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Systems modeling, simulation and analysis for robust operations and improved design of entrained-flow pulverized coal gasifiers

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ABSTRACT

Gasification processes with complex reaction systems typically require stable operating condition. However, variations of feedstock flow, composition of feedstock, and environmental factors, as well as other factors, may cause abnormal operating conditions. This work proposes a novel systems modeling and analysis method by combining computational fluid dynamics (CFD) and process simulation for the Shell pulverized coal gasifier. The proposed method considers the Shell pulverized coal entrained-flow gasifier with two parts: a gasification core zone and a heat exchange and water gas shift zone. High-fidelity CFD models of gasification core zone is developed to obtain characteristics of flow field, temperature field and composition profiles within the gasification core zone. An equation-oriented process simulation model is further developed for the heat exchange & water gas shift zone. The proposed hybrid method is validated by comparing with industrial operating data. Three cases for abnormal operating condition are further investigated with the proposed hybrid model. The most significant factors that influence the process operability are found to be the characteristics of gas and particles hydrodynamic behaviors of the inner layer of the gasification core zone. The results show that obvious vortex for the gas and particles is beneficial to the normal and abnormal operating conditions. To improve the operability of the entrained-flow gasifier under abnormal operating condition, it is crucial to keep the swirl zone of the vortex at the center of the reactor. In the end, an improved design for gasifier is presented by adjusting the bias angle of the nozzle to make the swirl zone of the vortex more obvious. According to the simulation results, the optimal bias angle is $5.0^*(\pi/180)$ rad for the gasifier under both nominal and abnormal conditions.

1. Introduction and background

1.1. Introduction

Coal gasification is one of the most efficient means to utilize coal, and it is an important part of the integrated gasification combined cycle [1,2]. The process combusts fuels with insufficient oxygen to convert the energy embedded in the fuel into thermal energy, or into chemical energy in the produced gases. There are three types of commercially available coal gasifiers, namely fixed-bed gasifier, entrained-flow gasifier, and fluidized-bed gasifier [3]. Among them, the entrained-flow one, which is an advanced coal gasification technology, exhibits high gasification efficiency and high carbon conversion efficiencies. Moreover, it produces less tar and phenolic compounds than other gasification processes because of its very high operating temperatures. At these elevated temperatures, gas-solid two-phase movement significantly affects slag flow, refractory life, and carbon conversion. In addition, it plays a key role in promoting the mass and heat transfer in the entrained-flow gasifier. However, the flow field, composition profile and the temperature inside the reactor are extremely difficult to measure. Therefore, an accurate and quantitative analysis of the flow and

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temperature field distribution, as well as the spatial distribution of the composition of inner reactor, is very important for improving the scientific understanding of multiphase transport phenomena in the quest of achieving higher gasifier efficiencies [4].

Computational fluid dynamics (CFD) has been used as a powerful tool in designing entrained-flow gasifiers and optimizing their operating conditions [5]. Most recent publications focus on the pilot-scale plant or experimental studies [6–13]. In the coal gasification process, the chemical reaction model mainly included coal pyrolysis, carbon gasification, and gas phase reaction [14,15]. In practice, the flow and temperature field distributions of pilot and industrial scale plants are usually quite different from the theoretical results. For a better understanding of the industrial scale gasifiers, investigation of the gas-particle flow in entrained flow gasifier receives many attentions [16–22]. However, existing CFD studies for entrained-flow gasifier is only considered in the reactor because of the limitation of computational power. In industry, the sensors for product distribution in this gasification process are installed after a series of heat exchangers. For example, the product composition is analyzed by gas chromatography and the sample is collected from the outlet of the last heat exchanger and sent into the chromatography. Thus, the results of the CFD models cannot be directly compared with the experimentally measured chromatography data. In general, water-gas shift (WGS) reaction and inverse water-gas shift (IWGS) reaction always occur after quench without catalysis, and this phenomenon is verified [23–26]. In addition, it should be noted that most CFD studies for gasifier is based on nominal operating conditions [4,19,22]. As gaseous-solid feedstock for entrained-flow gasifier, the feed flow rate always varies because of the fluctuations in the coal conveying line. Therefore, operability of entrained-flow gasifier, especially for Shell gasifier, should be investigated under the abnormal conditions.

This work aims to propose an effective systems approach to enhance the operability of Shell gasifier under nominal and abnormal conditions. We develop a novel hybrid model for entrained-flow coal gasifiers. In this hybrid systems model, the reaction core zone of the Shell gasifier is modeled by ANSYS-Fluent, and the heat exchange zone is simulated by MATLAB based on CFD results. The method is validated by comparing the results of the normal condition with the industrial data. Furthermore, operability analysis for abnormal condition is quantitatively investigated by the proposed method. The hybrid simulation model also helps to optimize the design of the gasifier by adjusting the bias angle of the nozzle. The simulation results suggest that the optimal bias angle is $5.0^*(\pi/180)$ rad for the gasifier under both nominal and abnormal conditions.

1.2. Background

Chemical reactions with coal particle in gasifiers can be simulated by the Shrinking-Core Shrinking-Particle Model (SCSPM) [27], or considered as heterogeneous reactions occurring inside the pore of a char particle [28], such as random pore model (RPM). In either case, this phenomenon in an entrained-flow gasifier is illustrate in Fig. 1. Red arrows in Fig. 1 are the direction of the movement of particles and gases. In Fig. 1(b) and (c), the yellow circles are products such as CO, H_2, CO_2, and CH_4. The black irregular symbols represent pores of the surface. The red straight arrows describe the motions in the gaseous phase. In addition, the white circles are reactants, and curve arrows describe the motion directions of the reactants or products in Fig. 1(c). The particles and gases move forward by the way of spiral rise with high speed at the same time because of the vortex in gasifier. Besides, the particles are rotating by themselves as shown in Fig. 1(a). During the process, gaseous phase is in touch with particles at the direction of the tangent as Fig. 1(b). There are many pores on the surface of the particle. Due to the tangential force, the reactants can be adhering to the surface or the pore of the surface. Meanwhile, the product on the surface or in the pore of the surface escape from its original position to the gaseous phase, as shown in Fig. 1(c). The site of the reaction can be substituted by new species and it promotes the heterogeneous phase reaction. From the viewpoint of the reaction mechanism, if there is more chance for the particles to contact with the gaseous reactant, the operability of the gasifier can be improved.

The novel contributions of this work are summarized below:

- Development of a novel hybrid model with high-fidelity CFD models and equation-oriented process simulation model for entrained-flow gasifier;
- Validation of the proposed hybrid model by comparing with industrial operating data;
- Identification of the key factors that influence the process operability by comparison of the flow pattern of different operating condition;
- Enhancement of the operability by adjusting the bias angle of the nozzle as an improved design for entrained-flow gasifier.

The rest of this article is organized as follows. Process description and submodels are presented in the following section. Next, the proposed method is validated and the operability analysis for nominal and abnormal operating conditions are investigated. Furthermore, the improved design is provided to enhance the operability of the gasifier. Finally, conclusions are drawn especially for abnormal operating condition.

2. Process description and submodels

The flowsheet of Shell gasification process is briefly described in Fig. 2. In this process, feedstock (raw coal) is ground into pulverized coal and dried to meet specifications first in a coal mill. Four gasification nozzles are set on the periphery of the gasification chamber as burners. Each pair of burners is symmetrically opposed, and the bias angle is $4.5^*(\pi/180)$ rad. Then the pulverized coal is injected into the gasifier through the center hole of each nozzle by the pressurized carrier gas CO_2 at 365 K. Meanwhile, oxygen at 450 K is injected into the surrounded holes. At the nominal condition, the high-speed feed jets form strong vortex field. With the role of strong vortex at the gasification zone, the pulverized coal is thermally decomposed into volatile matters and char. After the devolatilization, homogeneous and heterogeneous reactions in the gas and solid phases take place in the gasifier resulting in the production of syngas and ash as a byproduct. The temperature of the gasification zone is keeping at about 1773 K due to most of the dominating exothermic and fast reactions. Large amounts of ash stick to the gasifier wall as molten slag at the high temperature condition. The molten slag, which leaves the reactor via a hole in the bottom, is quenched in water, crushed in a submerged mill and then lock-hoppered out to atmospheric pressure. The reactor consists essentially of a pressure shell protected from the hot gases by a tube wall, in which saturated steam at 5 MPa is raised. The tube wall is in turn protected by a thin layer of a refractory material. The gases with the remaining ash leave the reactor and are quenched with solid free recycled synthesis gas of 1073–1173 K to solidify the entrained ash before they enter the waste heat boiler. The gases leave the waste heat boiler at a temperature of 593 K. In the waste heat boiler, superheated steam at 773 K and 5 MPa is raised. The waste heat boiler and the reactor tube wall have a common forced circulation system.

To obtain high-fidelity models of the entire gasification process, the gasification core zone and heat exchange & WGS reaction zone