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Detailed analysis of reacting particles in an entrained-flow gasifier

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ABSTRACT

For the development of reliable numerical models of entrained flow gasifiers it is crucial to understand and to model correctly the interactions between the hot gas-flow and the coal particles undergoing pyrolysis and char conversion. In this work a laboratory-scale entrained flow coal gasifier was investigated numerically. Based on the detailed analysis of the particle trajectories, the interaction between the flow field and coal particles of different sizes was carefully discussed and analyzed. For small, medium, and large particles, the primary regions for devolatilization, oxidation, and gasification were detected, and the conversion behavior for these particle fractions was quantified in terms of pyrolysis time, residence time, and overall conversion rate. Additional particle-resolved CFD calculations were carried out for representative particles of different sizes in order to study the heat and mass transfer of the isolated particles in detail. Pyrolyzing coal particles and combusting or gasifying char particles were considered at several positions in the reactor, where each location is characterized by different gas compositions and temperatures. For these particles, the flow field, and the species and temperature distributions in the boundary layer are discussed. The particle-resolved calculations demonstrate the impact of the particle Reynolds number and the influence of the mass flow from the particle to the surrounding gas on the overall heat and mass transfer.

1. Introduction

With the increasing availability of high-performance computing resources for the scientific modeling of both laboratory and pilot-plant-scale reactors, simulation has become a well-established tool for understanding and optimizing the complex reactive multiphase flow in coal gasification reactors. CFD simulations in particular now play an important part in the design process of advanced reactors. However, modeling coal gasification requires several mathematical submodels in order to describe the complex turbulent multiphase reacting flow [1,2]. The final simulation result depends directly on the validity and the applicability of these submodels and, especially in coal gasification, accurate description of the feedstock conversion is crucial.

Advanced, detailed phenomenological submodels have been developed for describing the transformation of the coal molecular structure at high temperature, allowing an accurate descriptions of the main transformations, i.e. pyrolysis [3–7] and char conversion [7–10]. However, these models generally require a great deal of computational work and cannot be easily integrated into the comprehensive CFD models, so in general simplified empirical models are used alternatively.

In previous works of the authors [11–13], two novel methodologies for bridging the gap between the detailed phenomenological models for coal transformation (pyrolysis and heterogeneous char conversion) and CFD were developed and tested using data from a laboratory-scale entrained flow gasifier at Brigham Young University (BYU) [14] and from a 5 pilot scale gasifier [15]. This experimental data set is especially suited for evaluating gasification models since in-reactor species measurements are available for various coals of different ranks.

Based on the results of the CFD simulations of the BYU gasifier [11,12], the current paper first analyzes in detail the interactions between the gas and the solid phase, focusing on the analysis of mass averaged carbon conversion. In particular, the influence of different particle sizes is investigated. Then, the boundary layers around the particles are analyzed by means of fully resolved CFD simulations of single particles. Several reference particles are investigated, taken at characteristic locations inside the reactor. The input conditions for the fully resolved single particle simulations, such as the gas and particle temperature, gas composition and Reynolds number, are consequently taken from the full CFD simulations of the reactor.

A similar investigation was performed by [16], who investigated the influence of the gasification reactions under oxy-combustion conditions and analyzing the influence of the particle trajectories. Similarly, [17] analyzed the impact of the particle size grinding on coal gasification.

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The paper is structured as follows: Section 2 presents a general overview of the numerical models used for simulating the entrained flow gasifier reactor and the single particle reacting flow during pyrolysis and char conversion. Section 3.1 briefly reports the operating conditions of the BYU gasifier and the main assumptions made for the numerical simulations. Section 3 reports the main results of the simulations of the BYU gasifier. In Sections 4.1 and 4.2 the coal devolatilization and char conversion is studied in detail based on particle-resolved CFD simulations.

2. Numerical models

2.1. Entrained flow gasifier modeling

The 2D axisymmetric RANS equations are solved using the CFD code ANSYS Fluent [18] with the SIMPLE algorithm. Convective fluxes in all transport equations are discretized with a second-order upwind scheme and the pressure gradients are discretized with a second-order accurate scheme. Turbulence is modeled using the realizable k-ε approach [19]. The Eddy Dissipation Concept (EDC) [20] accounts for the turbulence-chemistry interaction (TCI) in combination with a detailed kinetic mechanism [21] from the GRI-MECH suite, including 104 reactions among 22 species. The tar produced during pyrolysis reacts with O_2 and H_2O in the gas phase, decomposing into CO and H_2 [11,12]. This approach was used successfully for gaseous partial oxidation [22], for unconventional coal combustion [23,24], and coal gasification [11,12]. Soot formation is not included in the CFD model. Radiation was modeled with the P-1 model [25]. The radiating properties of the gas were modeled assuming a gray-band model, based on the Weighted Sum of Gray Gases (WSGG) model [26]. Absorption, emission, reflection and scattering from the 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 by means 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, e.g. [27,28], 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.

Devolatilization and char conversion are modeled in a consistent way with respect to the single particle simulations. The consistent modeling approaches are described in Section 2.3.

2.2. CFD modeling of single coal particle pyrolysis and char gasification

The numerical setup for single-particle calculations is similar to the one used in a previous work by the authors [29]. The two-dimensional, axisymmetric and steady-state Navier–Stokes equations, together with energy and mass conservation equations, are solved using ANSYS Fluent [18]. The two-dimensional steady-state approach is valid, since the flow field around spherical particles at Reynolds numbers below 210 remains steady-state and axisymmetric [30], see Section 4. The particle loading is low in the BYU gasifier (maximum volume fraction of particles is 0.1% in the char combustion zone, not illustrated here). For that reason it is valid to neglect particle-particle interactions, and hence to consider single particles. For reacting particles and for pyrolyzing particles, respectively, the pseudo-steady-state approach [31] is valid, since the particle shrinking, i. e. the movement of the reacting char surface, is slow compared to the gas-flow velocity. The particles are assumed to be spherical and non-porous. More details about modeling porous reacting particles are provided in [32,33].

The gas flow is treated as an ideal-gas incompressible media, thus the density is not affected by the local relative pressure field. The Richardson number is very small for the particle sizes considered here, so buoyancy effects are negligible [33]. The char particles consist of carbon only, and they are placed in an uniform mixture, whose composition is taken directly from reactor simulations. For this, different representative locations in the reactor were defined, and the corresponding cell values were used to define the composition and temperature of the gas phase in the single-particle simulations. For detailed information about the reaction mechanism and the implementation of heterogeneous reactions, see Section 2.3.

In this work, body-fitted quadrilateral meshes were utilized. In order to ensure grid-independent results, the numerical mesh used in this study was successively refined. The number of elements was increased to 21,000 and to 59,000, respectively, and the wall-resolution was reduced by factor of 2 with every refinement step. For an isolated 200 μm particle, the temperature and gas phase distribution normal to the forward stagnation point of the particle, and the overall carbon conversion rate was examined for the char conversion in an O_2/N_2 mixture at three temperatures between 1000 and 3000. For all three meshes, the difference in all control values was below one percent. In order to avoid blockage effects, the domain extends 40d in a radial direction, 30d in an upstream direction and 100d in a downstream direction. Details of the numerical setup, the governing equations and discretization were provided in Ref. [29]. The setup was validated against analytical models [34] in Refs. [35–37]. A comprehensive validation against different single-particle experiments including different gas temperatures, particles sizes, and gas-phase compositions [38,39], was reported in [29].

According to the reactor simulation, radiation was modeled using the P-1 radiation model, together with the Weighted Sum of Gray Gases model for the calculation of the absorption coefficient of the gas. Contrary to the previous studies, in which semi-global homogeneous reactions were applied, the numerical model here incorporates the DRM22 mechanism [21] to be consistent with the reactor simulations. The particle temperature was defined by evaluating particle data in the reactor simulation. This approach allows for taking into account that the particle temperature depends not only on the process under investigation, i.e. coal pyrolysis or char gasification, but also on previous processes such as heating or pyrolysis. Particle characteristics such as surface temperature, Reynolds number, and devolatilization rate are extracted from the particle trajectories in the reactor calculations, and are listed in Table 6 for pyrolysis and for char conversion.

2.3. Pyrolysis and char conversion kinetics

Pyrolysis is modeled with the empirical Competing 2 Step Model (C2SM) [40]. The parameters required by C2SM are evaluated according to the calibration procedure described in [11] using the in-house coal pyrolysis kinetic preprocessor (PKP), using the results of the detailed network-based Chemical Percolation Model (CPD) [3]. Volatile matter is considered as a mixture of light gases and heavy hydrocarbons (tar), which are released with a constant ratio during devolatilization. The volatile matter composition is estimated according to the method described in [23]. In particular the composition of the light gases is estimated using the method proposed by [41]. Tar is modeled using an equivalent formula $C_{3.36}H_{2.28}$, whose stoichiometric coefficients are obtained closing the elemental mass balance. The volatile matter composition is also assumed constant during the whole pyrolysis process. This is a reasonable hypothesis for entrained flow gasification, where pyrolysis occurs very quickly.

In addition, it is assumed that all the hydrogen, oxygen, nitrogen and sulfur fractions of the coal were released during pyrolysis and the char is