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Development of a modified equilibrium model for biomass pilot-scale fluidized bed gasifier performance predictions

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ABSTRACT

The objective of this work is to develop a thermodynamic model considering non-stoichiometric restrictions. The model validation was done from experimental works using a bench-scale fluidized bed gasifier with wood chips, dairy manure, and sorghum. The model was used for a further parametric study to predict the performance of a pilot-scale fluidized biomass gasifier. The Gibbs free energy minimization was applied to the modified equilibrium model considering a heat loss to the surroundings, carbon efficiency, and two non-equilibrium factors based on empirical correlations of ER and gasification temperature. The model was in a good agreement with RMS <4 for the produced gas. The parametric study ranges were 0.01 < ER < 0.99 and 500 °C < T < 900 °C to predict syngas concentrations and its LHV (lower heating value) for the optimization. Higher aromatics in tar were contained in WC gasification compared to manure gasification. A wood gasification tar simulation was produced to predict the amount of tars at specific conditions. The operating conditions for the highest quality syngas were reconciled experimentally with three biomass wastes using a fluidized bed gasifier. The thermodynamic model was used to predict the gasification performance at conditions beyond the actual operation.

1. Introduction

In recent decades, biomass has recently created attention as an alternative energy source to replace the use of fossil fuels and compensate for increasing energy consumption. On a daily or yearly basis, tons of lignocellulosic biomass, municipal solid waste (MSW), and human/livestock wastes are produced and processed at high cost. Even though many commercial technologies handle the wastes, a great deal of wastes are still buried underground or burned, especially in many underdeveloped or developing countries. The abundant biomass energy resources could be converted into different forms of useful products through various commercial technologies. A strong candidate for handling the mass production of biomass wastes could be a gasification technology, one of the thermochemical conversion processes [1].

After Zainal et al. [2] proposed a Gibbs free energy minimization model, many mathematical models for gasification processes have recently been developed based on chemical equilibrium [3–11]. However, thermodynamic equilibrium calculations are independent of the gasifier type, and the model is more suitable for process studies on the influence of the fuels and process parameters [12]. Some drawbacks present in the equilibrium models are: difficult to consider char and the formation of tar, the underestimation of CH_4, the overestimation of H_2 and product yield. In order to avoid these inaccuracies, authors introduced correction factors based on non-equilibrium phenomena from actual experiments. Li et al. [13] developed a correction system for an equilibrium model that described the amount of carbon and hydrogen which bypassed the equilibrium reactions in coal gasification in a fluidized bed. A similar correction system was introduced by Damiani et al. [14]. Some of basic modifications which were used by other researchers are consideration of the carbon conversion and tar formation [15].

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Barman et al. [16] validated an equilibrium model based on a consideration of a tar yield of 4.5% from the experimental results. Many modified models were developed to understand the effect of parameters on the final product compositions as follows: Antonopoulos et al. [17] developed a non-stoichiometric equilibrium model using an enthalpy change term (ΔH) included in the energy balance equation. The gasification temperature was manually changed until the ΔH reached zero, and the output parameters were calculated based on the predicted temperature at a constant ER = 0.45. Doherty et al. [18] developed an ASPEN Plus® model based on a Gibbs free energy minimization to create a sensitivity analysis of a circulating fluidized bed biomass gasifier. Due to the sequential modular approach of the program, stream thermodynamic conditions and mass flow rates were required in each process. Two unit operation blocks were examined for heterogeneous and homogeneous reactions for gasification reaction simulation. Im-orb et al. [19] also made a parametric study of a rice straw gasification system using two different gasifying agents, steam-air and steam-CO_2, and the model was developed using Aspen Plus based on the Fischer-Tropsch method. Schuster et al. [20] performed an extensive parametric study with operating conditions of temperature, fuel composition, and amount of fluidizing agent on a dual fluidized-bed steam gasifier. An equilibrium determination was calculated from three partial mass balances (C, H and O) and three equations for the chemical equilibrium of three independent reactions considering a restriction on the model, showing that the unconverted carbon increases when the temperature decreases. Ściążko and Stępień [21] formulated a modified Gibbs energy minimization model by introducing experimental concentrations of carbon monoxide and carbon dioxide to build a regression model, and found an exponential correction function that depended only on temperature. The resultant factor was multiplied by the Boudouard reaction equilibrium constant and a water-gas shift equilibrium correction factor of 2. The actual coal gasification experiments were also done using a circulating fluid bed reactor.

Developing new technologies would be difficult and costly without a prior modelling and simulation of the process. Many modelling tools can be used such as the stoichiometric model (the simplest method), the equilibrium model (more complicated method), and kinetic and CFD models (the most advanced and effective methods) [21]. Although several different gasification designs have been proposed based on experimental data, most models still have a limitation in predicting the syngas compositions at the out-of-range boundaries because of non-linear thermodynamic reaction behaviors. Zainal et al. [22] investigated the relationship between ER and reduction temperature using woodchip gasification in a downdraft gasifier. The relationship was linear and close to the theoretical gasification (ER = 0.19–0.43) obtained from a stoichiometric balance. Pinto et al. [23] conducted a steam gasification experiment using a pilot-scale reactor with different feedstocks of coal, pine wood, and polyethylene (PE) waste (main plastic present in MSW). Their optimum coal mixed ratio for co-gasification was 20% (w/w) of pine and 20% (w/w) of PE wastes at 900 °C. Sheth and Babu [24] tested sesame and rose wood in a downdraft gasifier to find the optimum ER of 0.21 to reach a calorific value of 6.3 MJ/Nm^3 of producer gas. Sharma [25] studied temperature profile, pressure drop, and gas composition across a reactor in both firing and non-firing mode. Ratnadhariya and Channiwala [26] tested woody biomass materials to study the distribution of CO/CO_2 and CO/H_2 ratios along the length of the gasifier. Then they developed a correlation using an Arrhenius equation to predict the molar distributions of each gas. The average absolute error was between 9.0 and 9.5% of the CO/CO_2 ratio and between 5.7 and 9.0% of the CO/H_2 ratio.

The overall goal of the present work is to develop a user friendly program coupled with a modified thermodynamic equilibrium model using EES (engineering equation solver) so that any gasification users with the program can predict the gas compositions with known operating variables. The modification of a model by using constant factors was based on the actual experimental gasification work using bench-scale and pilot-scale bubbling fluidized bed gasifiers at Texas A&M University (TAMU).

In this paper,

a) Experimental data was obtained from both bench-scale and pilot-scale reactors in order to achieve suitable correspondence to the actual system.
b) An equilibrium model was developed based on three modification factors based on the actual experimental results.
c) The effects of gasification parameters (ER, temperature and fuel) were investigated to improve the reaction operation to find an optimized condition for syngas quality.
d) A simple and rigorous model was implemented for predicting the gasification performance of a bubbling fluidized bed gasifier.

2. Experimental

The experimental data for high tonnage sorghum (HTS) and dairy manure (DM) was imported from Maglinao Jr. et al. [27] and Nam et al. [28]. Woodchip (WC) gasification was conducted for this work.

2.1. Sample preparation and characterization

HTS was introduced in a pilot-scale fluidized bed gasification system while WC and DM were utilized in a bench-scale fluidized bed gasification system. High-tonnage sorghum was planted and harvested at the Texas Agrilife farm in Burleson, Texas [27]. The HTS was an ES 5150 variety composed of low lignin content. The feedstock was shredded to an average particle size of less than 10 mm. The dairy manure was collected directly from an open pit at the Dairy Center at Tarleton State University in Stephenville, Texas [28]. The biomass wastes were initially air-dried. Then, only the dairy manure was further dried to reduce the moisture content enough to remove the sand bedding which was used at the dairy farm. A detailed sand removal study with manure from the Sierra Dairy in Texas was investigated [29]. The DM and WC were further milled through a 2 mm sieve using Wiley Laboratory Mill model #4 in order to be fed into a bench-scale gasifier. The characteristics of the three biomass samples were analyzed for their high heating value (HHV) using a Parr bomb calorimeter, a proximate analysis in accordance with ASTM standard E1775, ASTM D3175, and ASTM E871, and an ultimate analysis using a Vario MICRO Elemental analyzer.

The characteristics of biomass wastes used for the experimental gasification process are shown in Table 1. The HHV of the dry basis of the processed manure at 12.3 MJ/kg is comparable to the HHV of energy sorghum at 19.6 MJ/kg and its woodchip at 17.5 MJ/kg. The large difference in the HHV can be explained by the ash and carbon content. The carbon and ash contents were determined to be 33% and 36% for DM, and 46% and 16% for WC, while the HTS showed 42% carbon and 14% ash. The chemical composition can be expressed as $C_{3.52}H_{5.74}N_{0.02}O_{2.33}S_{0.002}$ for HTS, $C_{4.07}H_{6.6}N_{0.01}O_{2.79}S_{0.003}$ for the WC, and $C_{2.7}H_{2.5}N_{0.3}O_{1.53}S_{0.007}$ for the processed DM. This information is needed for the equivalence ratio (ER) calculations.