduced kinetics (dashed lines).

[3] van Oijen JA, Donini A, Bastiaans RJM, ten Thije Boonkkamp JHM, de Goey LPH. (2016). State-of-the-art in premixed combustion modeling using flamelet generated manifolds. Progress in Energy and Combust. Science 57: 30-74

[4] Goussis DA, Maas U. (2011). Model reduction for combustion chemistry. In Turbulent combustion modeling (pp. 193-220). Springer, Dordrecht.

[5] Bykov V, Maas U. (2007). The extension of the ILDM concept to reaction-diffusion manifold. Combust. Theory Model 11 (6): 839-862.

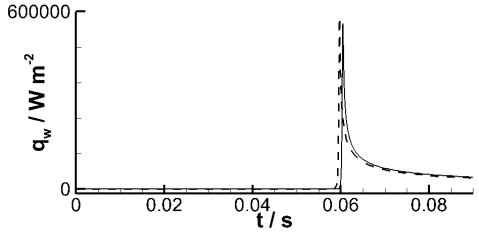

Figure 4: Heat flux density towards the wall (in $\mathrm{W/m^2}$) as a function of the time t (in s) for the detailed kinetics (solid lines) and reduced kinetics (dashed lines).

[6] Drost S, Aznar MS, Schießl R, Ebert M, Chen JY, Maas U. (2021). Reduced reaction mechanism for natural gas combustion in novel power cycles. Combustion and Flame, 223, 486-494.

[7] Kaczmarek D, Atakan B, Kasper T. (2019). Plug-flow reactor study of the partial oxidation of methane and natural gas at ultra-rich conditions. Combustion Science and Technology.

[8] Mariani A, Prati MV, Unich A, Morrone B. (2013). Combustion analysis of a spark ignition ic engine fuelled alternatively with natural gas and hydrogen-natural gas blends. International journal of hydrogen energy, 38(3), 1616-1623.

[9] Eubank CS, Rabinowitz MJ, Gardiner Jr WC, Zellner RE. (1981). Shock-initiated ignition of natural gasAir mixtures. In Symposium (International) on Combustion, 18 (1), 1767-1774.

[10] Mann M, Jainski C, Euler M, Böhm B, Dreizler A. (2014). Transient flamewall interactions: Experimental analysis using spectroscopic temperature and CO concentration measurements. Combustion and Flame, 161(9), 2371-2386.

[11] Wichman IS, Bruneaux G. (1995). Head-on quenching of a premixed flame by a cold wall. Combustion and flame, 103(4), 296-310.

[12] Strassacker C, Bykov V, Maas U. (2018). REDIM reduced modeling of quenching at a cold wall including heterogeneous wall reactions. International Journal of Heat and Fluid Flow, 69, 185-193.

[13] Maas U, Warnatz J. (1988). Ignition processes in hydrogen–oxygen mixtures. Combust. Flame 74(1): 53–69.

[14] de Charentenay J, Ern A. (2002). Multicomponent transport impact on turbulent premixed H_2/O_2 flames. Combust. Theory and Modelling, 6(3): 439–462

[15] Strassacker C, Bykov V, Maas U. (2018). REDIM reduced modeling of flame quenching at a cold wallThe influence of detailed transport models and detailed mechanisms. Comb. Sci. and Technol.: 1-15.

[16] Steinhilber G, Bykov V, Maas U.(2017). REDIM reduced modeling of FWI: Quenching of a premixed methane/air flame at a cold inert wall.Proc. Combust. Inst. 36:655-661.

[17] Strassacker C, Bykov V, Maas U. (2021). Reduced modeling of flame-wall-interactions of premixed isooctane-air systems including detailed transport and surface reactions. Proceedings of the Combustion Institute, 38(1), 1063-1070.

[18] Neagos A, Bykov V, Maas U. (2017). Adaptive hierarchical construction of reactiondiffusion manifolds for simplified chemical kinetics. Proc. Combust. Inst. 36: 663-672.