Bioresource Technology 206 (2016) 173–179

Contents lists available at ScienceDirect

Bioresource Technology

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

Thermodynamic modeling of small scale biomass gasifiers: Development and assessment of the "Multi-Box" approach

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HIGHLIGHTS

- Multi-stage and two-phase thermodynamic gasification model.
- Validation of the model with real data and comparison with single-stage model.
- Char and gases fractions were calculated for different stages of the gasifier.
- Realistic simulated final composition of the main gases.
- Multi-stage model is able to sustain a char yield throughout the process.

ARTICLE INFO

Article history:
Received 12 December 2015
Received in revised form 19 January 2016
Accepted 20 January 2016
Available online 25 January 2016

Keywords:
Thermodynamic modeling
Gasification
Small scale
Multi-phase
Biomass

ABSTRACT

Modeling can be a powerful tool for designing and optimizing gasification systems. Modeling applications for small scale/fixed bed biomass gasifiers have been interesting due to their increased commercial practices. Fixed bed gasifiers are characterized by a wide range of operational conditions and are multi-zoned processes. The reactants are distributed in different phases and the products from each zone influence the following process steps and thus the composition of the final products. The present study aims to improve the conventional 'Black-Box' thermodynamic modeling by means of developing multiple intermediate 'boxes' that calculate two phase (solid–vapor) equilibriums in small scale gasifiers. Therefore the model is named "Multi-Box". Experimental data from a small scale gasifier have been used for the validation of the model. The returned results are significantly closer with the actual case study measurements in comparison to single-stage thermodynamic modeling.

1. Introduction

Biomass could be described as a resource with a high level of complexity both on the micro- but also on the macro-molecular scale. On the other hand, the advantaging aspects of renewability and CO_2 neutrality should be pointed out. Thus a lot of interest has been raised in the thermochemical conversion processes of biomass for energy production (McKendry et al., 2002a,b). Gasification is a thermal process which, under sub-stoichiometric conditions, converts the input into mainly gaseous products. Contrary to combustion, the gaseous products of gasification have significant heating value due to the fact that the energy is packed into chemical bonds (Basu, 2010). Gasification is a preferable energy conversion process in small scale applications due to the higher electrical efficiency in comparison to standard technologies, mainly combustion (Dong et al., 2009).

Small scale gasification units can be defined as the ones which operate under the electrical production limit of 200 kWe. This distinction can mainly be justified from the straightforward designing and operating limitations, but also from the limits set by the legislation. For example, in Italy, since few years ago, the subsidization systems were promoting the production of electricity from renewable sources in power plants with a size lower than 200 kWe, which had easier access to subsidies (Italian Ministry of the Economic Development, 2012). In addition, a thermodynamic distinction is that small scale gasification is driven by solid–gas reactions where the solid phase is represented by char contrary to larger scale units where the final products composition are directly correlated to the operating conditions which dictate the thermodynamic equilibrium (Vakalis and Baratieri, 2015). Small scale gasifiers could be mainly characterized as autothermal, air-blown and fixed-bed designed (Rauch, 2003). Fixed bed gasifiers could be downdraft, updraft or cross-draft but in any case these fixed beds are separated in different reaction zones during

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http://dx.doi.org/10.1016/j.biortech.2016.01.060
0960-8524/

operation. The main zones can be identified as drying, pyrolysis, reduction and combustion and their distribution is dependent on the specific design of the gasification unit. In addition, the different reaction zones are characterized by a wide range of operating conditions and transitions in the state of the feedstock. Finally, gasifiers in general and fixed bed reactors in our specific case tend to produce several output streams, mainly producer gas, tar and char.

In the recent years, a rapid development of small scale biomass gasifiers has been observed (Rauch, 2003). Therefore the assessment of biomass gasifiers' performance and efficiency is a topic of high interest. Modeling is proved to be a relatively fast and economic solution compared to the direct construction of pilot units. Therefore several models have been developed in order to simulate fixed bed reactors, i.e. CFD, neural network, thermodynamic and kinetic, with the latter two being the most applied (Basu, 2010).

Kinetic rate models always contain parameters that limit their applicability to different plants. These parameters can be identified as the reactor design, the retention time and the prior knowledge of the reaction pathways (Bridgwater, 1995). The state-of-the-art of kinetic modeling of thermochemical conversion of biomass are primarily complicated nth-ranked models like the distributed activation energy model, i.e. DAEM, and the independent parallel reactions scheme, i.e. IPR (Sfakiotakis and Vamvuka, 2015). Therefore, the computation of these models is an extremely demanding process. In addition, as already mentioned above, fixed bed gasifiers have distinctive zones with pyrolysis being among them. The radiant surface temperature along with the size of the particles, are identified as the main factors of the pyrolysis rate (Di Blasi, 2008). Commercial scale fixed bed units, utilize G30–G50 wood chips which correspond to an average size between 3–16 mm and a corresponding particle area of 3 cm^2 (EN 14961:2010). In addition, as mentioned above, most commercial gasifiers are air-blown which means that the gasifying medium is air. As a result of the above, the process of pyrolysis takes place under a thermally thick regime which corresponds to a Biot number higher than 0.2. Thus gradients of temperature are formed during the heating of the particles and the particle's temperature can't be defined. This sets another constraining parameter to the applicability of kinetics in fixed bed gasifiers (Bryden et al., 2002).

Contrary to kinetic rate models, thermodynamic models have the ability to provide the final equilibrium products with fewer constraints. By means of this aspect, they are characterized by a higher level of flexibility and applicability. Moreover, less computational intensity is required in thermodynamic modeling (Puig-Arnavat et al., 2010). Thermodynamic equilibrium modeling has the aim to calculate the composition of highest stability of the products of a reaction, a condition defined as thermodynamic equilibrium that is met at the level of the products' minimum chemical potential. In practical applications, the lack of ideal conditions along with designing restrictions, i.e. retention time, prevent the output products to reach thermodynamic equilibrium (Bridgwater, 1995). Nonetheless, the calculation of the thermodynamic equilibrium may provide useful insights; the long residence time in fixed bed gasifiers suggest that the processes propagate in a rather slow rate and are not far from equilibrium (Baratieri et al., 2008). Various thermodynamic models have been developed and utilized and several of them provide results close to the experimental data.

A common approach to thermodynamic modeling is the application of calibration techniques so as to increase the accuracy of the corresponding methods. Several authors developed correction factors for the water–gas-shift reaction, where the rate of the reaction is corrected in order to match experimental data (Jarungthammachote and Dutta, 2007). Zainal et al. (2001) applied the RAND equilibration algorithm with the addition of several calibration factors, i.e. the surface reactivity of the char, the production of methane and assumed a linear correlation of moisture and hydrogen production. Li et al. (2004) utilized empirical equations for carbon conversion and the deviation from equilibrium. Correcting the rate of reactions has been a common and partially successful technique. Nonetheless, a large amount of experimental data is required for the development of calibration factors. This aspect also projects the lack of flexibility of these models, due to their inability to simulate several different fixed bed reactors.

The endeavor to describe better the gasification process led to the development of multi-stage models. Reed and Cowdery (1987) developed a two-stage model for stratified, i.e. open – top gasifiers. Nguyen et al. (2002) developed a three stages model where empirical data are used in addition to the reduction equilibrium reactions. This paper introduces the approach of combining different zones/processes with char–gas reactions. A similar approach is also applied from Giltrap et al. (2003) where the final gas composition is calculated from the char–gas reactions. Nonetheless, all the above mentioned multi-stage models are kinetic rate models. Except from the constraints of kinetic modeling in fixed bed gasifiers that are mentioned in previous paragraphs, multi-stage kinetic models face additional obstacles; the accuracy of these models is restricted from the representative elemental composition that is set as input in the reduction zone and application of empirical calibration factors which are always a potential aspect of bias and deviation from the actual fundamental mechanisms and reaction paths.

Finally several models have tried to describe the multi-phase nature of the gasification products from fixed bed gasifiers. Mendiburu et al. (2014) utilized carbon conversion efficiency as an input parameter. Parameters of similar nature have been applied also by other authors in order to return realistic results for the char yield (Zainal et al., 2001). Other studies have gone further by inserting representative tar compositions in order to add a third phase in the model (Barman et al., 2012). However, the development of tar compounds is not modeled and no data are retrieved concerning the behavior of the tar compounds along the different stages of the gasifier.

The aim of the present study is the development of a flexible multi-stage and multi-phase thermodynamic model which at the same time is as simple as possible concept-wise and can run on any processor of average capabilities. The main goal is the prediction of the final yield of the main gasification products in the different phases, i.e. gas–char–tar, and describes the fluctuation of the products along the different zones. In addition, the flexibility of the model is essential in order to increase the utilization of the model in several different fixed bed designs, i.e. updraft, downdraft etc. Finally the model aims to investigate the fundamental processes/pathways and thus no calibration or correction factors have been applied. The validation of the model has been done by applying it on a small scale gasifier. The monitoring campaign took place at San Leonardo, South Tyrol (Italy) and the details of the monitoring along with the full spectrum of the results analysis have been published by Patuzzi et al. (2015).

2. Methods

2.1. Development of the model

2.1.1. Thermodynamic equilibrium solver methods

A main sub-categorization of thermodynamic equilibrium models in the literature is in stoichiometric and non-stoichiometric models. The advantage of developing a non-stoichiometric model is that the prior knowledge of the reaction mechanism is not necessary. The only required input parameters are the elemental