Available online at www.sciencedirect.com
ScienceDirect
Energy Conversion and Management 49 (2008) 1345–1356
ENERGY CONVERSION & MANAGEMENT
www.elsevier.com/locate/enconman

Equilibrium modeling of gasification: Gibbs free energy minimization approach and its application to spouted bed and spout-fluid bed gasifiers

S. Jarungthammachote, A. Dutta *

Energy Field of Study, School of Environment, Resources and Development, Asian Institute of Technology, P.O. Box 4, Klongluang, Pathumthani 12120, Thailand

Received 16 May 2007; accepted 6 January 2008
Available online 4 March 2008

Abstract

Spouted beds have been found in many applications, one of which is gasification. In this paper, the gasification processes of conventional and modified spouted bed gasifiers were considered. The conventional spouted bed is a central jet spouted bed, while the modified spouted beds are circular split spouted bed and spout-fluid bed. The Gibbs free energy minimization method was used to predict the composition of the producer gas. The major six components, CO, CO_2, CH_4, H_2O, H_2 and N_2, were determined in the mixture of the producer gas. The results showed that the carbon conversion in the gasification process plays an important role in the model. A modified model was developed by considering the carbon conversion in the constraint equations and in the energy balance calculation. The results from the modified model showed improvements. The higher heating values (HHV) were also calculated and compared with the ones from experiments. The agreements of the calculated and experimental values of HHV, especially in the case of the circular split spouted bed and the spout-fluid bed were observed.

Keywords: Thermodynamic equilibrium model; Minimization of Gibbs free energy; Spouted bed; Spout-fluid bed

1. Introduction

Spouted beds have been found in many applications such as drying, granulation, blending and particle coating. Spouted beds are also widely used in combustion and gasification processes. The conventional spouted bed consists of a conical or conical cylindrical vessel that has an orifice at the center of the conical base. High velocity fluid injected from the orifice causes the particles to rise in the area, called spout. After reaching some level above the bed of solid particles, termed fountain, those particles fall back into the annular region between the spout and the vessel wall and move downward to the conical bed again. The details of spouted beds can be found in [1].

Modifications of the spouted bed have been done in many ways to improve the performance and overcome some limitations of the conventional design, e.g. inserting a draft tube. In order to design properly and scale up various spouted beds, the hydrodynamic behavior and flow model have been studied and presented in many literatures [2–6].

For spouted bed gasification, models for predicting the composition of the producer gas are rarely found. In gasification processes, Jarungthammachote and Dutta [7] demonstrated that the equilibrium model used by many researchers for the analysis of downdraft and fluidized bed gasifiers can be used not only in gasification process but also in combustion and phase equilibrium problems [8–10]. Some of those models were based on minimization of the Gibbs free energy. This is a constrained optimization problem that generally uses the Lagrange multiplier method. Another kind of equilibrium model is one based

* Corresponding author. Address: Biomass Conversion and Biofuels, Canada. Tel.: +662 524 5403; fax: +662 524 5439.
E-mail address: adutta@nsac.ca (A. Dutta).

0196-8904/$ - see front matter © 2008 Elsevier Ltd. All rights reserved.
doi:10.1016/j.enconman.2008.01.006

Nomenclature

A_j	total number of atoms of jth element in reaction mixture
a_{ij}	number of atoms of jth element in a mole of ith species
$\overline{C}_p$	specific heat at constant pressure, kJ/kmol · K
f	fugacity, atm
G^t	total Gibbs free energy of system, kJ
$\Delta\overline{G}^\circ_f$	standard Gibbs free energy of formation, kJ/kmol
$\overline{H}^\circ$	enthalpy, kJ/kmol
$\overline{H}^\circ_f$	enthalpy of formation, kJ/kmol
h_{fg}	enthalpy of vaporization, kJ/kg
HHV	higher heating value, MJ/kg
L	Lagrangian function
$\overline{LHV}$	lower heating value, kJ/kmol
n	numbers of moles
P	pressure, atm
R	universal gas constant, 8.314 kJ/kmol · K
$\overline{S}^\circ$	entropy, kJ/kmol · K
T	temperature, K
y_i	mole fraction of gas species $i = \frac{n_i}{n_{tot}}$

Greek letters

v	stoichiometric number
μ	chemical potential
ϕ	fugacity coefficient

Superscripts

_	quantity per unit mole
∘	standard reference state

Subscripts

fg	difference in property between saturated liquid and saturated vapor
i	ith gas species
j	jth chemical element
tot	total

on equilibrium constants. However, the equilibrium model based on minimization of the Gibbs free energy and the one based on equilibrium constants are of the same concept [7].

Li et al. [10] used a non-stoichiometric equilibrium model (minimization of Gibbs free energy) to predict the producer gas composition from a circulating fluidized bed coal gasifier. An equilibrium model for studying the biomass gasification with steam in a fluidized bed gasifier was presented by Schuster et al. [11]. They concluded that the accuracy of an equilibrium model is sufficient for thermodynamic considerations. However, they mentioned that thermodynamic equilibrium may not be achieved, mainly because of the relatively low operation temperature. A temperature more than 800 °C can meet the equilibrium condition [12]. However, lower temperatures than that may not completely meet the equilibrium condition. Li et al. [13] employed the equilibrium model to predict the producer gas compositions, product heating value and cold gas efficiency for circulating fluidized bed gasification. The prediction results showed good agreement with experimental data. From the literature review, it can be seen that an equilibrium model cannot give highly accurate results for all cases. However, it can give a satisfactory result, and it is not a too complicated method, such that several simulations can be done in a limited time.

A spouted bed is similar to a fluidized bed, but the difference is in the dynamic behavior of the solid particles [14]. A spout-fluid bed is a combination of a conventional spouted bed and a fluidized bed. Since various spouted beds are generally similar to fluidized beds, the equilibrium model should be able to predict the gas composition from a spouted bed gasifier. Additionally, from literatures surveyed, the authors could not find utilization of the minimization of the Gibbs free energy method for gasification processes in spouted beds or modified ones.

This paper aims to present the equilibrium model based on minimization of the Gibbs free energy, which is applied to three types of gasifiers; a central jet spouted bed, a circular split spouted bed and a spout-fluid bed. The composition of producer gas predicted from the model and those from the experiments reported in literatures are compared. The effect of carbon conversion is also taken into account in the model. The higher heating value (HHV) of the producer gas is calculated and compared with those from experimental data.

2. Gasification mechanism

Gasification is the conversion of solid fuel, called feedstock, to combustible gases by supplying a gasifying agent. Typical feedstocks are coal, wood, solid waste, etc., which mainly consists of carbon, hydrogen and oxygen. Normally, the oxidizing or gasifying agents are air, oxygen, steam and CO_2. The product gas from air gasification has, generally, a low heating value of around 4–7 MJ/N m^3. On the other hand, pure oxygen gasification produces higher quality gas (10–18 MJ/N m^3) but is disadvantageous due to the high production cost of oxygen [11].

The processes inside a gasifier can be categorized into four zones or four processes; drying zone, pyrolysis zone, oxidation zone and reduction or gasification zone. However, in some types of gasifier, e.g. fluidized and spouted bed, those zones cannot be separated because of good mixing, and all four processes can be regarded as occurring simultaneously throughout the reactor [14].