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Research paper

Evaluation of different biomass gasification modeling approaches for fluidized bed gasifiers

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ABSTRACT

To develop a model for biomass gasification in fluidized bed gasifiers with high accuracy and generality that could be used under various operating conditions, the equilibrium model (EM) is chosen as a general and case-independent modeling method. However, EM lacks sufficient accuracy in predicting the content (volume fraction) of four major components (H_2, CO, CO_2 and CH_4) in product gas. In this paper, three approaches—MODEL I, which restricts equilibrium to a specific temperature (QET method); MODEL II, which uses empirical correlations for carbon, CH_4, C_2H_2, C_2H_4, C_2H_6 and NH_3 conversion; and MODEL III, which includes kinetic and hydrodynamic equations—have been studied and compared to map the barriers and complexities involved in developing an accurate and generic model for the gasification of biomass.

This study indicates that existing empirical correlations can be further improved by considering more experimental data. The updated model features better accuracy in the prediction of product gas composition in a larger range of operating conditions. Additionally, combining the QET method with a kinetic and hydrodynamic approach results in a model that features less overall error than the original model based on a kinetic and hydrodynamic approach.

1. Introduction

Because of environmental and economic incentives, such as increasing energy prices and fossil fuel depletion, countries are changing their energy profiles toward more renewable and sustainable resources.

Thermochemical gasification of carbon-based solid and liquid materials, which results in product gas consisting of H_2, CO, CO_2, CH_4 and some light hydrocarbons, has been used and developed for nearly two hundred years [1]. This technology can convert renewable resources such as biomass or black liquor to energy products that substitute for fossil-based fuels.

Among the existing types of gasifiers, the fluidized bed gasifier has many advantages, such as easy scale-up, flexibility regarding feedstock type and size, uniform temperature distribution and high carbon conversion efficiency; therefore, it is suitable for the gasification of biomass. Biomass gasification in fluidized bed gasifiers is quite a complex process, which means that the operating parameters are influenced by a large number of variables. Therefore, process modeling and simulation of the gasification process is more cost effective than performing experiments.

According to the reviews by Puig-Arnavat [2]and Gomez Barea [3]and the study by Radmanesh [4], there are two major approaches to model gasification in fluidized beds: equilibrium modeling and dynamic modeling considering the kinetics and hydrodynamics of the bed. Dynamic modeling gives a better interpretation of the real case. However, this approach requires detailed information on the geometry and design of the reactor, which makes it dependent on measurements and estimation of these inputs for any further analysis of gasification process [5]. Due to the complex and quite fast flow regime of different phases in the gasifier, measuring and calculating residence time is necessary for developing a correct dynamic model. However defining this parameter close to reality is an issue which has been studied during years [3].

In contrast, equilibrium modeling (EM), which is based on thermodynamic analysis, does not require information on the dimensions, capacity and structure of the gasifier and therefore is suitable for concept studies, preliminary design and optimization of

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the process [5–7]. EM has been applied to the gasification process in different ways—for example, the entire gasification mechanism is considered to be at equilibrium [6], or only the pyrolysis stage is assumed to be at equilibrium [7,8].

EM is mostly applicable when the operating temperature is high and the retention time is longer than the time required for complete gasification. However, the model may not provide accurate results at low operating temperatures in the range of 750–900 °C [3]. EM also has limitations in predicting the amount of light hydrocarbons and unconverted solid carbon. Several studies have been performed on how to improve the accuracy of EM in gasification modeling. Some examples are related to the gasification of coal in a fluidized bed [9] and an entrained flow bed [10], whereas other examples are of biomass gasification in a downdraft gasifier [11] and fluidized bed gasifiers [6] [12,13].

In 2001, Kersten [12] reviewed and compared different quasi-equilibrium models for biomass gasification in fluidized bed gasifiers. He studied two methods: 1. implementing empirical correlations in the Schläpfer model [14] and 2. using the quasi-equilibrium temperature (QET) in the Gumz model [15] This method is explained more in Section 2.1. Kersten concluded that the Gumz model with QET yields better results. Li and his colleagues in different studies [6,16] have investigated different methods to improve the accuracy of EM for biomass air gasification in circulating fluidized beds (CFB). They found that adding empirical correlations for light hydrocarbons (mainly CH_4) and carbon conversion is a successful method for improving EM. Recently, Lim and Lee [13] also developed a quasi-equilibrium model for fluidized bed gasifiers. They built their model based on 43 experimental datasets, which were gathered from different CFB [17,18] and bubbling fluidized bed (BFB) [19,20] gasifiers. They concluded that to achieve a higher level of accuracy in quasi-equilibrium models, the empirical parameters in the correlations for improving EM models should be adjusted to the experimental data from the same plant that is modeled. Other attempts have been made to improve the accuracy of equilibrium models by considering reaction kinetics. In these studies, the pyrolysis step is assumed to be at equilibrium, whereas char gasification and part of the homogeneous reactions in the gasification are considered to be kinetically controlled. For example, Bilodeau et al. [8], Nikoo et al. [21] and Wang et al. [22]included different reaction kinetics and, in some cases, hydrodynamics of the bed to improve the results of EM.

According to the literature mentioned above and as Gomez and Leckner described in their review paper [3], the modification of EM (which is called pseudo-equilibrium in Ref. [3]) for the modeling of fluidized bed gasifiers can be categorized into three groups: 1. Modifying the equilibrium temperature by the QET method, 2. Using quasi-equilibrium by adding empirical correlations for specific components and 3. Introducing the kinetics for specific reactions and adding hydrodynamics of the bed. Gomez and Leckner [3] evaluated the capability of different modified EMs to predict the composition of the product gas at different operating conditions to measure the "generality" of those models. They concluded that pseudo-equilibrium models give the most accurate results for gas composition, whereas tar and char content cannot be predicted as generally as other components.

According to the mentioned studies, although the gasification system is quite complex and dependent on many interrelated and independent variables, the "generality" characteristic for a model is one of the major concerns in the field of gasification modeling—mostly, whether it is aimed to be used further in process design and simulation level. As discussed above, EM is independent of the gasifier size and type, which makes it suitable as a basis for developing a general model. However, addressing the limitations of this model to improve the accuracy of prediction results in some "non-generality" factors. Therefore, a systematic study to evaluate the advantages and disadvantages of different modification methods and mapping the barriers and complexities that result in this "non-generality" would be essential for any further development of any possible generic model. This is one of the major novel contribution of this study to the field of biomass gasification modeling. The investigation of further possibilities in improving the modeling of biomass gasification is another part of this study. All three modeling approaches presented above are included and are based on the results of this investigation along with new models suggested in this paper.

2. Methodology

In this study, three equilibrium-based models from the literature, one model for each modeling approach described in Section 1, have been selected for evaluation. Two of the models have also been further modified. The same set of experimental data have been used for the evaluation of all models.

The simulation tool ASPEN PLUS has been used for the evaluation. As a steady state simulation tool, ASPEN Plus has been widely used to implement EM to model biomass gasification in fluidized bed gasifiers [8,23] owing to its powerful database of thermodynamic and chemical properties [24]. According to Puig-Arnavat [2], ASPEN PLUS is chosen for modeling of gasifiers and further gasification processes to avoid complexity when principal gasification reactions and some fundamental physical characteristics are included.

The models evaluated in this study are called MODEL I, MODEL II and MODEL III, corresponding to the three different modeling approaches described in Section 1.

MODEL I, MODEL II and MODEL III are first replicated in ASPEN PLUS and verified by comparison with the model results in the original presented studies. Experimental data from different BFB and CFB gasifiers have been collected from the literature and used to evaluate the model performance, with the aim to test whether the models are also valid for experimental conditions other than those for which they were originally validated. The input data used for the simulations are biomass ultimate/proximate analysis, temperature, pressure, and biomass, air and steam flowrates (see Section 2.4). The detailed information on ultimate and proximate analysis of different biomasses used in this study can be found in the referred papers for each case, respectively.

To choose the suitable experimental data as the input for evaluating the models, 5 major input parameters have been compared. The parameters are gasifier type (CFB or BFB), equivalence ratio (ER) (is a dimensionless index for the ratio of the mass of air input to the stoichiometric amount of air needed for full combustion [25]), temperature, load (as an index for the size and residence time of the gasifier) and the mass ratio of steam to the moisture and ash free mass of biomass (S/B). These parameters are combinations of major operating parameters (ER, temperature, S/B) and variables that can limit the "generality" aspect of the model (gasifier type, load). The cases with input parameters in different ranges than those of the original validated experiments have been chosen for the evaluation step.

In the first part of the paper, the overall accuracy of the models in predicting the four major components in the product gas (H_2, CO, CO_2 and CH_4) is the focus. The main results in this part of the paper are from studying the sensitivity of the models to the major input parameters, which were mentioned earlier, and analyzing the variation of accuracy in different cases.

In the second part of the paper, based on the discovered limitations and "bottlenecks" in the existing modified EMs found and discussed in the first part, MODEL II and MODEL III are further