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Numerical modeling of a bubbling fluidized bed coal gasifier by kinetic theory of rough spheres

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HIGHLIGHTS

- Kinetic theory of rough spheres with reaction models is proposed in a coal gasifier.
- Concentrations, velocities and temperatures and gas compositions are predicted.
- Heterogeneous and homogeneous reactions mainly occur near the inlet of gasifier.

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ABSTRACT

Flow behavior and coal gasification are simulated using the kinetic theory of rough spheres with the coal reaction models in a steam-assisted bubbling fluidized bed coal gasifier. The collisions of inelastic rough spheres are modeled based on the kinetic theory of rough spheres with gas–solid interactions. The fluctuation kinetic energy of particles is introduced to characterize the random motion of particles as a measure of the translational and rotational velocities fluctuations. The coal gasification models compose of devolatilization model, char gasification model and gas phase reaction model. Simulations are carried out in a steam-assisted fluidized bed coal gasifier with a height of 2.0 m and a diameter of 0.22 m. The gasification performance has been predicted, and the distributions of concentrations, velocities, temperatures of gas and solids phases and gas compositions are analyzed in a 2D model of a steam-assisted bubbling fluidized bed coal gasifier. Predicted gas species concentrations are in agreement with experiments.

1. Introduction

The gasification technology is applicable to any type of hydrocarbon based feedstock, such as coal, heavy refinery residues, petroleum coke, biomass and municipal wastes [1]. The syngas produced from coal gasification by means of an incomplete combustion can be used as a fuel, or to make a synthetic natural gas, hydrogen gas or other chemical products. Fluidized bed gasifiers are applied to gasify coal due to high rates of heat and mass transfer. It becomes one of the most important developing directions for coal gasifiers [2]. Despite their widespread applications, most of the development and design of fluidized bed gasification reactors has been empirical because of the complex flow behavior of gas–solid flow by thermo-chemical processes in these systems. Thus, the evaluations of theoretical approaches and simulations are needed.

Computational fluid dynamics (CFD) is widely used to study the hydrodynamics of fluidized beds by means of the kinetic theory of granular flow (KTGF). This theory is basically an extension of the classical kinetic theory of dense gases to particulate flows, which takes non-ideal particle–particle collisions and gas–particle drag into account. Gidaspow [3] generalized the kinetic theory of granular flow to gas-particle flows. Associated with the random motion of the particles, a translational granular temperature θ_t is defined as $\theta_t = \langle \boldsymbol{CC} \rangle/3$, where $\boldsymbol{C}$ is the random fluctuating translational velocity of particles. However, the original KTGF model is derived for smooth, rigid, nearly elastic, spherical particles in translational motion, and does not allow for particle rotation. In realistic situation, particle surfaces cannot be perfectly smooth and particles are frictional as well as inelastic. To simulate flow of rough particles, two granular temperatures are introduced. The first is the translational granular temperature θ_t, which measures the energy associated with the translational velocity fluctuations. The second is the rotational granular temperature θ_r, which measures the energy associated with the angular velocity fluctuations, defined

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as $\theta_r = (1/3\ \mathrm{m})\ I_p\langle\Omega^2\rangle$, where I_p is the moment of inertia, Ω is the angular velocity fluctuation and m is the mass of a particle. Sun and Battaglia [4] implemented a model from the kinetic theory for rapid flow of identical, slightly frictional, nearly elastic spheres. In this model, the conservation of rotational granular energy is approximately satisfied by requiring that the net rate of energy production for the angular velocity fluctuations is zero. The influence of friction on the collisional transfer of momentum and translational energy is neglected. Recently, the kinetic theory for flow of dense, slightly inelastic, slightly rough sphere (KTRS) was proposed by Shuai et al. [5]. They found that the model captured the bubble dynamics and time-averaged bed behavior. However, the models mentioned above are without chemical reaction in the bubbling fluidized reactors.

In this work, a model is presented to describe the thermo-fluid dynamics of dense, reactive, gas–solid mixture. The kinetic theory of rough, inelastic, spherical particles proposed by Shuai et al. [5] was used to take the collisions and rotation of particles in the bubbling fluidized bed gasifier into account. Seven species transport equations are solved with three heterogeneous global reactions and four homogeneous reactions. The reaction rates of homogeneous and heterogeneous reactions are determined by the kinetics and the mass and heat exchanges between gas and solid phases caused by reactions. Simulations are carried out in a 2-D model of a steam-assisted bubbling fluidized bed coal gasifier. Flow patterns, gas and particles velocities, composition profiles of gas products are obtained. Simulations show the predicted outlet gas compositions are in agreement with the experiments.

2. Kinetic theory for granular flow of rough sphere (KTRS)

For simplicity, the gas–solid hydrodynamic and coal gasification models are assumed as follows: (1) The solids phase is a mixture including coal and char particles which have the same diameter and density. Thus, the mixture of coal and char particles has an identical velocity and temperature, (2) the mixture of particles is assumed as inelastic and monodispersed spheres. The diameter and density of coal and char particles is kept as constant during gasification and combustion, (3) the vertical section of bubbling fluidized bed gasifier is rectangular, which can be assumed as two-dimensional, and (4) the solid phase is dense and continuous in the bed, in which the mean free path of radiation is much smaller than the solid dimensions to limit the contribution of radiative heat transfer. The gas phase is assumed as transparent so that the radiative energy is neither absorbed nor emitted.

2.1. Governing equations with kinetic theory of rough spheres (KTRS)

The equations used in Euler–Euler modeling approach are a generalization of the Navier–Stokes equations for interacting media, which include the unsteady balance equations for mass, momentum, energy and species for gas and solids phases [3,5]. Here we briefly summarize the equation of solids fluctuating energy and models for heterogeneous and homogeneous reactions.

In the collision between frictional spheres, the collisional impulse has a tangential component. Thus, the frictional collision of particles is described by a normal restitution coefficient e and a tangential restitution coefficient β. Considering an ensemble of identical rough spherical particles with spherically symmetric mass distribution, the particle fluctuation kinetic energy is [5]

$$e_0 = < \frac{1}{3}C^2 + \frac{I_p\omega^2}{3m} > = (\theta_t + \theta_r) \tag{1}$$

The conservation equation of solids fluctuating energy is

$$\frac{3}{2}\left[\frac{\partial}{\partial t}(\varepsilon_s\rho_s e_o) + \nabla\cdot(\varepsilon_s\rho_s e_o u_s)\right] = \nabla\cdot(\kappa_s\nabla e_o) + (\nabla p_s I + \tau_s) : \nabla u_s - \gamma_s - D_{gs} - 3\beta_{gs}e_o \tag{2}$$

where the pseudo thermal conductivity for rough spheres k_s and fluctuation energy dissipation rate of solids phase γ_s are calculated by correlations proposed by Shuai et al. [5]. The interphase momentum transfer coefficient β_{gs} is predicted by Huilin–Gidaspow model given in FLUENT 14 [6]. The stress tensor of particles τ_s is expressed in terms of the solid shear viscosity and bulk viscosity which are predicted on the basis of fluctuation kinetic energy e_0 [5].

2.2. Chemical reactions

For the sake of simplification, the drying process is assumed to occur in parallel with devolatilization [7]. The volatile content of the coal is determined by the proximate and ultimate analysis. It is also assumed that the volatile matter is composed of CO_2, CO, H_2, H_2O and CH_4 gas species. The char from primary pyrolysis is assumed to consist of pure carbon. After the devolatilization process, the original dry-ash-free (daf) coal changes to volatiles V_1 and V_2, and residual char of R_1 and R_2 [8]

$$\text{daf coal} \begin{cases} \alpha_1 V_1 + (1-\alpha_1)R_1 & (R1) \\ \alpha_2 V_2 + (1-\alpha_2)R_2 & (R2) \end{cases} \tag{3}$$

where α_1 takes the value of volatile matter percentage obtained in proximate analysis of coal, and α_2 is given the value of 0.8 to reflect the characteristics of devolatilization at high temperature. The daf coal devolatilization rate is proportional to the mass of daf coal and takes the first-order kinetic model. The volatile release rate can be given as:

$$\dot{m}_v = -\alpha_1 m_d A_{v1}\exp\left(-\frac{E_{v1}}{RT_p}\right) - \alpha_2 m_d A_{v2}\exp\left(-\frac{E_{v2}}{RT_p}\right) \tag{4}$$

The parameters are selected as: $A_{v1} = 2\times10^5\ \mathrm{s}^{-1}$, $A_{v2} = 1.3\times10^7\ \mathrm{s}^{-1}$, $E_{v1} = 104.6$ kJ/kmol, $E_{v2} = 167.4$ kJ/kmol [9].

The reaction rate of char is predicted by assuming a shrinking core mechanism, which considers the three resistances: external film diffusion, diffusion through the ash layer, and the reaction at the surface of the unreacted core [9]. The kinetic rate constants for the char combustion (R3), gasification (R4) and Boudouard reaction (R5) are given in Table 1 [10,11], where p_i is the partial pressure of gas species, $\phi = (2+k)/(2+2k)$ and $k = 2512\exp(-6240/T_s)$ [9].

As long as oxygen is present, the combustion of the gaseous species CH_4, H_2 and CO will take place (reactions R6–R8). If oxygen is completely consumed, carbon monoxide and hydrogen could take part in the water–gas shift reaction (reaction R9).

Note that in present study, the kinetic rate expressions and associated kinetic constants have been selected for gasification reactions. The different kinetic equations may be found in the literature for each reaction considered. Further research efforts are required for the formulation of global models of char gasification to be valid over wide ranges of experimental conditions which can reliably describe the influence of the key parameters on char reactivity.

2.3. Boundary conditions and numerical solution procedure

The simulations are carried out with the CFD code KTRS-FIX (Kinetic Theory of Rough Spheres-Flow with Interphase eXchanges) which is based on K-FIX software code [5]. In the KTRS-FIX code written in FORTRAN language, the fluctuation