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Simulation of entrained flow gasification with advanced coal conversion submodels. Part 2: Char conversion

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HIGHLIGHTS

- Influence of char conversion modeling for entrained flow gasification CFD simulations.
- Calibration of CBK/G model kinetics using drop tube experiments.
- Single Nth-Order Reaction (SNOR) char conversion model used for CFD.
- SNOR calibrated with CBK/G according to the operating condition in the reactor.
- Validation of the methods using four coals with different ranks.

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ABSTRACT

CFD modeling results for entrained flow coal gasification using advanced submodels for coal conversion are presented and compared to detailed experimental data. The focus of this investigation is on the accurate modeling of the char conversion process. The CBK/E and CBK/G models are used for calibrating a simplified Single Nth-Order Reaction (SNOR) kinetic model, which is suitable for CFD calculations. The kinetics of the CBK/G model are fitted using char gasification data obtained from drop tube furnace experiments. CFD simulations are performed for the BYU entrained flow gasifier fired with four different coals varying significantly in rank ranging from bituminous coal to lignite. The comparison with the experiments generally gives good agreement in terms of flame stand-off, gas composition and carbon conversion when the kinetics of the CBK/G model calibrated with drop tube experiments is used. On the other hand, lower carbon conversion is obtained using the default correlation of the CBK/G model, which only allows to depict the overall tendency of the gasification reactivity with coal rank.

1. Introduction

With the increasing availability of high performance computing resources for scientific modeling both of laboratory and pilot-plant scale, simulation have become an well-established tool for understanding and optimizing the complex reactive multiphase flow in coal gasification reactors. Especially CFD simulations now represent an important part in the design process of advanced reactors. However, modeling of coal gasification requires several mathematical submodels in order to describe the complex turbulent multiphase reacting flow [1]. The final simulation result directly depends on the validity and the applicability of these submodels.

Generally, these submodels are developed and validated considering small scale experiments, focusing only on one phenomenon at a time. In particular, considering the processes in an entrained flow gasifier with pulverized coal particles in the range of about 1 μm to 200 μm, the existing different length scales cannot be completely resolved and hence it is necessary to model the processes on the smallest scales. For instance, the interactions between the gas phase chemistry and the turbulent flow as well as the boundary layers around the coal particles require a suitable (subgrid) model. In addition, the thermo-chemical transformations of the coal needs to be modeled as well.

However, in order to limit the computational requirements, CFD simulations of coal gasification generally consider only simplified modeling approaches. For instance, several effects, for example the particle shape or the Stefan flow, are often neglected, even if their impact may be significant. The thermo-chemical transformations of the coal are often accounted by simplified empirical correlations only.

In this multi-part work, entrained flow gasification is investigated using advanced submodels. The laboratory scale BYU gasifier [2], for which detailed in-reactor measurements are available, is used for validating and evaluating the computational submodels. The first part [3] focused on the modeling of pyrolysis. An

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advanced and accurate procedure was presented for calibrating the parameters required by empirical pyrolysis models using advanced network based models [4–6]. The second part here focuses on the modeling of the char conversion process. In particular, a Single Nth-Order Reaction (SNOR) model originally proposed by Liu and Niksa [7] is used for estimating char oxidation and gasification rates including an empirical effectiveness factor accounting for the reduction of reactivity in the late stages of the carbon burnout due to several phenomena such as ash inhibition, random pore evolution, annealing and char density changes. The kinetic parameters and the effectiveness factor of the model are calibrated by means of the advanced CBK/E [8] and CBK/G [7] models for char oxidation and gasification, respectively. CBK/E and CBK/G are the latest developments from the CBK (carbon burnout kinetics) family of models. A very good review of the CBK development history is given by Schurtz [9]. Numerical results are then validated with experiments by Brown et al. [2] considering different coal ranks and analyzed focusing on the influence of the char conversion.

The paper is structured as follows: Section 2.1 presents a general overview of the numerical models used for simulating entrained flow gasification. In particular Section 2.1.2 describes the SNOR model for modeling char conversion. Section 3 discusses the operating conditions of BYU gasifier and the numerical setup used for the simulations. Section 4 reports the results of the numerical simulations including a comparison with the experimental data investigating in detail different coal ranks and char conversion models.

2. Numerical models

2.1. CFD modeling of entrained flow coal gasification

The detailed description of the CFD code and of the main algorithms and models used for the simulations was described in detail in the first part [3] and here they are only briefly reported. The 2D axisymmetric RANS equations are solved using the CFD code ANSYS-Fluent [10] using the SIMPLE algorithm. Convective fluxes in all transport equations were discretized with a second-order upwind scheme and the pressure gradient with a second-order accurate scheme. Turbulence is modeled using the realizable $k-\varepsilon$ approach [11].

The Eddy Dissipation Concept (EDC) [12] accounts for the turbulence-chemistry interaction (TCI) in combination with a detailed kinetic mechanism [13] from the GRI-MECH suite, including 103 reactions among 22 species. It was successfully used for gaseous partial oxidation [14] and for unconventional coal combustion [15,16]. Advanced TCI models such as flamelet, CMC or PDF among others are not established yet for coal combustion and gasification. Some initial results with PDF [17,18] and flamelet modeling [19,20] approaches adapted for coal have been published recently. In addition, it was also demonstrated that the laminar flamelet approach can potentially be extended to include partial oxidation or fuel-rich conditions [21,22], which is of primary interest for coal utilization. Although initially developed for ignition and premixed flames, chemical mechanisms derived from the GRI-MECH family have been used for a wide range of coal combustion and gasification studies [22–24,16,15,19,21]. These investigations included detailed comparisons to experimental data for the validation of the numerical approach. Furthermore, the GRI-MECH mechanisms are often used for non-premixed flames, see e.g. [25,26].

Radiation was modeled with the P-1 model [27]. The P-1 model is the simplest version of the more general P–N approach, which is based on the expansion of the radiation intensity into an orthogonal series of spherical harmonics. The P-1 model has the main advantage of solving a transport equation for the incident radiation, requiring a limited computational effort but still being significantly more detailed than the optical thin limit. The radiating properties of the gas were modeled assuming a gray-band model, based on the Weighted Sum of Gray Gases (WSGG) model [28]. Absorption, emission, reflection and scattering from the disperse coal particles were considered in the radiative heat transfer calculation.

Coal particle trajectories are simulated using a Lagrangian approach. The Eulerian gas phase is coupled with the solid discrete phase exchanging mass, momentum and energy. The influence of the turbulent flow on the particle trajectories is accounted through a stochastic method including a random component of the turbulent velocity. The coal conversion is modeled according to the following sequence: drying, pyrolysis and finally char burnout, where a sequential approach is used here. For particle ignition, various authors [29,30] among others discussed non-sequential approaches under oxy-fuel conditions. However, considering the small particle sizes and high heating rates for the case investigated here (both leading to very fast pyrolysis), the standard sequential method is considered appropriate. The pyrolysis model and the procedure for calibration, which is the main topic of the first part [3], is briefly reported in Section 2.1.1, while the model for char oxidation and gasification is fully reported in Section 2.1.2.

2.1.1. Pyrolysis modeling

Pyrolysis is modeled with the empirical Competing 2 Step Model (C2SM) [31]. The parameters required by C2SM are evaluated according to the calibration procedure described in the first part [3], using the results of the detailed network based Chemical Percolation Model (CPD) [4]. Similar results were obtained considering the models FG-DVC [5] and FLASHCHAIN [6], respectively.

Volatile matter is considered as a mixture of light gases and heavy hydrocarbons (tar), which are released with a constant ratio during devolatilization, which is a reasonable hypothesis for entrained flow gasification, where pyrolysis occurs very quickly. In addition, it is assumed that char is composed only of pure carbon and the entire hydrogen, oxygen, nitrogen and sulfur fractions of the coal were released during pyrolysis.

The reaction of the volatiles gases are modeled using the EDC model as described above. No reactions in the direct vicinity of the particle during pyrolysis are considered that could potentially change the transport processes in the boundary layer. Such effects have been studied for char oxidation [32,16] and the resulting model was used in our previous paper [3]. This phenomenon should be studied in the future to quantify the influence on the particle heat balance.

2.1.2. Char conversion modeling

After pyrolysis, a porous char particle (including ash) remains. Char conversion involves heterogeneous reactions on the surface of the porous particle. Assuming that only carbon remains and reacts (which is often used but quite strong assumption), the following global reactions are usually regarded as important.

$$R_{s,1}: \quad C_{(s)} + \frac{\psi+1}{2}O_2 \rightarrow \psi CO_2 + (1-\psi)CO \tag{1}$$

$$R_{s,2}: \quad C_{(s)} + CO_2 \rightarrow 2CO \tag{2}$$

$$R_{s,3}: \quad C_{(s)} + H_2O \rightarrow CO + H_2 \tag{3}$$

$$R_{s,4}: \quad C_{(s)} + 2H_2 \rightarrow CH_4 \tag{4}$$

The first reaction $R_{s,1}$ (Eq. 1) is a combination of the partial and complete reaction of char with O_2, producing CO and CO_2. ψ is the fraction of char converted to CO_2. The oxidation is exothermic and generally faster than the other reactions, which are endothermic. The methanation reaction $R_{s,4}$ (Eq. 4) is usually generally much slower than all the other reactions.

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