Energy Conversion and Management 126 (2016) 717–723

Contents lists available at ScienceDirect

Energy Conversion and Management

journal homepage: www.elsevier.com/locate/enconman

A new model for coal gasification on pressurized bubbling fluidized bed gasifiers

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ARTICLE INFO

Article history:
Received 12 May 2016
Received in revised form 21 August 2016
Accepted 22 August 2016

Keywords:
Pressurized fluidized bed
Coal gasification
Gasifier simulation
Modeling

ABSTRACT

Many industries have taken interest in the use of coal gasification for the production of chemicals and fuels. This gasification can be carried out inside a fluidized bed reactor. This non-ideal reactor is difficult to predict due to the complex physical phenomena and the different chemical changes that the feedstock undergoes. The lack of a good model to simulate the reactor's behavior produces less efficient processes and plant designs. Various approaches to the proper simulation of such reactor have been proposed. In this paper, a new model is developed for the simulation of a pressurized bubbling fluidized bed (PBFB) gasifier that rigorously models the physical phenomena and the chemical changes of the feedstock inside the reactor. In the model, the reactor is divided into three sections; devolatilization, volatile reactions and combustion-gasification. The simulation is validated against experimental data reported in the literature and compared with other models proposed by different authors; once the model is validated, the dependence of the syngas composition on operational pressure, temperature, steam/coal and air/coal ratios are studied. The results of this article show how this model satisfactorily predicts the performance of PBFB gasifiers.

1. Introduction

Polygeneration is born from the necessity to generate cleaner and more efficient processes. In such plants, process integration is needed in order to maximize products and minimize residues. Some of the benefits of polygeneration are the higher overall value creation, higher overall thermal efficiency and feedstock utilization, synergistic usage of low grade steam and waste streams, enhanced reliability with potential to store syngas as a liquid fuel, among others [1]. The finite nature of worldwide petroleum reserves leads to the use of other technologies for the generation of fuels, energy and chemicals, like in the case of coal gasification. Coal gasification can be used to produce energy, ammonia, methanol, synthetic natural gas, Fischer-Tropsch products, among others [2].

Gasification is about converting a carbonaceous material into a combustible synthetic gas with the help of a gasifying agent. In contrast to combustion, gasification allows a more efficient removal of pollutants from the raw gas when the operation is at high pressure. The gasifiers used are generally classified according to the fluidization regime in the gasifier; moving bed, fluidized bed, and entrained flow. Thanks to the mixing of the different phases inside the reactor that facilitates the heat and mass transfer, the fluidized bed processes tend to have high efficiencies [3]. These kinds of reactors are complex to model because of the turbulent regime in which they operate. The implementation of new models to help predict the behavior of these gasifiers are of relevant importance since they ensure a better understanding of the phenomena taking place and also predict with precision the composition of the flue gas. These results lead to a better plant and process design.

Different kinds of approaches have been proposed to predict the behavior of fluidized bed gasifiers. When there is a need for simulations that yield a more detailed result about the heat, mass transfer, dynamic behavior or the influence of the geometry of the gasifier in the gasification process, the recommended tool is the use of computational fluid dynamics (CFD). Adamczyk et al. [4] used CFD to compare a hybrid Euler-Lagrange with a standard Euler-Euler approach for modeling particle transport in a circulating fluidized bed. By doing so, the authors realized that they needed to implement several user-defined functions (UDFs) to be

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http://dx.doi.org/10.1016/j.enconman.2016.08.066
0196-8904/

able to get the results they were seeking; but, by doing so the simulation became more complex and thus increasing the amount of computational time needed. The same authors, in other work, simulated the particle transport and combustion phenomena in a circulating fluidized bed boiler [5]. These authors indicated that many numerical simulations were focused on gathering experience on the proper use of the numerical techniques, the selection of the appropriate mesh size and distribution, as well as the time step size due to the introduction of all complexities involved in the model at one stage is not likely to result in a stable solution process. In the same way, several authors [6–9] have validated their models with experimental data to have better predictions and understandings of the system worked, but the computational cost, limitations of the software, and the complexity of the simulations are the disadvantages of CFD.

In order to predict the syngas composition, Arnavat et al. [10] used two different artificial neural networks (ANNs), one for modeling circulating fluidized bed gasifiers, and the other one for bubbling fluidized bed gasifiers. The ANNs were trained with published experimental data and the results obtained by the networks showed good approximations ($R^2 > 0.98$). Models like this are valid only for a certain range of operational conditions and are very dependent on how well the ANNs are trained.

Industrial process simulators such as Aspen Plus or Aspen Hysys have also been used to model gasifiers; since once the reactor is properly modeled, the users can continue with simulations of other plant operations allowing them to have an easier integration of the results, predict operational conditions and have better decision-making criteria. To be able to model a complex reactor such as this one, the use of several ideal reactors is recommended [11].

Emun et al. [12] demonstrated the advantages of working with these kinds of simulators by improving the performance of an integrated gasification combined cycle (IGCC) plant. Aspen Plus was used and RGIBBS reactors were implemented for the simulation of the combustion and gasification zones. Since the coupling of other units is possible in this process simulators, pinch analysis and process integration insights were employed to make topological changes minimizing operational costs. Nayak and Mewada [13] simulated a fluidized bed reactor using Aspen Plus. In their simulation, the model was based on the different chemical changes that the coal undergoes inside the reactor; these changes are: devolatilization, volatile reactions and combustion-gasification. The authors modeled the devolatilization with an RYIELD reactor, the volatiles reaction with an RGIBBS reactor and the combustion-gasification zone with a stoichiometric reactor. Bassyouni et al. [14] simulated a date palm waste gasifier using Aspen Hysys. The authors also used a model based on the different chemical changes that the biomass undergoes, but in their simulation they modeled the combustion and gasification zones with equilibrium and Gibbs reactors. The results were validated against experimental data from a lab scale gasifier. Same principle was applied by Niu et al. [15]. Aspen Plus was implemented to simulate the gasification process of municipal solid waste in a bubbling fluidized bed. In the simulation, the raw material was first dried in a stoichiometric reactor, then the devolatilization was carried out on a RYIELD reactor and lastly the combustion and gasification sections were done using RGIBBS reactors.

A similar approach was carried out by Doherty et al. [16] involving several reactors to model the different reactions that take place inside the fluidized bed gasifier, and a second gasifier to adjust the composition of the syngas to match the reported data in the literature. Another similar model was proposed by Nieto et al. [11], the fluidized bed was portrayed as a series of pairs of PFRs in series in Aspen Hysys. These models may explain the chemical changes that the coal undergoes, but do not take into account the physical phenomena that takes place inside the reactor, leading to less accurate results.

Jafari et al. [17] proposed a different approach to model the gasifier. The model considers the fluid dynamic behavior by taking into account the coexistence of the bubble and the emulsion phase inside the reactor. The movement of gas through bubbles in the fluidized bed was considered as plug flow while the movement of gas through the emulsion phase was considered as completely mixed. These assumptions and the selection of proper fluid dynamic and mass transfer equations, allowed this sequential modular approach to predict satisfactorily the flue gas concentration of fluidized bed gasifiers over a wide range of superficial gas velocities.

Sotudeh-Gharebagh et al. [18] tried to combine the two approaches, considering the reactions inside the gasifier and the hydrodynamics in Aspen Plus. Their model was based on a combination of yield, stochiometric, CSTR and Equilibrium reactors in series with some calculator blocks including a block called HYDRO, which calculated the mean void fraction in each section of the upper region and in the dense bed of the riser. By trying to combine the two approaches, the authors got results that satisfied their needs; but their hydrodynamic model still missed the mass transfer phenomena that takes place inside the reactor and the lack of robustness.

In the present article, a PBFB gasifier will be modeled in Aspen Plus. The proposed method will model the chemical changes that the coal undergoes, and the fluid dynamic behavior of the gasifier in order to have more realistic predictions with respect to other models available in the literature. Experimental data from the literature will be used to validate the model.

2. Methodology

2.1. Model assumptions and equations

A PBFB gasifier is a non-ideal reactor that will be modeled as a combination of several ideal reactors. The assumptions made in the present model are summarized below:

- Steady state.
- Isothermal process.
- Coal devolatilization takes place instantaneously.
- Char is composed of carbon and ash.
- Radial concentration gradients are negligible.
- No heterogeneous reactions take place in the bubble phase.
- In the emulsion phase both heterogeneous and homogeneous reactions are considered.
- The fluid dynamic behavior of both phases can be described by the two phase model proposed by Kunii and Levenspiel [19] with some modifications made by Cui et al. [20].
- Reactants and effluents mixing take place at the end of each section.
- Bubbles reach the equilibrium size quickly above the distributor. Meaning that their diameter is assumed constant.

The modifications made by Cui et al. [20] use a probability distribution model of the local voidage to describe and simulate the dynamic gas-solid distribution in the turbulent regimen of the gasifier. This helps the model from Kunni and Levenspiel have a better approximation to the actual phenomena happening inside pressurized bubbled fluidized bed gasifiers. The two-phase model (bubble-emulsion) was chosen over a three-phase model (bubble-cloud/wake-emulsion) because in the latter the mass transfer coefficient of bubble-emulsion has a contribution in a mass transfer bubble-cloud and cloud-emulsion phases, also there are heterogeneous chemical reactions taking place in the emulsion