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Three dimensional kinetic modeling of fluidized bed biomass gasification

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HIGHLIGHTS

- Three-dimensional kinetic modeling of a bubbling fluidized bed gasifier.
- The model is based on Eulerian–Lagrangian Computational Particle Fluid Dynamics (CPFD) concept.
- Complex gas–solid hydrodynamics is coupled with chemical reaction kinetics.
- Detail insight into the gasifier behavior including fluidization, thermal and chemical characteristics is obtained.

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ABSTRACT

Biomass gasification in fluidized bed system by using air–steam mixture as the gasifying agent is a promising way of utilizing biomass because it produces a gaseous fuel having relatively higher calorific value as well as higher hydrogen content with minimum or no heat addition to the gasifier. In the present work, a three dimensional numerical simulation of a bubbling fluidized bed biomass gasifier has been carried out. The numerical simulation is based on the Eulerian–Lagrangian approach where the fluid phase is solved by using a continuum approach and the solid is modeled by using Lagrangian computational particle model. The chemical reactions are coupled with the complex hydrodynamic calculation of gas–solid fluidized bed. The simulations are performed by varying the gasification temperature, equivalence ratio and steam-to-biomass ratio. Detail analyses of flow pattern, pressure distribution, and gas composition distribution have been presented. The complex three dimensional flow structures are revealed by plotting the results in different planes. The results provide a detail insight into the gasifier's behavior including fluidization, thermal and chemical characteristics. Simulated outlet gas compositions are compared with our own experimental data and a very good resemblance is observed.

1. Introduction

The promising future applications of fluidized bed gasification will require a continuous non-stop operation which can only be achieved through its optimum design. A comprehensive model can help to optimize both the gasifier design and the operation. In general two different types of modeling approaches are applied for gasification: (1) thermodynamic equilibrium modeling and (2) kinetic modeling. Thermodynamic equilibrium modeling is computationally inexpensive which is based on the concept of chemical reactions and phase equilibrium. Many researchers have studied the fluidized bed gasification process by using thermodynamic equilibrium model (Li et al., 2001; Prins et al., 2003; Pellegrini and Oliveira, 2007; Jurascik et al., 2010; Abuadala et al., 2010; Loha et al., 2011) because it provides an useful design aid in evaluating the possible limiting behavior of a complex reacting system. However, in equilibrium condition, rate of reaction is assumed to be very fast compare to the residence time of reactants, which does not occur in most of the cases. Besides, equilibrium model does not consider the hydrodynamics of the flow. Hence, for better understanding the gasification process, kinetic modeling is needed. Kinetic model takes into accounts the kinetics of pyrolysis, various homogeneous and heterogeneous reactions along with the hydrodynamic behavior depending on the reactor used. However, the development of kinetic based model is challenging depending on the level of detail required and this is determined by the type of kinetic model used. Most of the kinetic models for fluidized bed gasification reported in the open literature are one dimensional and steady-state, and the fluid dynamics is based on two-phase flow model (Chatterjee et al., 1995; Hamel

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and Krumm, 2001; Sadaka et al., 2002; Petersen and Werther, 2005; Corella and Sanz, 2005; Radmanesh et al., 2006; Barea and Leckner, 2010). In the two-phase flow model, the fluidized bed is divided into a bubble phase surrounded by an emulsion phase. However, in two-phase flow model the hydrodynamics of the fluidized bed is based on the semi empirical fluid dynamic correlations.

In this context, computational fluid dynamics (CFD) is perceived as an efficient tool for simulating the complex gas–solid hydrodynamics of fluidized bed system coupling with detail gasification reaction kinetics. Two different categories of CFD models (Loha et al., 2012) could be used for fluidized-bed simulation; Euler–Euler model and Euler–Lagrange model. In Euler–Euler approach, both gas and solid are treated as continuous phase. On the other hand, in Euler–Lagrange model, the gas is treated as continuous and solid as discrete phase. Because of complex mechanism of heat transfer and chemical reaction need to be modeled in coupling with complex fluidized bed hydrodynamics, relatively fewer studies on CFD modeling of fluidized bed gasification are available in the open literature. Euler–Euler CFD modeling of bubbling fluidized bed coal gasification process was carried out in two dimensional geometry (Yu et al., 2007; Armstrong et al., 2011) and three dimensional geometry (Wang et al., 2009) based on the experimental work of Ocampo et al. (2003). Euler–Euler CFD modeling was also used to simulate the fluidized bed reactor fast pyrolysis (Papadikis et al., 2008, 2009) and the fluidized bed steam reforming of glycerol (Dou et al., 2008; Dou and Song, 2010). However, in Euler–Euler model, several equations with semi-empirical parameters need to be solved simultaneously to get the solid phase properties and also it requires defining a separate solid phase for each diameter particle. But, the Euler–Lagrange model handles variable and time dependent particle size in a natural way by tracking each and individual particle. Sofialidis and Faltsi, 2001 simulated the fluidized bed biomass gasification where particles are modeled in Lagrangian frame in a prescribed porous medium and space occupied by the bubbles was calculated by semi-empirical relations. Oevermann et al. (2009) performed a two-dimensional Euler–Lagrange simulation of bubbling fluidized bed biomass gasification with limited members of particles. Therefore, the main advantage of Euler–Lagrange model has still not been explored due to high computational cost for simulating large numbers of particles in a high density bed which puts it at a disadvantage. The Euler–Lagrange simulation of entrained flow gasifier is adequate because of flow is relatively disperse and computational cost is less (Fletcher et al., 2000). Recently, a novel form of Euler–Lagrange approach i.e. Computational Particle Fluid Dynamics (CPFD) approach is applied for dense fluidized bed simulation. Eulerian–Lagrangian CPFD simulation is performed to study the heat transfer with chemistry in an example problem of large three-dimensional coal gasifier (Snider et al., 2011) and two-dimensional fast fluidized bed coal gasifier feeding section (Abbasi et al., 2011). Fluidized bed biomass gasification is also studied by Xie et al., 2012 using Euler–Lagrange CPFD simulation. But, (Xie et al., 2012) could not capture clearly the coalescence and eruption of bubbles due to high gas velocity in their simulation.

In the present work, a three dimensional numerical model is developed to study the bubbling fluidized bed gasification of rice husk. Eulerian–Lagrangian Computational Particle Fluid Dynamics (CPFD) approach called MP-PIC (multiphase-particle-in-cell) is used to simulate the complex gas–solid bubbling fluidized bed hydrodynamics together with gasification reaction kinetics. The hydrodynamic behavior of the fluidized bed is investigated in detail. Bubble formation, growth and eruption are captured by plotting gas–solid flow in three dimensional views as well as in two mutually perpendicular planes. The time-averaged particle volume fraction distribution is also obtained. The process of syngas generation is investigated by plotting the axial and radial variations of gas composition and outlet gas mass fraction variation with time. Simulations are performed by varying the gasification temperature, equivalence ratio and steam-to-biomass ratio. Some of the simulated results are compared with our own experimental data.

2. Experimental setup

Experiments were carried out in a laboratory scale bubbling fluidized bed gasifier described previously by Loha et al. (2013) and presented in Fig. 1. The experimental setup consists of a 50 mm internal diameter and 1200 mm length gasifier tube fitted with a single perforated type distributor plate at the bottom. The gasifier is placed inside an electric furnace. The furnace provides the necessary heat for gasification reaction with four numbers of electrically heating coils of capacity 2.0 kW each. The rice husk is chosen as the representative biomass material. The ultimate and proximate analysis of rice husk is given in Table 1. Rice husk is fed into the gasifier through two screw feeders with a hopper. The upper feeder is connected to a variable speed drive system that controls the feed rate and supplies the same to the lower screw feeder which is water cooled. The lower screw feeder is attached to the gasifier through a feeding port. It is maintained at a constant higher speed to feed the biomass immediately into the gasifier and thus the pyrolysis of biomass inside the screw feeder can be avoided. Silica sand is used as the inert bed material to help in

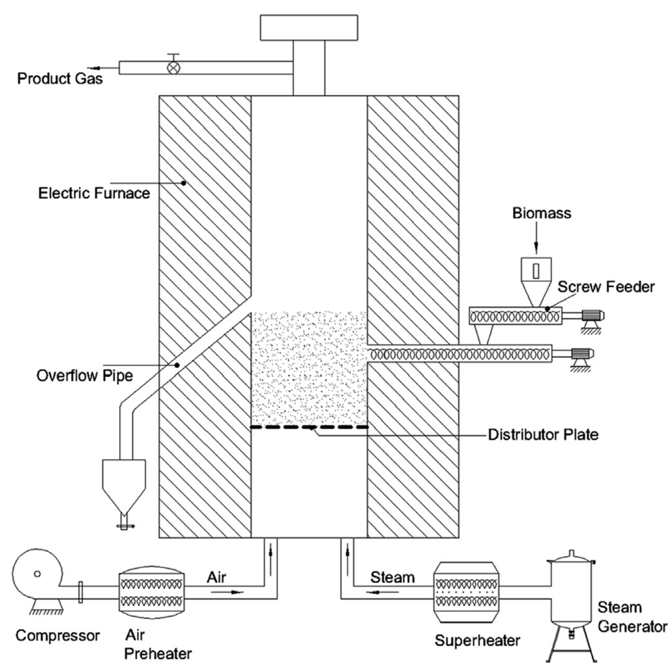

Fig. 1. Schematic diagram of the bubbling fluidized bed biomass gasifier.

Table 1
Ultimate and proximate analysis of rice husk.

Ultimate analysis	wt%	Proximate analysis	wt%
Carbon	38.43	Volatile matter	55.54
Hydrogen	2.97	Fixed carbon	14.99
Sulfur	0.07	Moisture	9.95
Nitrogen	0.49	Ash	19.52
Oxygen	36.36		
Ash	21.68		