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Effect of Operating Parameters in Air-Steam Gasification

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ABSTRACT

Biomass is a renewable energy source. Energy can be extracted from biomass through gasification, a thermo-chemical conversion process. The quantity and quality of the producer gas depend on the operating parameters like temperature, equivalence ratio and steam to biomass ratio. Enhancement of the quantity of hydrogen in producer gas is considered in the present context. A thermodynamic equilibrium model based on Gibbs free energy is developed to represent biomass gasification mathematically. This model is used to study the effect of the operating parameters on various gas yields, especially hydrogen. Air-steam gasification of coconut shell has been illustrated. Further a statistical software package, Design Expert is used to study the effect of parameter interaction on hydrogen yield based on the predictions made by the model. The study reveals that the hydrogen yield increases with increase in temperature and SBR. However, hydrogen yield decreases with increase in ER. A regression equation has also been obtained for hydrogen yield based on the operating parameters.

Keywords - biomass, renewable energy, air-steam gasification, design expert, hydrogen yield

1. INTRODUCTION

Rapidly depleting fossil fuels coupled with environmental apprehensions have encouraged the quest for new and renewable energy sources [1]. Biomass, a renewable source of energy is abundantly available and environment friendly. The use of biomass as an energy source is expected to play an important role in the generation of hydrogen, a potential energy carrier of the future. Biomass gasification, a thermo-chemical conversion process is being considered as one of the most promising technology for converting solid biomass into producer gas [2]. In Gasification, carbonaceous solid feedstock is partially oxidized into a mixture of hydrogen, carbon monoxide, carbon dioxide and methane. This partial oxidation process takes place in a reactor known as gasifier at temperatures above 800°C. Generally air or steam gasification is carried out. However, the quality of air gasification is improved injecting steam. Producer gas yield in air-steam gasification is influenced by reactor bed temperature (T), steam supplied (SBR) and air supplied (ER). A thermodynamic equilibrium model is developed to study the effect of these operating parameters on hydrogen yield.

Non-stoichiometric thermodynamic equilibrium models (NSTEM) have been developed to represent biomass gasification mathematically [3–5]. NSTEM is considered to study the effect of the operating parameters on quality and quantity of producer gas generated in air-steam gasification of coconut shell, a locally available biomass. Design expert - a statistical software package - is used to study the effect of various parameters.

2. MODELLING METHODOLOGY

2.1 Development of NSTEM

A non-stoichiometric thermodynamic equilibrium model (NSTEM) is developed to represent the biomass gasification process mathematically. It is based on minimizing Gibbs free energy in the system without specifying the possible reactions taking place. Total Gibbs free energy of a reaction system at constant temperature and pressure assumes a minimum value at the thermodynamic equilibrium. Hence the equilibrium composition of the reaction mixture can be obtained by the direct minimization of the total Gibbs free energy function subject to elemental mass balance constraints. Biomass gasification being a complex process, the formulation of the mathematical model requires certain simplifying assumptions. Assumptions are made regarding adequate residence time and reaction rates, isothermal and steady state nature of gasifier and ideal behavior of gases involved. It is further assumed that biomass molecule contains C, H and O only and the product gas contains only H_2, CO, CO_2, CH_4, N_2, and H_2O of which N_2 is inert.

2.2 Problem formulation and description

The total Gibbs free energy of a reaction system, based on thermodynamic principles can be expressed as given in equation (1).

$$G = \sum_j n_j \, \mu_j \tag{1}$$

G, represents the total Gibbs free energy and n_j the number of moles of species *j* in the reaction mixture. The chemical potential μ_j, of species *j* for an ideal gas mixture can be expressed as shown in equation (2).

$$\mu_j = G_j^o + RT \ln \frac{P_j}{P_0} = G_j^o + RT \ln \frac{y_j * P}{P_0} \tag{2}$$

G_j^o, denotes the standard Gibbs free energy of formation of species *j*. *R* and *T* represent universal gas constant and absolute temperature, respectively. 'G_j^o'can be obtained by finding out the standard enthalpy and entropy corresponding to absolute temperature T. P_j and P_o represent the partial pressure of species j and standard state pressure, respectively. However P_j can be expressed as the product of mole fraction (y_j) and total reaction system pressure (*P*). For an ideal gas reaction system maintained at an operating pressure of 1 atm and the standard pressure also at 1 atm chemical potential μ_j can be expressed as follows.

$$\mu_j = G_j^o + RT \ln \frac{n_j}{\sum n_j} \tag{3}$$

Here $\frac{n_j}{\sum n_j}$ represents the mole fraction y_j .

'n_j' denotes the number of moles of species *j and* $\sum n_j$ denotes the total number of moles of all the species in the reaction system.

Substituting the expression of μ_j in the original equation for total Gibbs energy (*G*) gives,

$$G = \sum_j n_j (G_j^o + RT \ln \frac{n_j}{\sum n_j}) \tag{4}$$

G_j^o for each temperature within normal gasification range (900 K to 1200 K) can be tabulated using Shomate equation which is an established method to calculate thermochemical data using polynomial equations. Shomate equation coefficients for various gas species were obtained from NIST Chemistry WebBook (Thermo-chemical tables) [6]. Having obtained the equation for Gibbs free energy (*G*) of the reacting system it is possible to find the values of n_j which minimize the objective function. The objective function obtained is modified as follows (as *R* and *T* are constants);

$$\frac{G}{RT} = \sum_j n_j \left(\frac{G_j^o}{RT} + \ln \frac{n_j}{\sum n_j}\right) \tag{5}$$

To obtain the constraints for minimization, law of conservation of mass in chemical reactions has been followed. Mathematical expressions for atomic mass conservation of each type of atoms entering and leaving the reactor can be expressed in the form of the linear equality constraints. Once the objective function and constraints are identified direct minimization of Gibbs free energy function can be carried out using FMINCON solver obtained from optimization toolbox provided by MATLAB. FMINCON is a non-linear solver that can find the constrained minimum of a function of several variables. Atomic mass conservation of atoms entering and leaving the reactor is based on the Global gasification equation (6).

$$n_b C_x H_y O_z + wH_2O + mO_2 + 3.76mN_2 + heat \rightarrow$$
$$n_{H_2} H_2 + n_{CO} CO + n_{CO_2} CO_2 + n_{CH_4} CH_4 + 3.76mN_2 + n_{H_2O} H_2O \tag{6}$$

2.3 Model validation and performance assessment

Deviations of model predictions from the experimental results are likely to occur due to the various assumptions considered during the model formulation. Modifications are incorporated into the models to increase the prediction accuracy. The accuracy of the model is checked using a statistical parameter, root mean square error (RMSE) [7] defined as,

$$RMSE = \sqrt{\frac{\sum (X_E - X_p)^2}{N}} \tag{7}$$

X_e, X_p and *N* are experimental data, predicted value, and number of observations, respectively.

Assessment of NSTEM is carried out by comparing it with the experimental results (EXP) based on the investigations by Turn et al.[8] for steam and air-steam gasification. Investigations were carried out with sawdust as the biomass is in a fluidised bed gasifier. The chemical characteristics of sawdust used in the experiment are presented in Table 1. Operating parameters considered are temperature (T), steam to biomass ratio (SBR) and equivalence ratio (ER). In steam gasification SBR is varied keeping T at 1073 K. In air-steam gasification SBR and ER are kept constant at 1.4 and 0.18, respectively, while the temperature is varied. A comparison between the gas yields in volume percentages during steam gasification and air-steam gasification is presented in Fig.1 and Fig. 2, respectively.

Table 1 Chemical characteristics of sawdust

Ultimate Analysis (% Wt.)				
Biomass	C	H	O	N
Sawdust	48.01	6.04	45.43	0.15
Proximate Analysis (%Wt.)				
Biomass	FC	MC	VM	AC
Sawdust	18.7	7.5	73.48	0.32

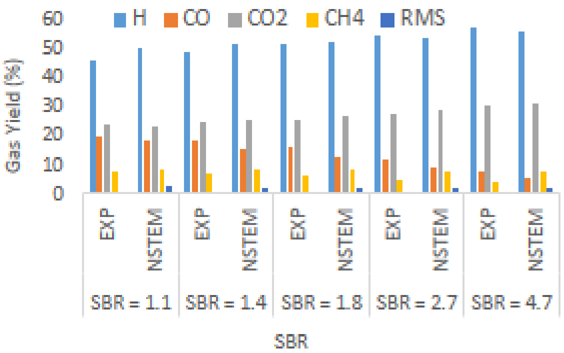

Fig. 1 Comparison of gas yield between the EXP and the NSTEM at 1073 K in steam gasification for different SBR

It is observed that the RMSE≤2.5 is obtained in steam gasification while RMSE≤5.5 is obtained in air-steam gasification. These values which are within the reasonable limits assure that the NSTEM developed based on minimization of Gibbs free energy can reasonably predict the quality and quantity of producer gas obtained in biomass gasification.

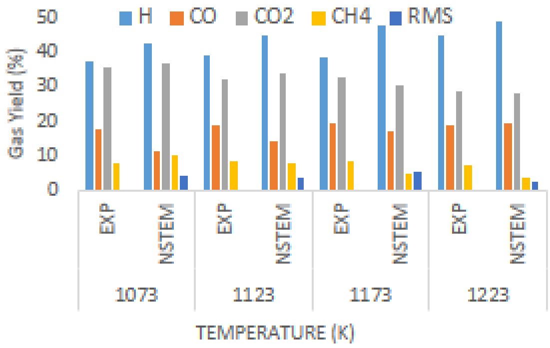

Fig. 2 Comparison of gas yield between the EXP and the NSTEM for air-steam gasification for different temperature at SBR=1.4 and ER =0.18

3. A STUDY ON THE INFLUENCE OF PROCESS PARAMETERS

Enhancement of hydrogen yield is important while considering biomass gasification. Hydrogen yield is mainly influenced by the operating parameters. NSTEM is used to predict the gas yield especially hydrogen yield of an air-steam gasification process using coconut shell powder as the biomass. Design Expert a statistical software tool is used to interpret the interaction of multiple variables enhancing hydrogen yield based on the model predictions.

Table 2 Chemical characteristics of coconut shell

Ultimate Analysis (% Wt.)				
Biomass	C	H	O	N
Coconut Shell	47. 17	5.82	46.84	0.17
Proximate Analysis (%Wt.)				
Biomass	FC	MC	VM	AC
Coconut Shell	16.1	12	68.5	3.4

The gasifier is proposed to be operated in the temperature (T) range 973 K to 1273 K, equivalence ratio (ER) range 0.15 to 0.4 and steam to biomass ratio (SBR) range 0.2 to 1.4. The chemical characteristics of coconut shell powder are given in the Table 2. Values obtained in the prediction are used in Design Expert software to analyse the interaction of the operating parameters.

4. RESULTS AND DISCUSSION

The influence of process parameters on gas yield (% composition) during air-steam gasification have been highlighted in Figs. 3 to 5. In Fig. 3, it can be observed that gas composition varies as a function of temperature (T) at constant ER and SBR. As temperature increases hydrogen and carbon monoxide yield increases while the yield of other gases decreases. The increase in H_2 and CO followed by decrease in CO_2 can be attributed to more intense endothermic gasification with increase in gasification temperature. However in Fig. 4, it can be observed that H_2 yield is decreasing with increase in ER. The decrease in H_2 yield with increase in ER can be attributed to the favourable oxidation condition (more air- indicated by the increase in Nitrogen yield) where more and more hydrogen is consumed in oxidation reactions.

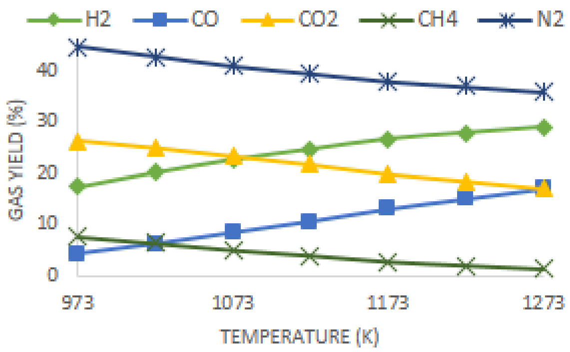

Fig. 3 Predicted gas yield for air-steam gasification for different temperature at SBR=0.8 and ER =0.25

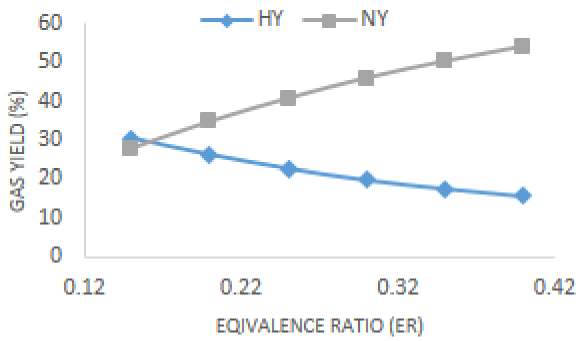

Fig. 4 Predicted hydrogen and nitrogen yield (%) for air-steam gasification for different equivalence ratios at SBR=0.8 and T =1073 K

In Fig. 5, the effect of steam to biomass ratio on gas yield at constant T and ER is presented. It is found that H2 and CO2 yield increases with increase in temperature while CO yield decreases with increase in temperature. This can be explained as the effect of the heterogeneous water gas reaction and the homogeneous water-gas shift reaction in the presence of more water. CH4 content remains more or less constant.

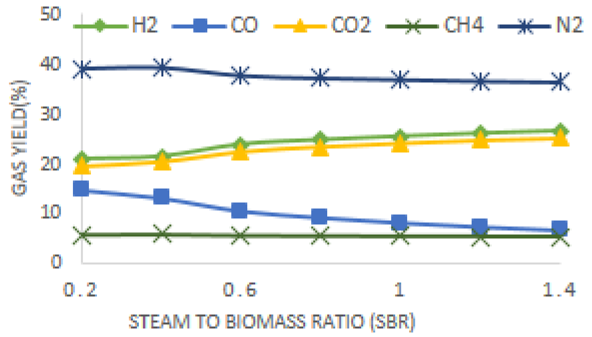

Fig. 5 Predicted gas yield for air-steam gasification for different steam to biomass ratio at ER= 0.22 and T =1073 K

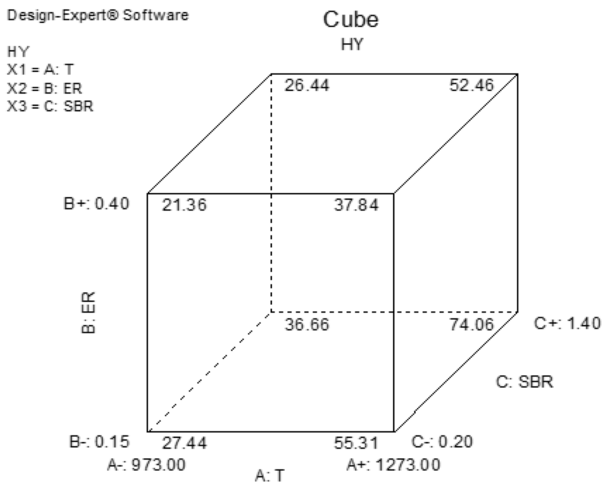

Fig. 6 Predicted ranges of hydrogen yield (g) for air-steam gasification for different ranges of T, ER and SBR using design expert software

A linear relationship between the process parameters for hydrogen yield has been developed based on the gas yield predictions made by the NSTEM with the help of Design Expert. This has been done to understand the influence of each operating parameter on hydrogen yield. Using the software the effect of individual process parameters and combined effect of the process parameters has been assessed. It is observed that hydrogen yield is predominantly influenced by T followed by ER and SBR. SBR has a positive effect while ER has a negative effect from the point of view of hydrogen yield. However, ER is effective in reducing the heat input into the gasification system. The influence of the process parameters on hydrogen yield (g) in the case of air-steam gasification using coconut shell is highlighted in Fig 6.

The liner relationship established is presented in equation (8). This linear relationship can be used to assess the hydrogen yield in air-steam gasification of biomass using coconut shell considering the operating conditions. These types of relations can be developed for different biomasses following the procedure adopted.

$$HY = -78.24 + 0.1104\,T + 126.13ER - 16.02\,SBR - 0.152\,T*ER + 0.0265T*SBR - 13.78ER*SBR \quad (8)$$

5. CONCLUSION

NSTEM developed based on minimization of Gibbs free energy has been validated with experimental results. The developed model is used to find the effect of operating parameters on hydrogen yield. Model values are further used to develop a liner relationship among the operating parameters with the help of a statistical software tool - design expert. This tool has been used further to verify that hydrogen yield is predominantly influenced by gasification temperature. The hydrogen yield increases with increase in temperature. SBR has a positive effect on hydrogen yield while the ER has a negative effect. The procedure adopted can be used to develop appropriate relation between the process parameters for different biomasses.

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