



Full Length Article

Evaluation of coal particle volatiles reaction by using detailed kinetics and FGM tabulated chemistry



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ABSTRACT

The method of Flamelet Generated Manifolds (FGM) coupled with a coal devolatilization model is investigated with regards to its capability to accurately predict the volatiles combustion process of a single coal particle which is exposed to hot product gases. In this approach the gas phase chemistry is mapped onto a three-dimensional manifold controlled by the mixture fraction, a reaction progress variable and the enthalpy. Comparisons to results obtained by a detailed gas phase chemistry simulation which serves as a reference solution are made. Thereby the same numerical setup (i.e., code and mesh) is applied in order to judge on the chemistry treatment by FGM. In the analysis emphasis is put on the chemical states and their description in the context of tabulated chemistry. Also, the influence of common simplifying assumptions regarding the volatiles composition onto the combustion process is investigated. The analysis includes both the overall volatiles conversion as well as the gas phase chemistry around the particle in detail. As the applied configuration setup has a strong non-stationary character, the limitations of the FGM approach based on stationary premixed flamelets are demonstrated. Conclusions regarding the validity of FGM modeling assumptions in single coal particle simulations are drawn.

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1. Introduction

Pulverized coal combustion contributes to a significant degree to the worldwide primary energy consumption [1]. In order to reduce its environmental impact by an effective usage, a comprehensive understanding of coal and its conversion is required, which is obtained by both experiments and numerical simulation techniques. In the early stages of the coal conversion process the coal particles are subject of rapid heating. Volatiles release, ignition and volatiles reaction are the main processes during this phase. Fundamental knowledge is required in order to design reliable models for an appropriate description of these phenomena. Experimental research on single particles is conducted to obtain this understanding and to evaluate the validity of models. For instance, data of particle ignition measurements in a hot laminar coflow by Shaddix and Molina [2,3] are widely used as reference. Levendis et al. [4] focus on a phenomenological description of the partly strong differences in the combustion behavior of coals of different rank. Köser et al. [5] applied planar OH-LIF – measurements for the characterization of single particle combustion. Further examples of experimental investigations can be found in the literature

(e.g., [6–8]). Research on single coal particle ignition and volatiles combustion is also conducted numerically. For instance, a detailed study of coal particle ignition was carried out by Vascellari et al. [9]. In their work, the authors compared detailed chemistry simulations with non-premixed flamelet model results with overall good agreement both between the detailed chemistry and the flamelet simulation and with regards to experimental findings. Goshayeshi and Sutherland [10] evaluated the predictive capability of less elaborated models by comparing them to a detailed gas phase reaction mechanism coupled with a detailed coal kinetics model. It could be observed that the simplistic models are capable of reproducing trends but show less quantitative agreement with the detailed chemistry treatment. In their study, the authors also took the ignition delay as a decisive metric to judge on the agreement with experimental data. It was found, that the detailed models are well-suited to predict the ignition delay correctly.

In our previous work [11] we simulated the ignition and volatiles reaction of single coal particles in a premixed flat flame configuration using a Flamelet Generated Manifold (FGM) approach. In the applied setup, particles cross a closed flame front and hence, are subject of rapid heat up due to the exposure to hot product gases. In our study, it was one of the aims to numerically reproduce the experimentally found particle ignition heights. Good agreement could be found regarding the global behavior. However, a

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quantification of the accuracy of the combustion process around the particle and the justification of modeling assumptions remained an open question. In particular the accurate description of the non-premixed combustion regime around the particle with a stationary and premixed flamelet base as well as the substitution of the complex volatiles by the simple surrogate methane were the issues. In order to evaluate the former and to approximate the flat flame burner situation as good as possible, the same premixed flamelet-database was chosen in the present study.

The aim of this work is threefold: Firstly, the accuracy in the description of the transient volatiles combustion process within the FGM context gets evaluated against a simulation that adopts a detailed gas phase reaction mechanism, which serves as a reference solution. Therefore, the same numerical setup (i.e., code and mesh) is applied. Conclusions regarding the validity of the FGM approach in strong non-stationary single coal particle combustion simulations are drawn. Differently to the work of Vascellari et al. [9], a premixed flamelet tabulation method under consideration of heat losses is used. Secondly, an analysis of the volatiles reaction process of single coal particles is given. Emphasis is put on the chemical states present during the volatiles combustion process and their description in the context of tabulated chemistry. Thirdly, the impact of different volatiles compositions on ignition and volatiles reaction gets examined.

The outline of this work is as follows: In Section 2, numerical methods within the applied CFD-code are briefly exposed. Furthermore, the FGM modeling strategy and the mathematical description of the detailed chemistry approach are provided. Section 3 outlines the numerical configuration. Results are presented in Section 4 which is split into a description of the physical processes during the volatiles conversion process, an analysis of the impact of different assumed volatiles compositions and a comparison between FGM and detailed gas phase chemistry simulation results. At the end a summary is given.

2. Modeling and numerical methods

2.1. CFD-code FASTEST

The academic block-structured CFD-code FASTEST is based upon 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, mass transfer between the phases is considered by particle source terms S_{prt} , which get detailed in Section 2.4. The coal particles are modeled by a Lagrangian approach. Hence, they are treated as spatially non-resolved discrete elements, which interact with the gas phase (2-way coupling). The temporal evolution of each particle is computed by an adaptive, explicit Runge-Kutta scheme of fourth order [12], whereas the time integration of the gas phase is performed by using an explicit, three-stage Runge-Kutta scheme of second order. Multi-dimensional Taylor-series expansion with second order accuracy [13] is used for the spatial discretization of the velocity. To ensure boundedness of scalar quantities the TVD-limiter suggested by Zhou et al. [14] is applied. Continuity is satisfied by solving a pressure correction equation within each Runge-Kutta stage.

2.2. FGM tabulated chemistry

The FGM approach belongs to the group of flamelet models, which means that a turbulent flame is assumed to be an ensemble of laminar 1D-flames [15]. Initial formulations for premixed laminar flames within the flamelet context go back to de Goey and Thijse Boonkkamp [16]. The development of the FGM approach originates from the work of van Oijen [17], van Oijen and de Goey [18] and van Oijen et al. [19]. The parallel development of the similar Flame-Prolongation of Intrinsic Low-Dimensional Manifolds (FPI) approach was conducted by Gicquel et al. [20]. Within the framework of FGM, detailed kinetics are considered for the gas phase reaction by computing laminar one-dimensional flames under premixed conditions prior to the actual CFD simulation. These flamelets then get tabulated on the basis of only a few control variables, which in turn have to be transported by the LES solver. In the present work, these are the mixture fraction f , the enthalpy h and a reaction progress variable Y_{CO_2} .

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

$$\frac{\partial \rho h}{\partial t} + \frac{\partial(\rho u_j h)}{\partial x_j} = \frac{\partial}{\partial x_j} \left(\frac{\lambda}{c_p} \frac{\partial h}{\partial x_j} \right) + S_{\text{prt},h} \quad (4)$$

$$\frac{\partial}{\partial t} (\rho Y_{\text{CO}_2}) + \frac{\partial}{\partial x_j} (\rho u_j Y_{\text{CO}_2}) = \frac{\partial}{\partial x_j} \left(\rho \mathcal{D} \frac{\partial Y_{\text{CO}_2}}{\partial x_j} \right) + \dot{\omega}_{\text{CO}_2} \quad (5)$$

In this work, the flamelet computation is done by using the 1D detailed chemistry flame code CHEM1D [21,22] adopting the GRI 3.0 reaction mechanism [23]. Air and methane are oxidizer and fuel, respectively. Especially the simplifying choice of methane as fuel is of interest here, since it determines the volatiles composition. In our previous work [11] methane was also taken since coal combustion was assisted by a methane flame. In such gas assisted coal flames a further table dimension would be required for realistic volatiles compositions, which did not correspond with the model development state. Furthermore, the real volatiles composition was unknown. In this work this simple fuel gets validated against realistic volatiles compositions (Section 4.2) in order to judge on the impact of such simplifications.

The mixture fraction f is defined as the sum of the elemental mass fractions of carbon and hydrogen ($f = Z_C + Z_H$). The enthalpy h consists of the sensible and the standard formation enthalpy and is therefore a conservative quantity. As the corresponding transport equation does not include a source term, no resolution requirements for the latter have to be met in LES computations, which makes this enthalpy form more advantageous for the treatment within the tabulated chemistry approach. As it is detailed in [24], the CO_2 mass fraction is chosen as the reaction progress variable as a compromise between thermo-chemical accuracy and resolution requirements. Since carbon dioxide is not part of the assumed volatile composition, the transport equation of the progress variable (Eq. (5)) does not include a particle source term. For the tabulation, the flamelet computation is repeated for different equivalence ratios within the flammability range and also for varying enthalpy levels to account for heat transfer effects between the phases and towards walls. For an in depth description of the tabulation technique particularly with regards to the inclusion of enthalpy, the reader is referred to Ketelheun et al. [25]. A Lewis number of unity is assumed both for the flamelet computation and within the detailed chemistry CFD simulation, which is described in the following section.

The manifold was extended to the full mixture fraction range by adopting an extrapolation technique given by Ketelheun et al. [26] to account for mixing processes. Within the approach, a

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