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Modelling of solid waste gasification process for synthesis gas production

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This study presents a mathematical model to predict synthesis gas ($CO+H_2$) composition from selected solid wastes (municipal waste, animal waste and agricultural waste) in a downdraft fixed bed reactor. This model assumes chemical and thermodynamic equilibrium with products inside the reactor. Effect of temperature in gasification zone, equivalence ratio and moisture content of biomass on gas composition was investigated. Model helps to know the behaviour of different biomass types and is a useful tool for predicting operating parameters of downdraft gasifiers with this biomass.

Keywords: Equilibrium, Equivalence ratio, Municipal solid waste, Synthesis gas

Introduction

Gasification is one of the efficient ways to convert energy embedded in biomass. Conversion of municipal solid wastes (MSW) to electrical energy can conserve more valuable fuels and lessen any harmful impact on environment. Production of transportation fuels or hydrogen from MSW through gasification is an attractive option both economically and environmentally. Countries like India, where there is no national power grid, distributed generation (DG) of power has a great potential for supplying power to remote areas[1], where energy resources are available locally. In a downdraft fixed bed, biomass undergoes combustion, pyrolysis and gasification[2]. Babu & Chaurasia[3,4] reported modelling and simulation of various zones in gasification process. Altafini *et al*[5] simulated an equilibrium model based on minimization of Gibbs free energy for wood waste. Melgar *et al*[6] combined chemical equilibrium and thermodynamic equilibrium of global reaction to predict final composition of synthesis gas. Zainal *et al*[7] studied an equilibrium gasification model based on equilibrium constants, to simulate gasification process in a downdraft gasifier.

This study presents a mathematical model to predict synthesis gas ($CO+H_2$) composition from selected solid wastes (MSW, animal waste and agricultural waste) in a downdraft fixed bed reactor.

Experimental Section

Biomass Characteristics

Various biomasses [MSW, animal waste (AW) and agricultural waste {groundnut shell (GS)}] that differ in composition were selected as feedstock for this model. MSW is heterogeneous in nature containing combustibles (paper, yard clippings, wood waste, food waste, plastics and textiles) and non-combustibles (glass, metals and other inorganic wastes). It has less carbon compared to AW and GS. Also, ash content is more in MSW than AW and GS. Increase of ash content in biomass decreases potential value for synthesis gas production. These biomass fuels were tested in order to investigate synthesis gas composition at different gasification temperatures.

Methodology in Model Formulation

Formulation of mathematical model was based on following assumptions: i) All carbon content in biomass is converted into gaseous form and residence time is high enough to achieve thermodynamic equilibrium; ii) Ash in feedstock was assumed inert in all gasification reactions; iii) All gaseous products are assumed to behave as ideal gases; iv) Reaction was auto-thermal and no external source of heat was applied, process is completely adiabatic so that no heat losses occur from gasifier and amount of air was varied to achieve desired reaction temperature in gasifier; and v) Sulphur and chlorine contents in biomass were neglected. Chemical composition of biomass was taken to be in the form $CH_xO_yN_z$ and gasification reaction can be written as

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$CH_xO_yN_z+m_wH_2O+x_g(O_2+3.76N_2) \rightarrow x_1CO+x_2H_2+ x_3CO_2+x_4H_2O+x_5CH_4+(z/2+x_g3.76)N_2$ é (1)

Where, moles of water vapour m_w can be calculated as

m_w = Molecular weight of biomass (Mb) * [Moisture content of biomass (m) / [18 (1 – Moisture content of biomass (m) é (2)

Major reactions that occur inside gasifier are as

$C + CO_2 \leftrightarrow 2CO$ é (3)
$\Delta H_f°$ (298) = 172.61 kJ/mol (Boudouard Reaction)

$C + H_2O \leftrightarrow CO + H_2$ é (4)
$\Delta H_f°$ (298) = 130.41 kJ/mol (Water Gas Reaction)

Eqs (3) and (4) can be combined as single reaction known as water-gas shift reaction as

$CO + H_2O \rightarrow CO_2 + H_2$ é (5)
$\Delta H_f°$ (298) = -42.2kJ/mol

Other prominent reactions in gasification process are as

$C + 2H_2 \leftrightarrow CH_4$ …(6)
$\Delta H_f°$(298) = -74.9 kJ/mol (Methanation Reaction)
$CH_4 + H_2O \rightarrow CO + 3H_2$... (6a); $\Delta H_f°$ (298) = 205.31 kJ/mol (Steam reforming of methane)

Where C is assumed as pure solid and activity is taken as unity.

Eqs (5) and (6) are two major reactions that occur in gasification process. Equilibrium constant for these equations as function of their molar composition can be written as

$$K_1 = \frac{P_{CO_2} P_{H_2}}{P_{CO} P_{H_2O}} = \frac{n_{CO_2} n_{H_2}}{n_{CO} n_{H_2O}} = \frac{X_3 X_2}{X_1 X_4} \quad \text{é (7)}$$

$$K_2 = \frac{P_{CH_4}}{\left(P_{H_2}\right)^2} = \frac{n_{CH_4} n_{tot}}{n^2_{H_2}} = \frac{X_5}{X_2^2} n_{tot} \quad \text{é (8)}$$

Gibbs free energy [Eq. (9)] is used in determining value of K_1 and K_2. For a given ideal gas, Gibbs free energy is a strong function of reaction temperature and a weak function of pressure[8].

$$\ln K(T) = \frac{-\Delta G_T}{RT} \quad \text{é (9)}$$

$$\Delta G_T = \sum_i X_i \Delta G^o_{f,T,i} \quad \text{é (10)}$$

Where, $\Delta G^o_{f,T,i}$ is empirically calculated as

$$\Delta \bar{g}^o_{f,T,i} = \bar{H}^o_{f,i} - aT\ln T - bT^2 - \frac{c}{2}T^3 - \frac{d}{3}T^4 + \frac{e}{2T} + f + gT$$

Values of a-g and enthalpy of formation at standard reference state of 298 K and 1 atm pressure are taken from Probstein & Hicks[9]. Eqs (11-13) can be written by balancing C, H and O moles, respectively as

$x_1+ x_3 + x_{5=} =1$ é (11)

$2x_2+ 2x_4 +4x_5= x+2m_w$ é (12)

$x_1+ x_4 +2x_3= y+m_w+2x_g$ é (13)

Total enthalpy content in any chemical species is sum of its chemical enthalpy and sensible enthalpy and can be written at reference temperature and pressure of 298 K and 1 atm as

$$H^o_{f-Biomass} + m_w\left(H^o_{f_{H2O(l)}} + H_{(vap)}\right) = X_1\left(H^o_{f_{CO}} + \int_{298}^{T_g} C_{P_{CO}}\, dT\right) + X_2\left(\int_{298}^{T_g} C_{P_{H2}}\, dT\right) + X_3\left(H^o_{f_{CO2}} + \int_{298}^{T_g} C_{P_{CO2}}\, dT\right) + X_4\left(H^0_{f_{H2O}} + \int_{298}^{T_g} C_{P_{H2O}}\, dT\right) + X_5\left(H^o_{f_{CH4}} + \int_{298}^{T_g} C_{P_{CH4}}\, dT\right) + \left(\frac{z}{2} + 3.76 X_g\right)\left(\int_{298}^{T_g} C_{P_{N2}}\, dT\right) \quad ...(14)$$

Eq. (14) acts as constraint for gasification process and forms basis for adjusting amount of air to be supplied. Amount of air is adjusted in such a way that total enthalpy of reactants is equal to that of products in gaseous form[10]. In this study, LHV is calculated in dry basis of biomass and was calculated using Eq. (9) as LHV = 4.187(81C+300H-26(O-S)-6(9H+m)) (kJ/kg), where C, H, O, S are carbon, hydrogen, oxygen and sulphur fraction in biomass respectively and m is moisture content in biomass on dry basis. C_p can be determined using an empirical relation as

$C_p(T) = c_1+c_2T+c_3T^2+c_4T^3$ (kJ/kg) é (15)

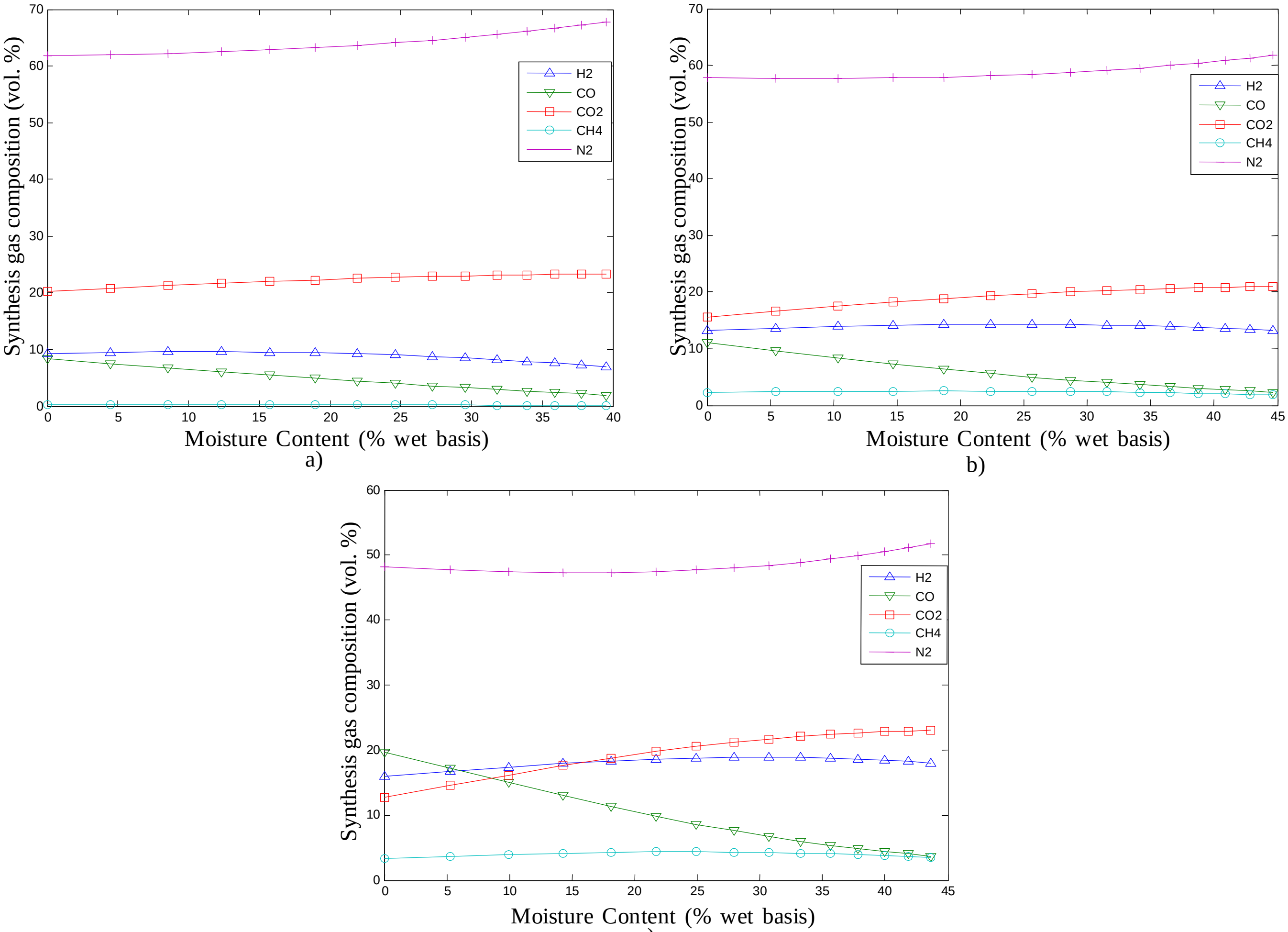
Sensible heat of each gas species was found by integrating Eq. (15) from ambient temperature to

Table 1ð Ultimate analysis for selected biomass feedstocks (dry basis, wt%)

Sl No.	Biomass	C %	H %	O %	N %	Ash %
1	Municipal solid waste (MSW)	30.3	3.4	35.8	1.4	29.1
2	Animal waste (AW)	42.7	5.5	31.3	2.4	18.1
3	Ground nut shell (GS)	48.3	5.7	39.4	0.8	5.9

Table 2ð Synthesis gas composition at 15% moisture content and at 800°C for various biomass feedstocks

Sl No.	Biomass	H_2	CO	CO_2	CH_4	N_2
1	Municipal solid waste	10.63	4.06	23.80	1.34	60.14
2	Animal waste	14.16	7.25	18.28	2.51	57.77
3	Ground nut shell	17.92	13.01	17.60	4.12	47.33



a)

b)

c)

Fig. 1ð Effect on synthesis gas composition at 800°C of moisture content in: a) typical municipal solid waste; b) animal waste; and c) ground nut shell

gasification temperature. Values of c_1-c_4 are taken as reported by Reid *et al*[11].

Model was run with elemental composition obtained from ultimate analysis of biomass, gasification temperature, moisture content and equivalence ratio as inputs for MSW, AW and GS feedstocks. Synthesis gas composition was determined by solving 6 equations (Eqs 7-8, 11-14) using MATLAB[12] programming by Newton-Jacobi iteration method.

Results and Discussion

Table.1 presents ultimate analysis for selected biomass feedstocks (dry basis, wt%)[13,14]. Table.2 gives synthesis gas composition at 15% moisture content and

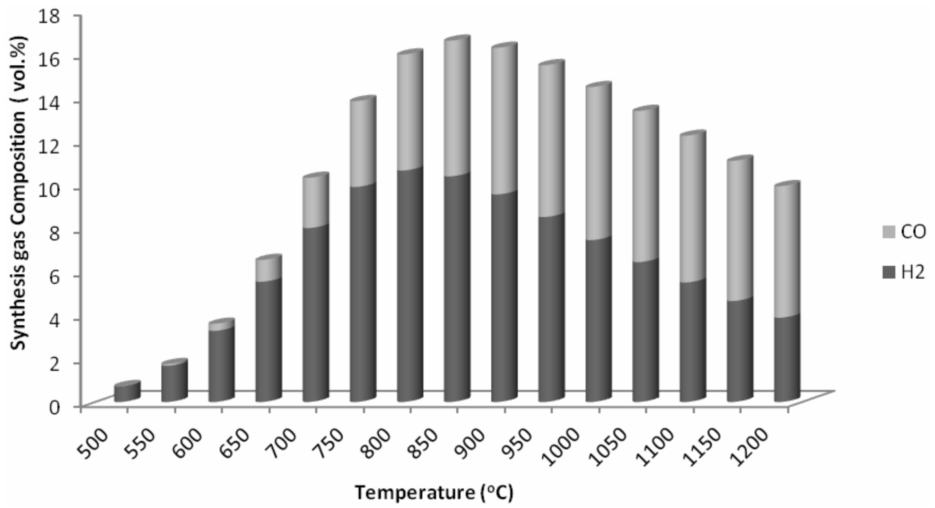


Fig. 2ð Effect of temperature on dry synthesis gas composition in selected range of temperatures (500-1200°C)

at 800°C for various biomass feedstocks obtained from Model.

Effect of Moisture Content on Synthesis gas Composition

Biomass moisture is often expressed on a dry basis. If W_{wet} kg of wet biomass becomes W_{dry} after drying, its dry basis (M_{dry}) is expressed as $M_{dry} = W_{wet} – W_{dry} / W_{dry}$. This can give a moisture percentage greater than 100% for very wet biomass, which might be confusing. Therefore, basis of moisture should always be specified. Wet-basis moisture is $M_{wet} = W_{wet} – W_{dry} / W_{wet}$. Increasing moisture content (0-28 wt%), concentration of hydrogen (H_2) increased for MSW (10.32-10.67 vol%; Fig. 1a), AW (13.21-14.29 vol%; Fig. 1b) and GS (13.78-15.35 vol%; Fig. 1c), and started decreasing thereafter with further increase in moisture content. Whereas carbon mono oxide (CO) decreased for MSW from 7.19 to 1.39 vol%, for AW from 10.99 to 2.33 vol% and for GS from 19.71 to 3.6 vol%, with an increase in moisture (0-45 wt%). With increase in moisture content (0-45 vol%), carbon di oxide (CO_2) concentration increases for MSW (21.97-24.42 vol%), for AW (15.64-20.94 vol%) and for GS (12.71-23.06 vol%). Highest percentage of methane (CH_4) is found associated with GS followed by AW and MSW. Variation of methane% in all feedstocks is almost constant.

As assumed that the process is completely adiabatic, additional air flow is required with an increase in moisture content to generate heat required to sustain desired temperature. This can be seen in increase in concentration of N_2 with increase in moisture content. In an actual gasification process, if this air flow is not supplemented, a decrease in gasifier temperature is observed. Small increase in H_2 concentration is overshadowed by rapid decrease of CO with an increase in moisture content.

Effect of Temperature on Synthesis gas Composition and on Gasification Process with Municipal Solid Waste (MSW)

Gasifier temperature was varied from 500°C to 1200°C. At very low temperature (500°C), carbon present in MSW (Fig. 2) is not utilized completely so synthesis gas production is not good but with increasing temperature more carbon is oxidized and rate of conversion increases. At low temperatures both unburnt carbon and CH_4 are present in synthesis gas but as temperature increases, carbon is converted into CO in accordance with Boudouard reaction. CH_4 is converted into H_2 by reverse methanation reaction, resulting in increasing operating temperature of gasifier that favours production of H_2 and CO, consequently heating value of gas improves. According to Boudouard reaction, as gasifier temperature increases, volume fraction of CO increases and that of CO_2 decreases. Water gas reaction suggests that high temperature increases production of both CO and H_2. According to methanation reaction, volume fraction of CH_4 in synthesis gas decreases and that of H_2 increases with increase in temperature. At higher temperatures, yield of H_2 and CO starts reducing, also attributed to water gas reaction. CH_4 production decreases sharply at temperature above 500°C.

Effect of Equivalence Ratio (ER) on Synthesis gas Composition

ER is defined as the ratio of the amount of air actually supplied to gasifier and stoichiometric amount of air. ER (<1.0)$_{gasification}$ = (air/biomass) / (air/biomass)

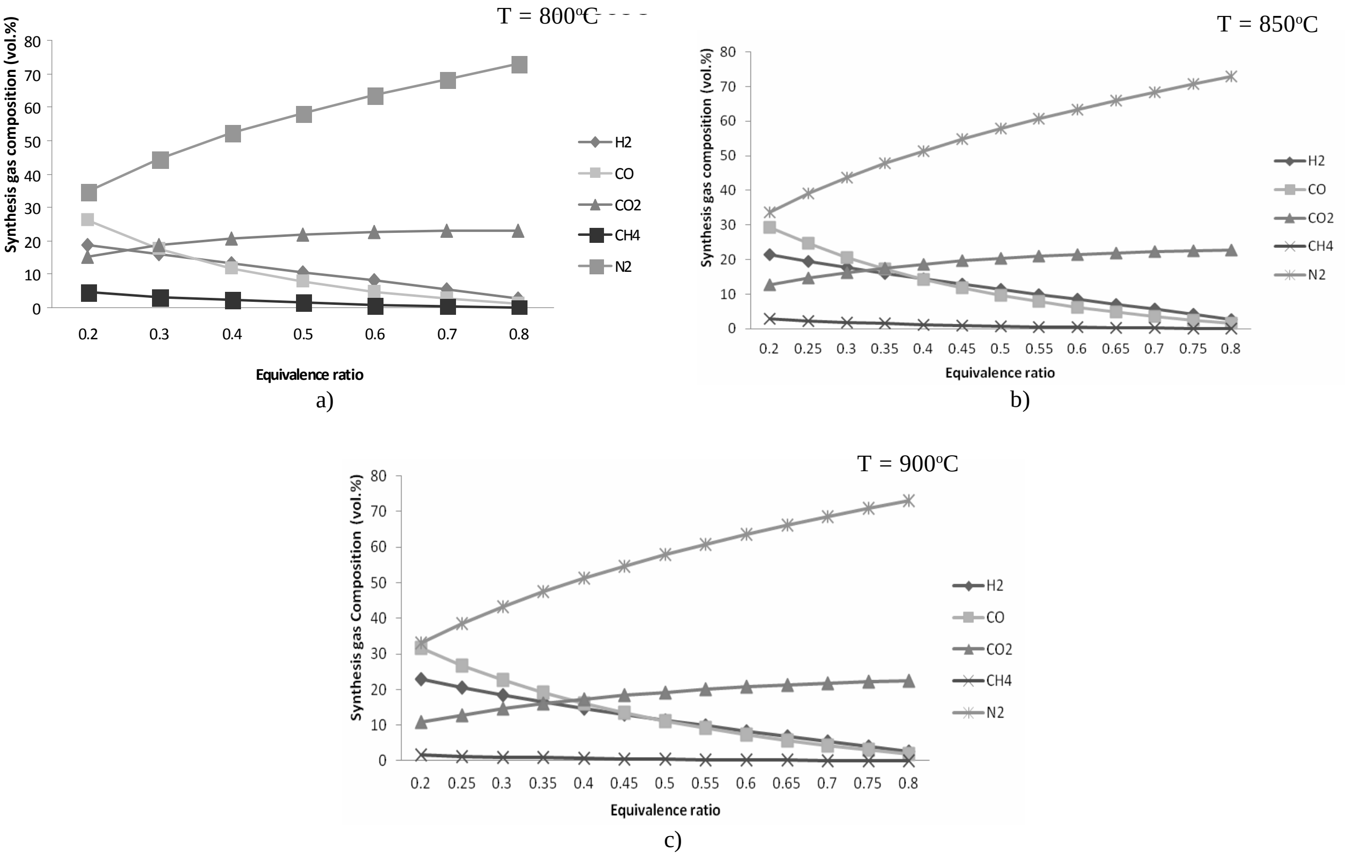


Fig. 3ð Effect of equivalence ratio on dry synthesis gas composition at gasification temperature of: 800°C; b) 850°C; and c) 900°C

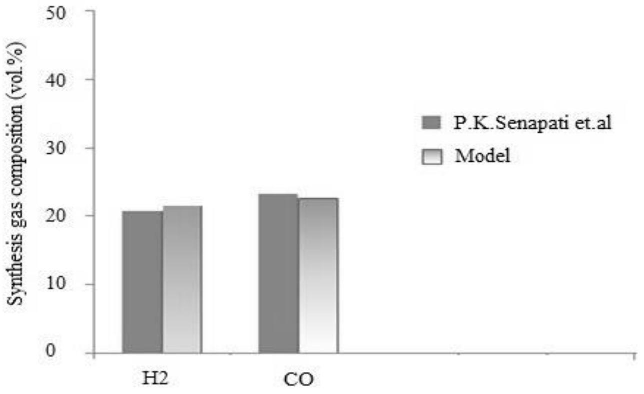


Fig. 4ð Comparision of synthesis gas composition obtained from model to experimental results

stoichiometric. As ER is increased, amount of oxygen supplied to gasifier increases, due to which conversion of carbon present in the fuel increases. But excess amount of oxygen oxidizes fuel completely and production of synthesis gas declines. ER in gasifier has been varied from 0.2 to 0.8. Initially, amount of CO and H_2 is comparatively high due to increased conversion of fuel but after a certain limit (0.3), production of synthesis gas decreases due to complete combustion of feed. Graphs plotted at three different temperatures [800°C (Fig. 3a), 850°C (Fig. 3b), and 900°C (Fig. 3c) for MSW, indicated that the maximum synthesis gas composition was observed at ER ranging 0.3 to 0.4 at all temperatures.

Model Validation

Comparing this model with the work of Senapati & Behera[15], predicted results from the model were found in good agreement with experimental results (Fig. 4). However, relations become less accurate with increase in ash content in biomass materials because a reaction with ash and heat absorbed by ash is ignored in the model. Also, perfect adiabatic conditions are difficult to achieve in practical gasifiers, resulting in some discrepancy between predicted and experimental results. As temperature increases, predicted values from this model and relation become more realistic.

Conclusions

Concentration of H_2 in synthesis gas increases with increase in moisture content and it attains maximum at 28-30%. Concentration of CO decreases with increase in moisture content. With increase in temperature, concentration of H_2 and CO in synthesis gas increases and attains maximum at 800-900°C. Concentration of H_2 and CO in synthesis gas decreases with increase in ER from 0.2 to 0.8 at all temperatures. Maximum values attained at lower ER around 0.3. Model predicted composition of synthesis gas matches well with experimental data reported in literature. Though chemical or thermodynamic equilibrium may not be reached within gasifier, this model provides designer with a reasonable prediction of maximum achievable yield of a desired product. However, it cannot predict influence of hydrodynamic or geometric parameters, like fluidizing velocity, or design variables, like gasifier height by using this model.

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