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Particle-resolved numerical study of char conversion processes in packed beds

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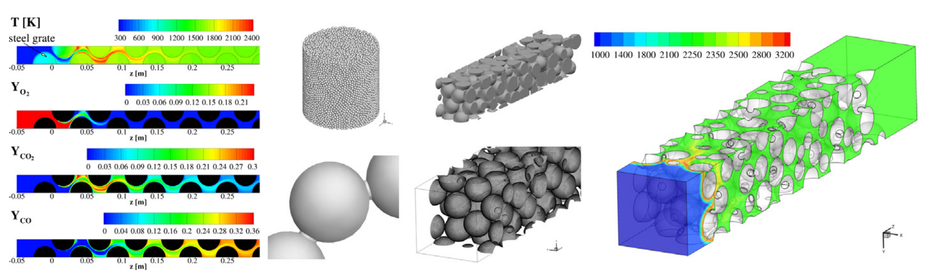
HIGHLIGHTS

- Particle-resolved CFD calculations of fixed-bed gasification.
- Different packed beds are analyzed based 2d and 3d configurations.
- The influence of the void space on temperature and species distribution is studied.
- Different atmospheres and Reynolds numbers are considered.

GRAPHICAL ABSTRACT



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ABSTRACT

For the design and operation of fixed bed gasifiers the understanding of the occurring physicochemical phenomena is essential. In this work, to study the fluid flow, heat and mass transfer as well as chemical reactions a particle-resolved CFD-model is presented. The two-dimensional approach was validated against experiments and simulations for different conditions were conducted and the resulting local temperatures, species mass fractions and carbon mass flux are discussed. Furthermore, the basic two-dimensional approach is compared to three-dimensional representation of packings considering two different configurations, namely random packed bed and simple cubic packed bed. The random packed bed was generated by a sedimentation utilizing Discrete-Element-Method. Furthermore, conditions which can be found in a British Gas Lurgi (BGL) gasifier were applied to simulate carbon conversion in a packing at a pressure of 40 bar. It was found that the results from the basic model are in good agreement with those of the random packed bed. Furthermore, the 3-d distribution of particles in a bed shows significant influence on the fluid flow, heat and mass transfer which is discussed through the flame length.

1. Introduction

The fixed-bed gasification of coal is a highly exothermic process to preferably produce synthesis gas consisting of CO and H_2. For the large-scale production of synthesis gas two process have been proved to work economically, the Lurgi Fixed Bed Dry Bottom gasification process and the British Gas Lurgi (BGL) process. For the gasification processes the overall efficiency is dependent on the overall carbon conversion. Since the conversion of coal is carried out at high temperatures and pressures the construction and operation of such plants require high costs. Here, modeling can play a crucial role for the development, design and operation of these reactors.

Some of the first works directed at the numerical modeling of fixed-bed gasifiers were done by Yoon et al. [1], Amundson et al. [2], Bhattachyra et al. [3] and Hobbs et al. [4]. In most of the models a gas/solid plug flow in the reactor is assumed and the gas temper-

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ature is equal to the temperature of the solid phase. The next widely-used simplification is the neglection of the gas phase kinetics. More recently, Cooper and Hallet [5] presented a one-dimensional model for the combustion of char particles in a packed bed. Their heterogeneous model, which was coupled with a particle shrinkage effect, includes the gas phase kinetics of the CO oxidation. However, one-dimensional models are not capable of representing phenomena occurring between the particles and on the particles surfaces within the fixed-bed, including flow behavior and gas phase reactions.

The rapid increase of computational resources and numerical methods to solve basic conservation equations describing fluid flow coupled with heat and mass transfer have made computational fluid dynamics (CFD) a standard tool for understanding and predicting flow behavior in packed beds.

Furthermore, the coupling of CFD with the Discrete Element Method (DEM) [6,7] allows to resolve the motion of individual particles and subsequently the distribution of particle-induced sources and sinks, respectively [8–12]. Utilizing these methods, the conversion of solid particles on a forward acting grate was studied by Simsek et al. [13] and Mahmoudi et al. [14]. Furthermore, these numerical models were applied to investigate particle-gas flows in blast furnaces [15,16] and stoves [17,18].

Additionally, it should be noted that the interior of fixed bed reactors, especially gasifiers operating at high pressures, is difficult to access and experimental studies are not always capable of characterizing the basic features of flow and the phenomena inside the reactor. From this point of view numerical simulations can play the role of 'numerical-experiments' enabling the processes to be seen 'in situ'.

Focusing on the detailed simulation of the gas phase within the void space, e.g. see the review by Dixon et al. [19], the majority of CFD modeling has been dedicated to fluid flow in the void space and interphase heat transfer. Up to now, there are only a few numerical works featuring reacting flows in packed-beds of chemically reacting particles. For instance, Freund et al. [20] studied the three-dimensional flow field and local concentration in a randomly packed isothermal bed applying the Lattice-Boltzmann method, where a first-order reaction was considered on the solid surface. Dixon et al. [21] investigated the flow in a 120° segment of a packed tube taking into account intraparticle reactions and gradients for the steam reforming process. Kolaczkowski et al. [22] used CFD to model the catalytic combustion of propane within catalytic pellets placed in a row, representing a packed bed. Behnam et al. [23] carried out CFD simulations of catalyst deactivation in the propane dehydrogenation process, where the carbon deposition was modeled on and within the catalyst pellet coupled with chemical reactions, external and intraparticle heat and mass transfer. Recently, the dry reformation of methane in a packed bed was studied by Wehinger et al. [24] and Eppinger et al. [25].

An analysis of recent works shows that the spatial distributions of the reactive flow inside packed beds taking into account homogeneous and heterogeneous reactions remain to be studied, especially for gasification processes. In particular, the primary interest of this work is the spatial distribution of the temperature and species concentrations in the so-called combustion and gasification zone of a fixed bed, where the oxygen, carbon dioxide and water vapor react with char particles. Therefore, this work is devoted to the particle-resolved numerical simulation of the combustion/gasification of carbonaceous particle in a packed bed configuration. In contrast to the work of Sahu et al. [26] presenting a 2-d approximation of a reacting structured packing of carbon particles, here, a two-dimensional axisymmetric modeling approach is utilized with the aim to represent general packing structures. Subsequently, this approach is validated against published experimental data [27]. Furthermore, the influence of three-dimensional effects is studied and compared to the basic setup. The configurations of a randomly packed bed and a simple cubic packing are chosen to represent three-dimensional packings. Finally, simulations are conducted for the conversion within a BGL gasifier applying high temperatures and pressures.

2. Problem formulation

In a countercurrent fixed-bed gasifier, coal is fed in the top of the gasifier, while the feed gas is supplied at the bottom. Four zones are established at different heights within the gasifier, corresponding to drying, pyrolysis, gasification and combustion. The combustion zone differs from the gasification zone that oxygen is present. In this study spherical coal char particles placed in a stationary position in a reactive environment are considered. Thus, the particles are in a region that corresponds to the combustion zone overlapping with the gasification zone. The gas flow is forced to pass around the spherical particles within the void space. The inflow velocity is assumed to be uniform and is determined by means of the Reynolds number, calculated as

$$Re = \frac{\rho_{in} u_{in} d_p}{\mu_{in} \epsilon} \tag{1}$$

where ρ_{in} and μ_{in} are the density and molecular viscosity, respectively, corresponding to the inflow temperature T_{in} and the gas composition. The porosity is expressed by ϵ.

2.1. Chemical reactions

The chemistry is modeled using semi-global homogeneous and heterogeneous reactions [28]. The heterogeneous reactions are the partial oxidation reaction with oxygen, the Boudouard reaction and the heterogeneous water–gas reaction:

$$C + \frac{1}{2}O_2 \rightarrow CO \qquad h^0_{R1} = -9.2\ \text{MJ kg}^{-1}\ \text{C} \tag{R1}$$

$$C + CO_2 \rightarrow 2CO \qquad h^0_{R2} = 14.4\ \text{MJ kg}^{-1}\ \text{C} \tag{R2}$$

$$C + H_2O \rightarrow CO + H_2 \qquad h^0_{R3} = 10.9\ \text{MJ kg}^{-1}\ \text{C} \tag{R3}$$

The homogeneous reactions comprise the oxidation of CO and the forward and backward reaction of the reversible water-gas shift reaction:

$$CO + \frac{1}{2}O_2 \rightarrow CO_2 \qquad h^0_{R4} = -10.1\ \text{MJ kg}^{-1}\ \text{CO} \tag{R4}$$

$$CO + H_2O \rightarrow CO_2 + H_2 \qquad h^0_{R5} = -1.47\ \text{MJ kg}^{-1}\ \text{CO} \tag{R5}$$

$$CO_2 + H_2 \rightarrow CO + H_2O \qquad h^0_{R6} = 1.47\ \text{MJ kg}^{-1}\ \text{CO} \tag{R6}$$

3. Modeling approach

According to Wehinger et al. [24], the particles in this work are considered as spatially and temporally fixed, which allows for a detailed numerical study of the heat and mass transport processes in the particle boundary layers. In addition, the pseudo-steady-state (PSS) approach [29] is considered. It states that the shrinking of the particle is negligibly slow compared to the heat and mass transport phenomena at the particle surface. For instance, the ratio of the gas velocity from the particle (Stefan flow) and the velocity of the shrinking particle surface is high. Precisely, it is the density ratio between particle and gas. The validity of this approach was confirmed by Stauch and Maas [30], who conducted transient simulations. They concluded that the combustion process is only dependent on the current particle diameter. Thus, particle shrinkage is not included into the model. Despite this model assumption, particle shrinkage occurs in general and leads to the traveling of