

Combined Transport and Kinetic Modeling of Downdraft Biomass Gasifier

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Abstract

Kinetics-free equilibrium models can predict the exit gas composition of the biomass gasifier, given the solid composition and the equilibrium temperature, but they cannot be used for reactor design. Hence, there is a need to develop a combined transport and kinetic model which takes into account of the kinetics of homogeneous and heterogeneous chemical reactions, transport of volatiles produced, heat and mass transfer between solid and gaseous phase and pyrolysis reactions. Taking into account of the importance of downdraft biomass gasifier and its commercial applications, it is essential to have a complete model for such a configuration. In the present study, a transient one-dimensional model is developed for the throated close-top downdraft biomass gasifier. The model takes into account of the drying, pyrolysis, secondary tar reactions, homogeneous gas reactions and heterogeneous combustion/gasification reactions. The experimental data obtained in our earlier study are used to validate the simulation results of the complete combined transport and kinetic model. The fraction of initial moisture content, air flow rate, temperature of the drying & pyrolysis zone, and chemical composition of the biomass are required as input data for the model to predict the composition of producer gas. The variation of molar fraction of producer gas components with time is predicted and compared with the experimental data. It is concluded from the present study that the developed model can predict the performance of the biomass gasifier, *a priori*. The results of this study are also useful in the design of a downdraft biomass gasifier.

1. Introduction

Bio-energy is now accepted as having the potential to provide the major part of the projected renewable energy provisions of the future. Gasification is one of the efficient

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technologies to convert the energy embedded in the biomass (Babu and Sheth, 2004). Gasification is a process of conversion of solid carbonaceous fuel into combustible gas by partial combustion. Downdraft gasification is comparatively cheap method of gasification that can produce a product gas with very low tar content (Giltrap et al., 2003). The understanding of the chemical and physical mechanisms during gasification is of fundamental importance for the optimal design of biomass gasifier (Babu and Chaurasia, 2004a-d). Modeling of biomass gasification implies the representation of chemical and physical phenomena constituting drying, pyrolysis, combustion, and reduction in the mathematical form (Babu and Sheth, 2005). The models of downdraft biomass gasification can be categorized into two groups: (1) Equilibrium models and (2) Combined transport and kinetic models. Equilibrium models are important in order to predict the thermodynamic limits of chemical reactions describing the gasification process. Kinetics-free equilibrium models can predict the exit gas composition, given the solid composition and the equilibrium temperature, but they cannot be used for reactor design (Sheth and Babu, 2009a). A transient one-dimensional model for the throated close-top downdraft biomass gasifier has been developed by Sheth and Babu (2009a). The model takes into account of the pyrolysis, secondary tar reactions, homogeneous gas reactions and heterogeneous combustion/gasification reactions. The drying and pyrolysis phenomena are modeled together as one zone. The drying zone is indirectly incorporated in the pyrolysis zone model. The pyrolysis model is divided into two subsystems, i.e., gas phase inside the bed and the individual particles. The model for single particle, developed by Babu and Chaurasia (2004c), is used in the complete gasifier model (Sheth and Babu, 2009a). The composition of volatiles is found using the experimental data of Boroson et al. (1989), which predicts the release of mainly water vapor from the pyrolyzing particle below 120 °C. Di Blasi (1998) also reported that at low temperatures the degradation rates are much slower than the drying rate. The presence of moisture is seen to delay wood pyrolysis and ignition. Therefore, drying and pyrolysis can be seen as two separate (sequential) processes in the biomass gasification (Di Blasi, 1998).

In the present study, the drying zone of the biomass gasifier is modeled independently and incorporated into the model proposed by Sheth and Babu (2009a). A model of

moisture evaporation and transport phenomena is presented to account for the drying. The drying model is divided into two subsystems, i.e., the bulk phase in the bed and the individual particles. Bulk phase modeling is carried out by a transient mass balance for water vapor. Single particle model incorporates the conservation of moisture, water vapor and energy. The kinetic model of drying developed by Chan et al. (1985) for wood pyrolysis is used in the present study. The simulated model can predict the performance of the biomass gasifier, *a priori* which is useful in the design of a downdraft biomass gasifier.

2. Mathematical Model

A transient one dimensional model is developed for the throated close-top downdraft biomass gasifier. The model takes into account of the pyrolysis, secondary tar reactions, homogeneous gas reactions and heterogeneous combustion/gasification reactions. Eight gaseous species namely O₂, N₂, CO₂, CO, H₂O, H₂, CH₄ and tar are considered in the gas phase. In the pyrolysis and combustion zone, the solid phase is a biomass, whereas in the reduction zone it is a charcoal. The developed model is divided into four parts according to four different zones formed: (1) drying, (2) pyrolysis, (3) oxidation, and (4) reduction.

2.1 Drying

The first zone in which the feed comes in contact in biomass gasifier is the drying zone. Basically drying is a mass transfer operation resulting in the removal of water moisture by evaporation from a solid or semi-solid. In the drying zone, feed descend into the gasifier and moisture is removed using the heat generated in the zones below by evaporation. The water vapor flows downward in the gasifier. Part of it may be reduced to hydrogen in the reduction zone and the rest will end up as moisture in the gas. The rate of drying depends on the surface area of the fuel, the temperature difference between the feed and the hot gases, the re-circulation velocity, relative humidity of these gases, and the internal diffusivity of moisture within the fuel (Dogru et al., 2002). In this zone, no chemical reaction takes place and only the water removal is carried out.

Drying zone is modeled as a stack of particles in one dimension. The model presented here considers temperature gradient both in the bed and also inside the single particles. Thus the entire bed is divided into two subsystems, i.e., vapor phase inside the bed and the individual particles. The assumptions made in this model are: (1) the moisture released from biomass particles flow downward, (2) unsteady state operation, (3) velocity varies along the bed, (4) solid biomass does not move downward during the operation, and (5) porosity of the bed remains constant.

2.1.1 Transport Model for Vapor Phase in Drying Zone

The continuity equation for the water vapor in a packed bed is given by Eq. (1).

$$\begin{aligned} \varepsilon_{bed} \frac{\partial \rho_{w,bed}}{\partial t} = & -\varepsilon_{bed} \left[v_{w,bed} \frac{\partial \rho_{w,bed}}{\partial z} + \rho_{w,bed} \frac{\partial v_{w,bed}}{\partial z} \right] \\ & + \frac{\partial}{\partial z} \left[\varepsilon_{bed} D_{w,eff,bed} \frac{\partial \rho_{w,bed}}{\partial z} \right] + a_p \dot{m}_{w,p} \end{aligned} \quad (1)$$

where, ε_{bed} is the porosity of the bed, $v_{w,bed}$ is the velocity of the water vapor (m/s), $\rho_{w,bed}$ is the density of the water vapor in packed bed gas phase (kg/m³), $\dot{m}_{w,p}$ is the mass transfer rate of water vapor from particle to the gas phase (kg/m² s), $D_{w,eff,bed}$ is the effective diffusivity of water vapor in packed bed gas phase, and a_p is the specific surface area of particle (m²/m³).

The initial and boundary conditions are given below by Eq. (2) and Eq. (3) respectively.

Initial Conditions:

$$\text{at } t = 0; \quad \rho_{w,bed} = 0; \quad v_{w,bed} = 0 \quad (2)$$

Boundary Conditions:

$$\text{at } z = 0; \quad \rho_{w,bed} = 0; \quad v_{w,bed} = 0 \quad \text{for all } t > 0 \quad (3a)$$

$$\text{at } z = L; \quad \frac{\partial \rho_{w,bed}}{\partial z} = 0 \quad \text{for all } t > 0 \quad (3b)$$

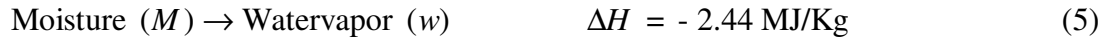
The water vapor generated from the biomass particle flows downward and its velocity is computed using Eq. (4).

$$v_{w,bed} = \left(\frac{\text{Flow rate}}{\text{Area}} \right) = \left(\frac{\rho_{w,bed} A \Delta z}{\text{Density of gaseous mixture}} \right) \left(\frac{1}{\Delta t} \right) \left(\frac{1}{\text{Area}} \right) \quad (4)$$

2.1.2 Single Particle Model in Drying Zone

Drying of a particle is carried out using an unsteady state one dimensional variable property model of transport phenomena. It includes heat (conductive, convective and radiative modes) and mass (diffusive modes) transport of the water vapor released within the solid. An Arrhenius type kinetic reaction proposed by chan et al. (1985) and subsequently modified by Bryden et al. (2002) describing the mechanism of evaporation is considered in the model.

Equations (5) and (6) describe the reaction of moisture evaporation and kinetic rate expression respectively.



$$k = A \exp\left(\frac{-E}{RT}\right) \quad A = 5.13 \times 10^{10} \text{ s}^{-1} \quad E = 88 \text{ KJ/Mol} \quad (6)$$

The equation for conservation of moisture is given by Eq. (7).

$$\frac{\partial C_M}{\partial t} = -kC_M \quad (7)$$

where, C_M = Density of moisture in solid phase

The conservation of water vapor is given by Eq. (8).

$$\frac{\partial(\epsilon C_w)}{\partial t} = D_{ew} \left(\frac{b-1}{r} \frac{\partial C_w}{\partial r} + \frac{\partial^2 C_w}{\partial r^2} \right) + kC_M \quad (8)$$

The conservation of energy is given by Eq. (9).

$$\frac{\partial(\rho C_p T)}{\partial t} = k \left(\frac{b-1}{r} \frac{\partial T}{\partial r} + \frac{\partial^2 T}{\partial r^2} \right) - \left(D_{ew} \frac{\partial C_w}{\partial r} \right) C_{p,w} \frac{\partial T}{\partial r} + (-\Delta H) \left(-\frac{\partial \rho}{\partial t} \right) \quad (9)$$

The initial and boundary conditions are given by Eqs. (10-13).

$$\text{At } t=0; \quad C_M = C_{M0}; \quad C_w = 0; \quad T(r,0) = T_0 \quad (10)$$

Particle boundary condition:

$$\text{At } t > 0,$$

$$\text{At } r = 0; \quad \frac{\partial C_w}{\partial t} = 0; \quad \left(\frac{\partial T}{\partial r} \right)_{r=0} = 0 \quad (11)$$

$$\text{At } r = R; \quad \left(D_{ew} \frac{\partial C_w}{\partial r} \right) = K_{m,w} (C_{w0} - C_{w1}) \quad (12)$$

$$\text{At } r = R; \quad K \left(\frac{\partial T}{\partial r} \right)_{r=R} = h(T_f - T) + 6\epsilon(T_f^4 - T^4) \quad (13)$$

2.2 Pyrolysis

Pyrolysis is a process by which a biomass feedstock is thermally degraded in the absence of oxygen/air to produce solid (charcoal), liquid (tar and other organics) and gaseous (H₂, CO₂, CO, etc.) products. Released volatiles from each biomass particle flow downward in packed pyrolysis bed. Rate of volatiles release depends on the particle size and temperature within a single particle. Pyrolysis bed is modeled as a stack of particles in one dimension. The model presented here considers temperature gradient both in the bed and also inside the single particles. Thus the entire bed is divided into two subsystems, i.e., gas phase inside the bed and the individual particles. The assumptions made in this model are: (1) the volatiles released from biomass particles flow downward, (2) unsteady state operation, (3) released volatiles is a mixture of CO, CH₄, CO₂, H₂, H₂O and tar, (4) velocity varies along the bed, (5) solid biomass does not move downward during the operation, and (6) porosity of the bed remains constant.

2.2.1 Transport Model for Gas Phase in Pyrolysis Zone

The continuity equation for the gas phase in a packed bed is given by Eq. (14).

$$\frac{\partial \epsilon_{g,bed} \rho_{g,bed}}{\partial t} = - \frac{\partial}{\partial z} [\epsilon_{g,bed} \rho_{g,bed} v_{g,bed}] + a_p \dot{m}_p \quad (14)$$

where, $\epsilon_{g,bed}$ is the porosity of the bed, $v_{g,bed}$ is the gas velocity (m/s), $\rho_{g,bed}$ is the density of the gas phase (kg/m³), \dot{m}_p is the mass transfer rate from particle to the gas phase (kg/m² s), and a_p is the specific surface area of particle (m²/m³).

The species conservation equation is given by Eq. (15).

$$\begin{aligned} \varepsilon_{g,bed} \frac{\partial \rho_{ig,bed}}{\partial t} = & -\varepsilon_{g,bed} \left[v_{g,bed} \frac{\partial \rho_{ig,bed}}{\partial z} + \rho_{ig,bed} \frac{\partial v_{g,bed}}{\partial z} \right] \\ & + \frac{\partial}{\partial z} \left[\varepsilon_{g,bed} D_{i,eff,bed} \frac{\partial \rho_{ig,bed}}{\partial z} \right] + a_p \dot{m}_{i,p} \end{aligned} \quad (15)$$

where, $\rho_{ig,bed}$ is the density of the species i in packed bed gas phase, $D_{i,eff,bed}$ is the effective diffusivity of species i in packed bed gas phase, and $\dot{m}_{i,p}$ is the mass transfer rate of species i from particle to the gas phase ($\text{kg/m}^2 \text{ s}$).

The initial and boundary conditions are given below by Eq. (16) and Eq. (17) respectively.

Initial Conditions:

$$\text{at } t = 0; \quad \rho_{ig,bed} = 0; \quad v_{g,bed} = 0 \quad (16)$$

Boundary Conditions:

$$\text{at } z = 0; \quad \rho_{ig,bed} = 0; \quad v_{g,bed} = 0 \quad \text{for all } t > 0 \quad (17a)$$

$$\text{at } z = L; \quad \frac{\partial \rho_{ig,bed}}{\partial z} = 0 \quad \text{for all } t > 0 \quad (17b)$$

Pyrolysed gas generated from the biomass particle flows downward and its velocity is computed using Eq. (4).

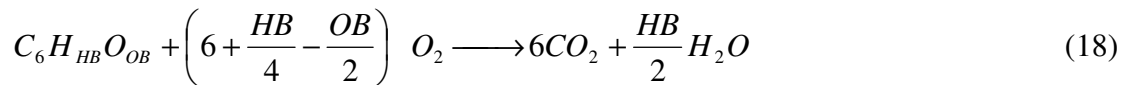
2.2.2 Single Particle

To describe the chemical process of pyrolysis in a single solid particle, an unsteady state one dimensional variable property model of transport phenomena is required. It should include heat (conductive, convective and radiative modes), mass (diffusive and convective modes) and momentum transport of the products formed within the solid (volatiles and gases). Babu and Chaurasia (2003 a-b; 2004 a-d) carried out exhaustive modeling and simulation studies on the pyrolysis of single solid particle. The model developed and modified by Babu and Chaurasia (2003 a-b; 2004 a-d) uses physically measurable parameters and practically explainable kinetic scheme, incorporating the convective and diffusion effects. Babu and Chaurasia (2004c) proposed three models for the pyrolysis of biomass under two categories namely, (1) Generalized reference model (Model-I), and (2) Simplified models (Model-II & Model-III). In most practical situations of industrial pyrolysis reactions, the contributions of the bulk motion of gases inside the pores of the particle are insignificant. Because the resistance offered by the pores in the

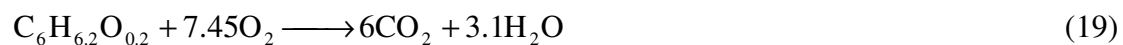
solid particle is so high, the transport of these gases would take place essentially by a diffusion mechanism but not by bulk motion (i.e. convection). Taking this situation into consideration, Model –II is used in the present study, which is based on the assumption that there is no bulk motion contribution (i.e. convective transport is neglected) to the temperature profile and the product yield predictions.

2.3 Combustion

The biomass present in the oxidation zone reacts with oxygen to form carbon dioxide, which provides heat for the subsequent gasification reactions. In complete combustion, carbon present in biomass is completely converted to carbon dioxide while hydrogen is converted to water vapor. It is an exothermic reaction and yields temperatures in the range of 1000 °C to 1500 °C. In the present model, complete combustion of biomass is assumed which can be ensured by supplying excess air (usually around 20%) than stoichiometrical requirement. The combustion reaction therefore is represented as given by Eq. (18)



The volatile products generated in the pyrolysis zone flow downwards and enter into the oxidation zone where a part of volatiles gets oxidized. It is assumed that the tar present in the pyrolysed gas mixture completely gets decomposed due to very high temperature present in the oxidation zone. The tar decomposition is represented by Eq. (19).



2.4 Reduction

The main components of the gaseous mixture leaving the combustion zone are carbon dioxide, water vapor, inert nitrogen, carbon monoxide, hydrogen and some amount of low molecular weight hydrocarbons such as methane, ethane, ethylene etc. In the reduction zone, the gaseous mixture passes through the hot porous charcoal bed resting above the grate. The reduction zone is often referred as gasification zone. Giltrap et al. (2003) developed a model of reduction zone of downdraft biomass gasifier to predict the composition of producer gas under steady state operation. The accuracy of the model is limited by the availability of data on the initial conditions at the top of the reduction zone. Moreover they assumed that the char reactivity factor (*CRF*) which represents the

reactivity of char and the key variable in simulation is constant throughout the reduction zone. Giltrap's model (2003) is modified by incorporating the variation of CRF along the reduction zone of downdraft biomass gasifier in our earlier study (Babu and Sheth, 2006). It is assumed that CRF is exponentially increasing along the bed length of the reduction zone. Solid carbon in the form of char is assumed to be present throughout the reduction zone. Modeling equations of single particle model of pyrolysis (Babu and Chaurasia, 2004c) and reduction model proposed by Babu and Sheth (2006) are not presented in the present article to reduce the length of the article.

3. Experimental Studies

The main equipment of the experimental set up is an Imbert downdraft biomass gasifier. An Imbert downdraft biomass gasifier is the one, which has throated combustion zone and different diameter for pyrolysis and reduction zones unlike stratified downdraft biomass gasifier in which diameter of the gasifier is uniform through out (Reed and Das, 1988). Biomass is fed from top of the gasifier and air is introduced through nozzle in the combustion zone. The downdraft gasifier converts the solid biomass into a combustible gas, generally known as a producer gas. Biomass undergoes pyrolysis and gets oxidized in the combustion zone near air inlet. The pyrolysed gas mixture and the gases produced due to combustion passes over the charcoal bed resting above the grate and generate producer gas. The details of the experimental set up, procedure and operating variables are reported in our earlier study (Sheth and Babu, 2009b).

4. Results and Discussion

The experimental data reported in our earlier study (Sheth and Babu, 2009b) are used to validate the simulation results of the complete combined transport and kinetic model. The initial moisture content fraction, air flow rate, temperature of the pyrolysis zone, and chemical composition of the biomass are required as an input data for the model to predict the composition of producer gas. The combined transport and kinetic model is validated using the parametric values as given in Table-1.

Table 1 Details of the biomass gasification experiments

Experimental No	Air flow rate (m ³ /h)	Initial moisture content (wt fraction, wet basis)	Biomass consumption Rate (kg/h)	Equivalence ratio(Φ)
1	2.7765	0.1145	2.10	0.2533
2	3.3935	0.0437	3.63	0.1791
3	1.8510	0.0437	2.12	0.1673
4	2.7765	0.0437	2.67	0.1992
5	2.7765	0.073	2.59	0.2054
6	1.8510	0.10	1.00	0.3546
7	2.7765	0.1518	2.20	0.2418
8	2.1595	0.07	1.488	0.278
9	2.1595	0.044	2.12	0.1951
10	2.1595	0.1167	1.1626	0.3558
11	2.1595	0.164	1.0424	0.3968

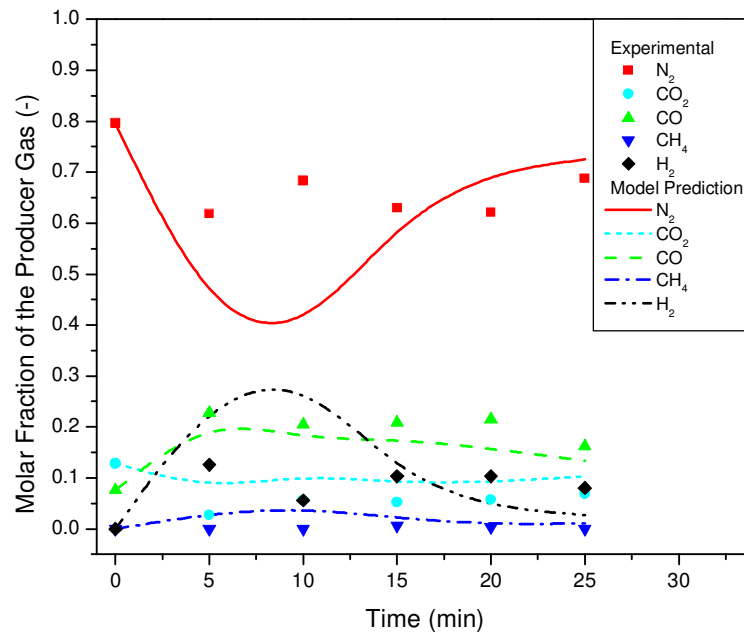


Fig. 1 Comparison of model predicted producer gas composition with experimental values of the present study ($\Phi = 0.2533$)

The variation of molar fraction of producer gas components with time is predicted and compared with the experimental data. Fig. 1 show the comparison of model predicted molar fractions of producer gas components with those found experimentally for an equilibrium ratio of 0.2533. It is found that the model predicted molar fraction of nitrogen decreases first during the few initial minutes (5-10 min) of gasification. After that it increases and attains a steady value (after 10-15 min). The molar amount of nitrogen is constant for a particular flow rate of air as nitrogen acts as an inert but its composition varies due to the changes in molar amount of other components of gaseous mixture. It is found that the model predicted molar fractions of carbon monoxide and hydrogen increase first with time and after that it decreases and attains a steady value. It is observed that the model predicted molar fraction of methane is very less and almost remains constant. It is also found that the model predicted molar fraction of carbon dioxide decreases a little and attains a steady value.

The simulation results of the molar composition of various components of the producer gas match well with the experimental data of 10 minutes or higher from the start of run. For the experimental data of 5 min and 10 min, the simulation results differ more. This is because of the assumption taken in the model that all the gas generated in pyrolysis or reduction zone travel downwards in the gasifier. However, it is observed while carrying out the experiments that the gas produced in the pyrolysis zone first travels upwards and occupies the empty space above the biomass. After 5 - 10 minutes from the start of the run, the accumulated gas builds up a pressure and the producer gas gets started flowing downwards. Because of this, the model predicts higher concentration of hydrogen and carbon monoxide and lower concentration of nitrogen in comparison to the experimental data for initial 5 -10 minutes from the start of a particular experimental run. Fig. 2 shows the model predicted composition profile of gaseous phase across the gasifier at 5 min from the start of the experiment for the first run of the present study. Figs. 3 and 4 show the similar profiles at different times from the start of the experiment (run 1). The pyrolysis zone in the gasifier is represented by first 100 mm, oxidation zone by 100 to 140 mm and reduction zone by 140 to 270 mm in Figs. 2 to 4.

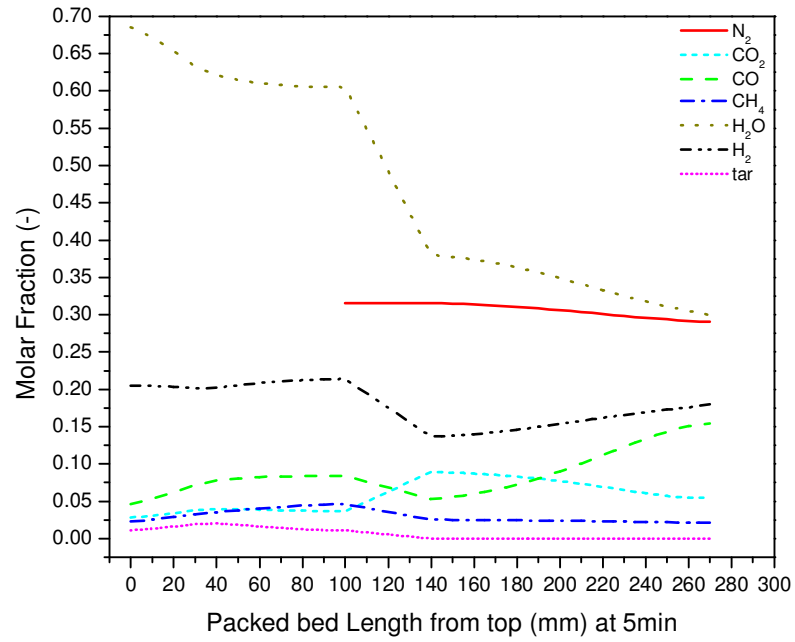


Fig. 2 Simulated composition profile across the gasifier at 5 min from the start of the experiment for the present study ($\Phi = 0.2533$)

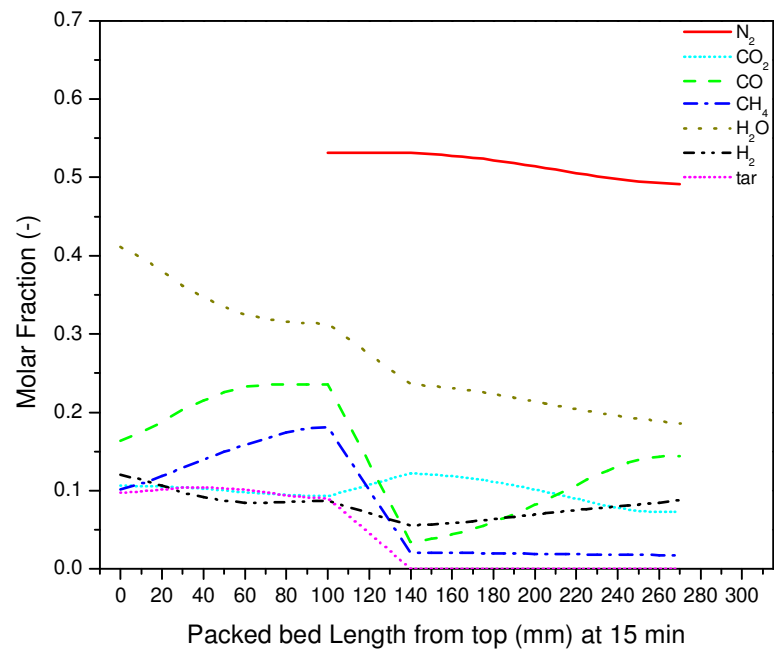


Fig. 3 Simulated composition profile across the gasifier at 15 min from the start of the experiment for the present study ($\Phi = 0.2533$)

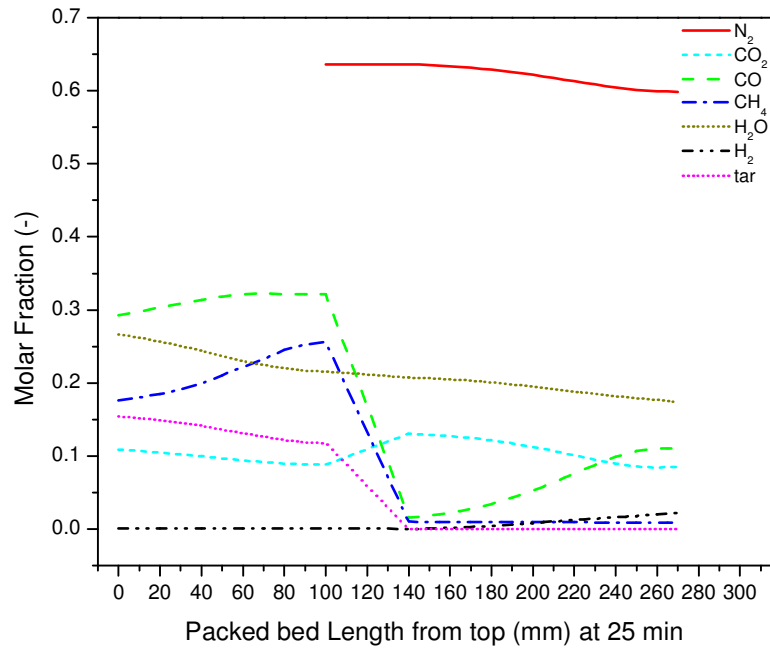


Fig. 4 Simulated composition profile across the gasifier at 25 min from the start of the experiment for the present study ($\Phi = 0.2533$)

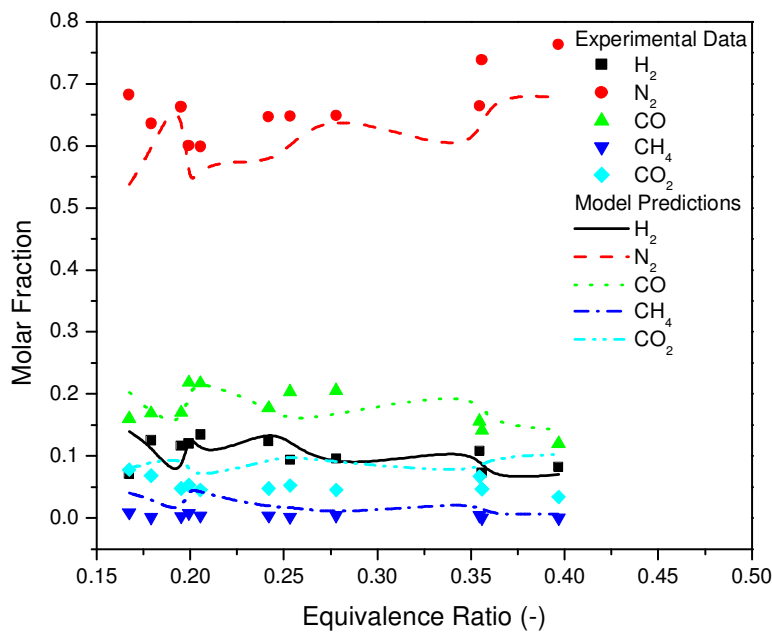


Fig. 5 Comparison of experimental data of present study with model predicted composition of producer gas

It shows the variation of molar fraction of the main components of the producer gas, i.e. nitrogen, carbon monoxide, carbon dioxide, methane, water vapor, hydrogen, and tar, with time in the gasifier. It is found that the composition of water vapor in the gaseous phase is the highest in pyrolysis zone (0-100 mm) and decreases in oxidation zone (100-140 mm) and reduction zone (140-270 mm) of the gasifier, when it travels through these zones (Figs. 2 to 4). It is also observed that the molar fraction of water vapor decreases with time in all zones of the gasifier. The molar fractions of CO and CH₄ in the gaseous phase increase in the pyrolysis zone as gas travels through it.

It is found that the molar fractions of CO, H₂, and CH₄ decrease in oxidation zone due to combustion. The molar fraction of CO₂ increases and that of tar decreases due to the high temperature oxidation. The molar fraction of nitrogen almost remains constant in the oxidation zone due to the constant supply of air. In the reduction zone of gasifier, the molar fractions of CO and H₂ increase and those of CO₂ and N₂ decrease. The molar flow rate of nitrogen does not change but due to the water gas reaction, methane formation reaction, and Boudouard reaction, formation of hydrogen and carbon monoxide occurs and the composition of nitrogen decreases in the reduction zone.

It is also found that the composition of carbon monoxide, methane, hydrogen and tar increases and that of water vapor decreases with time in the pyrolysis zone of the gasifier due to successive increase in the temperature of the pyrolysis zone. The simulated composition profiles shown in Figs. 2 to 4 at different times from the start of the experiment give proper insight of the gasifier. These simulated variations of the molar fraction of gaseous components with time match with the theory of downdraft biomass gasification. To study the variation of the simulated composition of the combined transport and kinetic model with equivalence ratio, the composition of producer gas is averaged over 25 minutes. Fig. 5 shows the comparison of the average composition of producer gas with those found experimentally as a function of equivalence ratio.

5. Conclusions

Based on the results obtained in the present study, the following conclusions are drawn:

1. The proposed combined transport and kinetic model is successfully validated with the experimental data reported in the literature.

2. The model predicted composition of producer gas matches very well with the experimental data reported in the literature.
3. The molar fractions of CO, CH₄ and tar increase and that of water vapor decreases with time in the pyrolysis zone of the gasifier due to a subsequent increase in the temperature of pyrolysis zone.
4. The molar fraction of water vapor in the gaseous phase is the highest in the pyrolysis zone and decreases as it travels through the oxidation and reduction zones of the gasifier.
5. The molar fractions of CO and CH₄ in the gaseous phase increase in the pyrolysis zone as gas travels through it. However, the molar fractions of CO, H₂, tar, and CH₄ decrease in the oxidation zone due to high temperature oxidation and hence the molar fraction of CO₂ increases.

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