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Description of the char conversion process in coal combustion based on premixed FGM chemistry

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ABSTRACT

This work presents and assesses a tabulation approach to represent the complex coal combustion chemistry at low computational costs. It should enable to include the process of volatiles conversion and char burnout in scale resolving simulations (such as large eddy simulations) of realistic coal combustion chambers. It is based on premixed flamelets and gets investigated with respect to its capability to accurately describe char conversion. In this approach the gas phase chemistry is mapped onto a four-dimensional manifold controlled by two mixture fractions, the enthalpy and a reaction progress variable. Accordingly, mixing between oxidizer, volatiles and gaseous char conversion products is accounted for besides non-adiabatic physics and finite rate chemistry effects. In a previous work (Knappstein et al., 2017), several modeling assumptions with regard to the description of the volatiles reaction using tabulated chemistry were already assessed. For the full description of the coal combustion process the model functionality was extended to account also for char conversion in the present work. Here, special emphasis is therefore put on aspects related with the conversion of char. The consistency of the model formulation and its implementation is demonstrated by the examination of mass, species and energy balances in generic test cases for which analytical solutions are derivable. Furthermore, results of a simulation adopting the presented model are compared against a detailed chemistry reference solution accounting for the full reaction mechanism. This situation approximates a particle essentially consisting of char that is exposed to hot oxygen-containing product gases. Thereby, capabilities of the presented modeling approach with respect to prediction accuracies for the model's intended application in LES can be estimated.

1. Introduction

The combustion of pulverized coal is still one of the main primary energy conversion mechanisms worldwide [1]. Particularly in the context of carbon dioxide emission reduction goals the effective usage of the fuel and an adaption of the combustion technology is mandatory. The application of oxyfuel environments in the combustion process is an example for the latter. In order to obtain a deeper understanding and gain insight into the mechanisms of realistic coal combustion chambers the utilization of simulation techniques, that resolve turbulent structures in space and time such as large eddy simulations (LES), is of increasing importance (e.g., [2–5]). The treatment of the chemical reaction is a severe difficulty within simulations of complex devices since it is impossible to fully resolve all scales and variables required. Tabulated chemistry methods such as flamelet generated manifolds (FGM) represent already a good approximation in many situations and are already widely used in pure gaseous combustion simulations. A review

of FGM combustion modeling can be found in [6]. The development of these methods towards their applicability in coal combustion simulations is on the one hand desirable because of the good accuracy in combination with reasonable numerical costs and on the other hand challenging due to the complexity of the coal's combustion process.

In recent years, flamelet based models were increasingly adopted for pulverized coal combustion. Single particle simulations were done by Vascellari et al. [7,8] as well as Xu et al. [9], who applied and compared flamelet based models with results obtained by resolved chemistry simulations. The authors demonstrated that the flamelet models proposed therein are well capable of predicting the ignition and the flame structure around single coal particles. Wen et al. [10] also investigated the characteristics of flamelets in coal flames. The authors further proposed a multi-regime flamelet based model for two-phase flows and applied it to a coal jet flame configuration [11]. In the work of Watanabe et al. [12] an approach is proposed, which employs two different mixture fractions to account for the varying fuel composition resulting

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out of the volatiles release and the char conversion. Later on, this concept was further extended by a third mixture fraction additionally considering moisture release from the particle [13], however, it was not reported to what extent this affects the simulation results. A flamelet model with two mixture fractions was also proposed by Rieth et al. [4,5,14]. Depending on whether the simulated configuration is a gas assisted or a self-preserving coal flame the second mixture fraction accounts either for the gaseous fuel [14] or the char burnout products [4,5], whereas the first one represents the volatiles. In Rieth et al. [14] a multiple mixture fraction flamelet model was coupled with a detailed treatment of the particle chemistry for the first time.

A model for coal combustion which is comparable to the one presented in this work was also proposed by Wen et al. [15]. However, differences exist. In [15], the authors employed non-premixed flamelets for their chemistry look-up table and investigated a classical counter-flow configuration. The model introduced here relies on premixed flamelets. Furthermore, a generic char conversion configuration is investigated, in which it is approximated that a char particle is exposed to hot product gases consecutively to volatiles combustion. Further differences in the model exist. Different enthalpy levels are also considered by [15] by accounting for differently heated fuel. Thereby, a certain range of thermo-chemical states is covered. In the present work instead, the full physical range down to room temperature is represented in the manifold over the full reaction range for all mixing states. This way, enthalpy losses below the extinction limit can be accounted for which can become relevant if a group of particles quenches a chemical reaction.

The volatiles reaction was already investigated in our previous works [16,17]. Here, a FGM modeling approach is presented that describes both, volatiles reaction and char conversion, and is therefore suited for the application in real coal combustion chambers. As part of the approach the physics of the process are represented by a reduced set of variables. At this, the different coal conversion products, the consumption of oxygen during char burnout, finite rate chemistry effects and non-adiabatic physics are accounted for.

The aim of this work is the presentation and assessment of a chemistry reduction strategy for coal combustion with particular focus on char conversion. In the investigated configurations we excluded the physical aspect of turbulence. This was done in order to solely evaluate the chemistry reduction under conditions of reduced complexity. However, the study's informative value is also transferable to turbulent systems making use of the separation of chemical and turbulent scales in flamelet based models so that the chemistry reduction itself stays unaffected by turbulence.

The work is structured as follows: In Section 2, the theoretical background of the physical processes and their modeling are given. Furthermore, the mathematical description of the detailed chemistry approach is provided. Section 3 is dedicated to the assessment of consistencies in terms of mass, species and energy balances. In Section 4, the approach gets analyzed with the aim to judge on its capability to reproduce the reference solution given by a fully resolved, detailed chemistry simulation. Thereby, the focus solely lies on the conversion of the char. For this purpose single char particle conversion is investigated in a generic domain. A summary and conclusion is given at the end. In the appendix, numerical aspects related with a non-equidistant tabulation in the context of the applied CFD (computational fluid dynamics) code are discussed.

2. Theory and modeling

For the computations the academic block-structured CFD-code FASTEST was used. It relies on the 3D finite volume method and solves the incompressible, variable density Navier–Stokes equations

$$\frac{\partial \rho}{\partial t} + \frac{\partial(\rho u_j)}{\partial x_j} = S_{\text{prt},m}, \quad (1)$$

$$\frac{\partial \rho u_i}{\partial t} + \frac{\partial(\rho u_i u_j)}{\partial x_j} = \frac{\partial}{\partial x_j} \tau_{ij} - \frac{\partial p}{\partial x_i} + \rho g_i + S_{\text{prt},u_i}. \quad (2)$$

Herein, the interaction between the phases is considered by particle source terms S_{prt} , which get detailed in Section 2.3. The particle phase is treated by a Lagrangian approach. Hence, particles are spatially non-resolved discrete elements, which interact with the gas phase (2-way coupling). Their temporal advancement is computed by an adaptive, explicit Runge–Kutta scheme of fourth order [18]. For the time integration of the gas phase an explicit, three-stage Runge–Kutta scheme of second order is used. Spatial discretization of the velocity is done by multi-dimensional Taylor-series expansion with second order accuracy [19]. To ensure boundedness of scalar quantities the TVD-limiter suggested by Zhou et al. [20] is applied. In order to satisfy continuity a pressure correction equation is solved within each Runge–Kutta stage. The solver is based on an ILU matrix decomposition and uses the strongly implicit procedure proposed by Stone [21]. In FASTEST, chemical kinetics can either be treated by computing the fully resolved, detailed chemical mechanism or by extracting the thermo-chemical state from a pre-generated lookup table. This allows for comparing identical setups while only adjusting the treatment of the chemistry. These different chemistry treatments are outlined in the following two sections, whereat emphasis is put on model developments with respect to the consideration of char conversion.

2.1. Detailed chemistry (DC)

For the simulation of detailed chemical kinetics, transport equations for all considered species Y_k

$$\frac{\partial}{\partial t}(\rho Y_k) + \frac{\partial}{\partial x_j}(\rho u_j Y_k) = \frac{\partial}{\partial x_j} \left(\rho \mathcal{D} \frac{\partial Y_k}{\partial x_j} \right) + \dot{\omega}_k + S_{\text{prt},Y_k}. \quad (3)$$

are solved. Here, a Lewis number being unity is assumed which results in equal diffusion coefficients for all species. This simplification is commonly made within the chemistry reduction being a reasonable approximation for many fuels within a certain operation range. It avoids modeling difficulties related to complex differential diffusion effects (curvature, instabilities) and their - partially compensating - interaction with turbulence (e.g., [22–24]). Removing the associated uncertainties allows a more distinct assessment of the FGM model with respect to description of the char process being the subject of this work. The chemical source terms $\dot{\omega}_k$ in Eq. (3) follow from the elementary reactions of the applied reaction mechanism according to

$$\dot{\omega}_k = \mathcal{M}_k \sum_{j=1}^{N_r} (\nu_{k,j}'' - \nu_{k,j}') \left(k_{f,j} \prod_{k=1}^{N_s} c_k^{\nu_{k,j}'} - k_{b,j} \prod_{k=1}^{N_s} c_k^{\nu_{k,j}''} \right). \quad (4)$$

In this work, the GRI 3.0 reaction mechanism [25] is used, which accounts for $N_s = 53$ species and $N_r = 325$ elemental reactions. The stoichiometric coefficients on the educt and product side are indicated by $\nu_{k,j}'$ and $\nu_{k,j}''$, respectively. The reaction constants of the forward reactions ($k_{f,j}$) follow from Arrhenius approaches, whereas the backward reaction constants ($k_{b,j}$) are obtained from the forward rates divided by the equilibrium constants. \mathcal{M}_k and c_k are the molar mass and the molar concentration of species k , respectively.

Laminar viscosity and heat conductivity are obtained from the empirical temperature dependent equations ([26]):

$$\frac{\mu}{c_p} = 1.67 \cdot 10^{-8} \left(\frac{T}{298 \text{ K}} \right)^{0.51}, \quad \left[\frac{\mu}{c_p} \right] = \text{kg}^2 \text{ K}^{-1} \text{ m}^{-1} \text{ s}^{-1}, \quad (5)$$

$$\frac{\lambda}{c_p} = 2.58 \cdot 10^{-5} \left(\frac{T}{298 \text{ K}} \right)^{0.69}, \quad \left[\frac{\lambda}{c_p} \right] = \text{kg m}^{-1} \text{ s}^{-1}. \quad (6)$$

The chemical source terms get separately integrated within each Runge–Kutta stage by using the Livermore solver LSODE [27]. Additionally the sensible enthalpy is transported in DC computations where the

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