Energy Conversion and Management 78 (2014) 367–373

Contents lists available at ScienceDirect

Energy Conversion and Management

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

Kinetic modeling of reduction zone in biomass gasification

Samreen Hameed [b,*], Naveed Ramzan [a], Zaka-ur Rahman [a], Muhammad Zafar [b], Sheema Riaz [b]

[a] Department of Chemical Engineering, University of Engineering & Technology, Lahore, Pakistan
[b] Department of Chemical Engineering, University of Engineering & Technology, KSK Campus, Lahore, Pakistan

ARTICLE INFO

Article history:
Received 19 March 2013
Accepted 20 October 2013
Available online 23 November 2013

Keywords:
Kinetics
Mathematical modeling
Optimization
Simulation
Isothermal
Bioprocess

ABSTRACT

Gasification of biomass is becoming common technology now a days; it is convenient to apply numerical simulation to the process to save time and energy as compared to the lengthy experimentation.

Syngas produced as a result of gasification has many applications. Keeping in view those applications the objective of this work is to maximize the yield of syngas, using five different biomass like bagasse, wood sawdust, douglas fir bark, peanut hull and rice husk. The maximum yield of syngas is calculated using rate equations under isothermal and non-isothermal conditions. For isothermal conditions, the kinetic model is simulated over the temperature range of 1000–1300 K by taking a step size 50 K to estimate optimum temperature. For non-isothermal conditions, the kinetic equations are solved for heating rate range of 25–75 K/s by taking a step size 10 K/s to assess optimum value of heating rate.

1. Introduction

Energy plays a vital role in the development of living standards. The primary energy sources are solar, biomass, wind, hydro, tidal, geothermal and fossil. With the advance of using biomass as an alternative to the fossil fuels it is becoming most promising renewable energy source. Biomass is helping in meeting the present world's energy demand because it is abundant, environment friendly and renewable [1]. Thermochemical conversions of biomass include three methods; combustion, pyrolysis and gasification [2]. Among these processes, *gasification* is considered to be an effective process for the production of energy.

Gasification converts biomass into high proportions of gaseous products (CO_2, water, CO, H_2 and gaseous hydrocarbons) and small quantities of char (solid product), ash, and condensable compounds (tars and oils). This conversion is achieved in a gasifier, at a higher temperature and with a controlled amount of oxidizing agent, so that combustion may be prevented [2]. Among different types of gasifier, downdraft gives the minimum tar production. It includes three stages; biomass gets enter into the pyrolysis zone and the products obtained are solid (Charcoal), liquid (tar and other organics) and gases. These products are then oxidized in the presence of some oxidizing agent like oxygen, air, etc. The charcoal is converted into syngas by reduction reactions in the last zone of gasifier [3]. Every zone of the gasifier is independent and plays significant role in the gasification of biomass but the reduction zone is important among all. The reactions in this zone are slow and they control the overall conversion of biomass [4]. All these three zones are shown in Fig. 1 [12]:

The primary focus of this work in the biomass thermochemical conversion was directed towards the optimization of the process to reduce the amount of unwanted products and maximize the syngas production. Several researchers have worked on the reduction zone of biomass gasifier [5–9]. Simulation has been done on the equilibrium models of reduction zone [3,4,9–11] and kinetic models [8], whereas Sharma has studied a combined effect of both in his work [5]. This study is entirely about the simulation of kinetic rate models under both isothermal and non-isothermal conditions for different kinds of biomass such as douglas fir bark, rice husk, peanut hull, bagasse and wood sawdust. The different types of models available for the simulation of gasifier are: [12]

- Kinetic or Diffusion Rate Models.
- Thermodynamic Equilibrium Models.
- Neural Network Models.
- Computational Fluidised Models.

Kinetic rate models were selected for the reduction zone of the gasifier, and parameters such as equilibrium constants $K_{eq,i}$, rate constants, k_i for the five reactions of reduction zone were calculated. The rate equations were then simulated using numerical simulation technique. As a result, compositions of the components char, CO, CO_2, H_2O, CH_4 and H_2 were obtained under isothermal and non-isothermal conditions. The kinetic rate models were simulated and the maximum yield of syngas was optimized.

* Corresponding author. Tel.: +92 3334918330.
E-mail address: samreenhameed@yahoo.com (S. Hameed).

0196-8904/$ - see front matter © 2013 Elsevier Ltd. All rights reserved.
http://dx.doi.org/10.1016/j.enconman.2013.10.049

Nomenclature

r_i	rate of reaction i (mol fraction/s)	x_{CO}	mole fraction of CO
A_i	frequency factor for reaction, i	x_{CO_2}	mole fraction of CO_2
C_{RF}	char reactivity factor	x_{H_2O}	mole fraction of H_2O
E_i	activation energy of reaction, i (J/mol K)	x_{H_2}	mole fraction of H_2
R	gas constant (J/mol K)	x_{CH_4}	mole fraction of CH_4
k_i	rate constant for reaction i		
$K_{eq,i}$	equilibrium constant for reaction i	*Subscripts*	
$\boldsymbol{T}$	temperature (K)	i	reaction number

2. Methodology

The simulation of reduction zone of gasifier is done in the sequence shown in Fig. 2:

In the reduction zone of the gasifier several reactions take place; the major reactions and the kinetic rate models for these reactions, selected from the previous research work of Sharma [5] are as follows:

Reaction 1: Boudouard reaction

$$C_{(s)} + CO_{2(g)} \Longleftrightarrow 2CO_{(g)} \quad \Delta H_R^\circ = 172.6\ \text{kJ/mol}$$

$$r_1 = C_{RF} k_1 \left(x_{CO_2} - \frac{x_{CO}{}^2}{K_{eq,1}} \right)$$

Reaction 2: Water gas reaction

$$C_{(s)} + H_2O_{(v)} \Longleftrightarrow CO_{(g)} + H_{2(g)} \quad \Delta H_R^\circ = 131.4\ \text{kJ/mol}$$

$$r_2 = C_{RF} k_2 \left(x_{H_2O} - \frac{x_{CO} \cdot x_{H_2}}{K_{eq,2}} \right)$$

Reaction 3: Methanation Reaction

$$C_{(s)} + 2H_{2(g)} \Longleftrightarrow CH_{4(g)} \quad \Delta H_R^\circ = -75\ \text{kJ/mol}$$

$$r_3 = C_{RF} k_3 \left(x_{H_2}^2 - \frac{x_{CH_4}}{K_{eq,3}} \right)$$

Reaction 4: Steam reforming reaction

$$CH_{4(g)} + H_2O_{(v)} \Longleftrightarrow CO_{(g)} + 3H_{2(g)} \quad \Delta H_R^\circ = 206.4\ \text{kJ/mol}$$

$$r_4 = C_{RF} k_4 \left(x_{CH_4} \cdot x_{H_2O} - \frac{x_{CO} \cdot x_{H_2}^3}{K_{eq,4}} \right)$$

Reaction 5: Water gas shift reaction

$$CO_{(g)} + H_2O_{(v)} \Longleftrightarrow CO_{2(g)} + H_{2(g)} \quad \Delta H_R^\circ = -41.1\ \text{kJ/mol}$$

$$r_5 = C_{RF} k_5 \left(x_{CO} . x_{H_2O} - \frac{x_{CO_2} x_{H_2}}{K_{eq,5}} \right)$$

Reaction (5) is the shift reaction in which CO and H_2O are converted into CO_2 and H_2. According to Wang and Kinoshita [13], the shift reaction should not be included as it does not affect the rate for that particular moisture to biomass ratio, but here in this study the shift reaction was included because of the fact it is one of the gasification reactions [1].

2.1. Initial conditions

Initial conditions of the reduction zone are the end conditions of oxidation zone. Rate constants and equilibrium constants are calculated to find out the residence time for the reduction zone. C_{RF} is the char reactivity factor. Extents of reactions in reduction zone depend upon the reactivity of char, which is represented by C_{RF}. It indicates the degree of burn-off and number of active sites on char and its particle size [6]. The value of C_{RF} may vary between 10 and 10,000 and sometimes exponentially or linearly, for the present models it is taken as 100. The compositions of the species leaving the pyrolysis zone are taken as the initial compositions of the reduction zone. The overall process of gasification can be represented by a single reaction as [13]:

$$CH_\alpha O_\beta + yO_2 + zN_2 + wH_2O = x_1C + x_2H_2 + x_3CO + x_4H_2O + x_5CO_2 + x_6CH_4 + x_7N_2$$

where $CH_\alpha O_\beta$ is the chemical representation of dry biomass. The subscripts α and β were determined from ultimate analysis of biomass feedstock.

y, z, w, x_i are the molar numbers of various components.

At $t = 0$ when the reactants enter into the reduction zone the initial compositions of CO and H_2 entering in the reduction zone are assumed to be zero by some researchers, here the initial

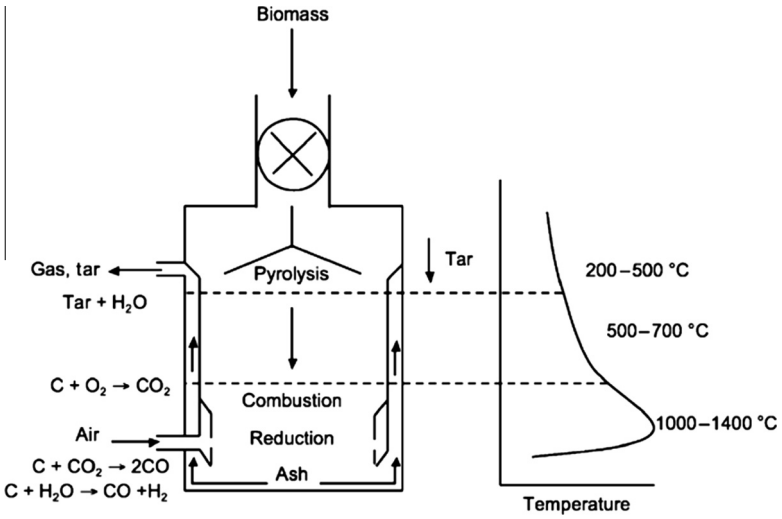

Fig. 1. Downdraft gasifier.