

Simulation of Reduction Zone of a Downdraft Biomass Gasifier

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Abstract

Bio mass gasification has become a common technology now days for the production of synthesis gas. Synthesis gas produced as a result of gasification has many applications. The numerical simulation techniques can be applied to the gasification process to save time and energy from lengthy experimentation. Simulation of reduction zone of a downdraft biomass gasifier was carried out for three different biomasses, Wheat Straw, Rice Husk and Corn Stover. The kinetic parameters were simulated and optimized, based on the maximum yield of CO and H₂, for the three biomass materials under isothermal conditions, using kinetic models over the temperature range of 1000-2000K.

For all three biomasses, the maximum composition of CO and H₂ in producer gas was obtained at a temperature of 1400 K under isothermal conditions. Furthermore, the composition of CO and H₂ and char utilization was at maximum in the case of wheat straw.

Keywords: Gasification, Kinetics, Modeling, Optimization, Reduction, Simulation

Nomenclature

- r_i = rate of reaction i (mol fraction/s)
 A_i = frequency factor for reaction, i
 C_{RF} = char reactivity factor
 E_i = activation energy of reaction, i (J/mol K)
 R = gas constant (J/mol K)
 k_i = rate constant for reaction i
 $K_{eq,i}$ = equilibrium constant for reaction i
 T = temperature (K)
 x_{CO} = mole fraction of CO
 x_{CO_2} = mole fraction of CO₂
 x_{H_2O} = mole fraction of H₂O
 x_{H_2} = mole fraction of H₂
 x_{CH_4} = mole fraction of CH₄

Subscripts

- i reaction number

Introduction

Energy plays a vital role in the development of living standards. The primary sources include fossil fuels, solar energy, biomass, wind energy, hydro energy, tidal energy and geothermal energy. Biomass is becoming the most promising, renewable energy alternative to fossil fuels since it is abundantly available, renewable and environmental friendly [1]. Combustion, Pyrolysis and Gasification are the three methods for thermochemical conversions of biomass [2], among which, Gasification is considered to be an efficient process for the production of energy.

In gasification, the biomass is partially oxidized at elevated temperatures to produce a mixture of gases (mainly CO, H₂, and CO₂), tars (i.e. condensable products) and typical pollutants such as sulphurous compounds. The composition of the effluent gas of the gasifier is affected by a number of factors, including biomass composition, operating

temperature and pressure of the gasifier, the gasifying medium and flow rate, gasifier design. These operating parameters can be manipulated to achieve a high yield of synthesis gas (CO+H₂) instead of the so-called producer gas (i.e. a mixture of CO, H₂, CO₂, CH₄ and N₂). To avoid combustion of biomass, gasification is carried out at a higher temperature, with a controlled amount of oxidizing agent [2]. The reaction temperature controls the reaction rates and the directions of various reactions and, hence, the efficiency of thermochemical conversion [3]. A typical gasifier consists of (a) pyrolysis zone, (b) oxidation zone, and (c) reduction zone. Common types of gasifiers include updraft, downdraft, cross flow, and fluidized bed gasifiers. In the downdraft design, pyrolysis and combustion occurs simultaneously and tar production is low, while the pyrolysis, oxidation and reduction reactions take place in separate regions in updraft designs. The schematic diagram of a typical downdraft biomass gasifier is shown in Fig. 1 [3].

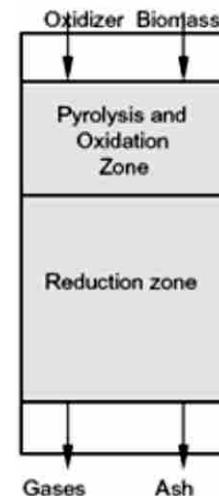


Figure 1: Downdraft Gasifier

The reduction zone is the most significant zone in a gasifier for the production of producer gas since the reactions in reduction zone are slow and control the overall conversion of biomass [3]. Extensive research has been done on the reduction zone of biomass gasifier [4, 5, 6, 7, 8, and 9] using the equilibrium models [3, 5, 9, and 10] as well as the kinetic models [8].

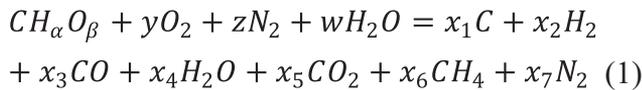
The present study is aimed towards the optimization of the reduction zone process, using kinetic models, under isothermal conditions for three biomass; Wheat Straw, Rice Husk and Corn Stover, to maximize CO and H₂ composition among the different components of producer gas.

Methodology

Kinetic rate models were selected for the reduction zone of the gasifier. Initial conditions were specified for the rate models, the equilibrium constants and rate constants were calculated and the models were simulated using Fourth-Order Runge-Kutta Method in Matlab 7.0 [11].

Initial Conditions

The initial temperature of the reduction zone was taken as 1000 K since the temperature variation lies in the range 1000–2000 K in the reduction zone. Rate constants and equilibrium constants were calculated in this temperature range to evaluate the residence time for the reduction zone. Char reactivity factor, C_{RF}, affects the extent of reactions in reduction zone. The value of C_{RF} was taken as 100 [6]. The conditions at the exit of the pyrolysis zone were taken as the initial conditions of the reduction zone. The overall process of gasification can be represented by a single reaction as [12]:



Where CH_αO_β is the chemical representation of dry biomass (α and β were evaluated from ultimate analysis of biomass feedstock) and y, z, w, x_i are molar numbers of components.

At t = 0 when the reactants enter into the reduction zone, the initial compositions of CO and H₂ entering in the reduction zone are assumed to be zero. Also, the nitrogen entering in the gasifier acts as an inert component.

$$x_{2,0} = 0, x_{3,0} = 0, x_{7,0} = z$$

and

$$x_{5,0} + x_{1,0} + x_{6,0} = 1 \quad (2)$$

$$2x_{4,0} + 4x_{6,0} = \alpha + 2w \quad (3)$$

$$x_{4,0} + 2x_{5,0} = 2y + \beta + w \quad (4)$$

The eq. 2, 3, and 4 were simultaneously solved after specifying the compositions from the ultimate analysis of the three biomass materials.

Calculation of Equilibrium Constants and Rate Constants:

The major reactions occurring in the reduction zone of a downdraft gasifier, along with their kinetic rate models

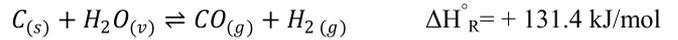
are as follows [5]:

Reaction 1: Boudouard Reaction



$$r_1 = C_{RF}k_1 \left(x_{CO_2} - \frac{x_{CO}^2}{K_{eq,1}} \right) \quad (5)$$

Reaction 2: Water Gas Reaction



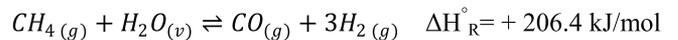
$$r_2 = C_{RF}k_2 \left(x_{H_2O} - \frac{x_{CO}x_{H_2}}{K_{eq,2}} \right) \quad (6)$$

Reaction 3: Methanation Reaction



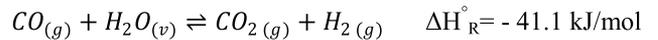
$$r_3 = C_{RF}k_3 \left(x_{H_2}^2 - \frac{x_{CH_4}}{K_{eq,3}} \right) \quad (7)$$

Reaction 4: Steam Reforming Reaction



$$r_4 = C_{RF}k_4 \left(x_{CH_4} \cdot x_{H_2O} - \frac{x_{CO}x_{H_2}^3}{K_{eq,4}} \right) \quad (8)$$

Reaction 5: Water Gas Shift Reaction



$$r_5 = C_{RF}k_5 \left(x_{CO} \cdot x_{H_2O} - \frac{x_{CO_2}x_{H_2}}{K_{eq,5}} \right) \quad (9)$$

CO and H₂O are converted into CO₂ and H₂ in the water gas shift reaction (equation 9). The shift reaction does not affect the rate for particular moisture to biomass ratio [12], but is included in the current study since it is one of the gasification reactions [1].

The equilibrium constants, K_{eq,i}, and rate constants, k_i, for the five reactions (equations 5–9) of reduction zone were calculated. The rate equations were then simulated using numerical simulation technique. As a result, compositions of the components char (C), CO, CO₂, H₂O, CH₄ and H₂ were obtained under isothermal conditions. The kinetic rate models were simulated and the maximum yield of CO and H₂ was optimized.

Since the equilibrium constant is a temperature dependent factor, it was calculated using the Gibbs Function [3]. The relation for the equilibrium constants for five reactions (equations 5–9) can be given as:

$$K_{eq,1} = e^{-\left(\frac{\Delta G_1^{\circ}(T)}{RT}\right)} = e^{-\left(2\frac{g_{CO}^{\circ}(T)}{RT} - \frac{g_{CO_2}^{\circ}(T)}{RT} - \frac{g_C^{\circ}(T)}{RT}\right)} \quad (10)$$

$$K_{eq,2} = e^{-\left(\frac{\Delta G_2^{\circ}(T)}{RT}\right)} = e^{-\left(\frac{g_{CO}^{\circ}(T)}{RT} + \frac{g_{H_2}^{\circ}(T)}{RT} - \frac{g_{H_2O}^{\circ}(T)}{RT} - \frac{g_C^{\circ}(T)}{RT}\right)} \quad (11)$$

$$K_{eq,3} = e^{-\left(\frac{\Delta G_3^{\circ}(T)}{RT}\right)} = e^{-\left(\frac{g_{CH_4}^{\circ}(T)}{RT} - 2\frac{g_{H_2}^{\circ}(T)}{RT} - \frac{g_C^{\circ}(T)}{RT}\right)} \quad (12)$$

$$K_{eq,4} = e^{-\left(\frac{\Delta G_4^{\circ}(T)}{RT}\right)} = e^{-\left(\frac{g_{CO}^{\circ}(T)}{RT} + 3\frac{g_{H_2}^{\circ}(T)}{RT} - \frac{g_{H_2O}^{\circ}(T)}{RT} - \frac{g_{CH_4}^{\circ}(T)}{RT}\right)} \quad (13)$$

$$K_{eq,5} = e^{-\left(\frac{\Delta G_5^\circ(T)}{RT}\right)} = e^{-\left(\frac{g_{CO}^\circ(T)}{RT} + \frac{g_{H_2O}^\circ(T)}{RT} - \frac{g_{H_2}^\circ(T)}{RT} - \frac{g_{CO_2}^\circ(T)}{RT}\right)} \quad (14)$$

While,

$$\frac{g_i^\circ(T)}{RT} = Ag_i + Bg_iT + Cg_iT^2 + Dg_iT^3 + Eg_iT^4 + \frac{Fg_i}{T} + Gg_i \ln T \quad (15)$$

The data for the constants A, B, C, D, E, F and G in eq. 10 - 15 was taken [4], equilibrium constants were calculated over a range of temperature and graphs were plotted (Fig. 2 and 3).

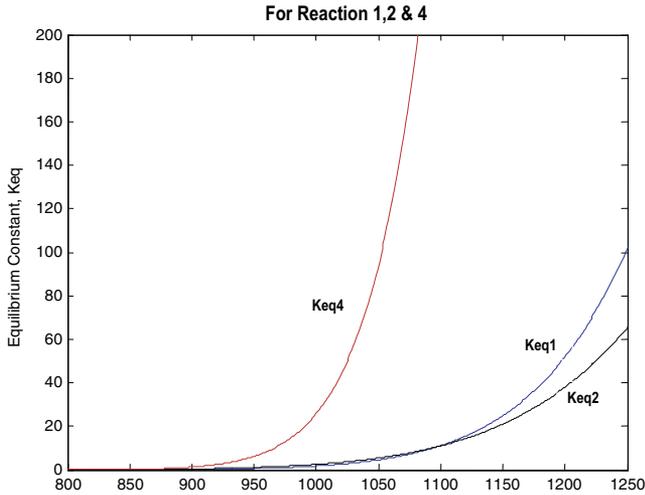


Figure 2: K_{eq} for Endothermic Reactions

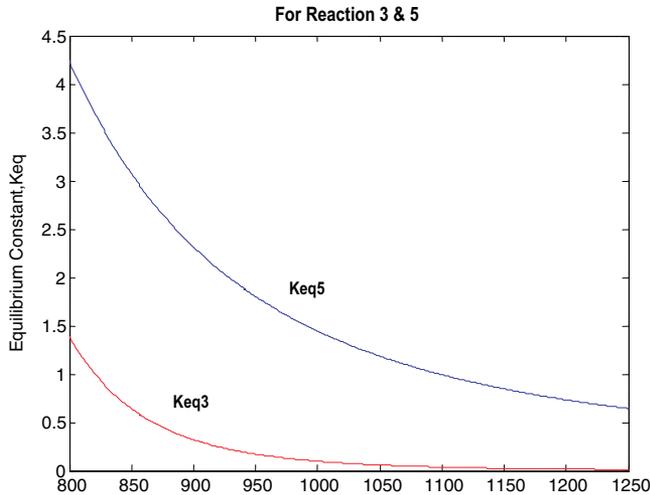


Figure 3: K_{eq} for Exothermic Reactions

As evident from Fig. 2 and 3, the values of equilibrium constants increased with the increase in temperature for endothermic reactions, while, the reverse was true for exothermic reactions.

The temperature dependency of the rate constant is given by Arrhenius Law. For equations 5 - 9 of the reduction zone, the rate constants were calculated using activation energy (A_i) and frequency factor (E_i) data [1], and the resultant values are provided in Table 1:

Table 1: Activation Energy and Frequency Factor Data

Reaction	Activation Energy A_i (1/s)	Frequency Factor E_i (kJ/mol)
Reaction 1: Boudouard Reaction	3.616×10^1	77.39
Reaction 2: Water Gas Reaction	15170×10^4	121.62
Reaction 3: Methanation Reaction	4.189×10^{-3}	19.21
Reaction 4: Steam Reforming Reaction	7.301×10^{-2}	36.15
Reaction 5: Water Gas Shift Reaction	2.842×10^{-2}	32.84

The values of rate constant were calculated for a range of temperature and graph was plotted (Figure 4). The trend of Fig. 4 was in accordance with the reported literature [12].

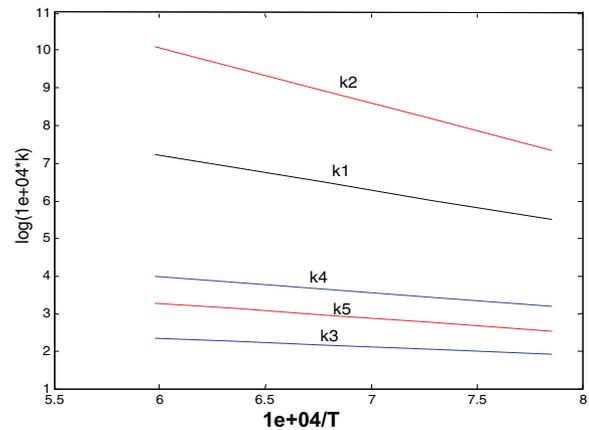


Figure 4: Rate constants for Reduction Reactions

Simulation of Kinetic models:

The initial values of temperature, char reactivity factor, equilibrium constant and the rate constant were substituted in the rate equations (equations 5 - 9) of the reduction reactions. The kinetic models were simulated, using Fourth Order Runge-Kutta method in Matlab-7.0, to calculate the producer gas composition leaving the reduction zone. Under isothermal conditions, the rate equations were simulated for all biomasses in the temperature range of 1000 -2000 K with an increment of 100 K. Rate of formation of producer gas for the three biomass materials was calculated. The temperature, at which the maximum production of $CO + H_2$, i.e. the synthesis gas, was achieved, was determined and designated as optimum temperature. The rate equations were simulated at the optimum temperature to get final composition of the producer gas having the following components: *char*, *CO*, *CO₂*, *H₂O*, *CH₄* and *H₂*.

Results and Discussions

The simulation of kinetic rate models under isothermal

conditions requires the calculation and selection of equilibrium constants and rate constants. Char reactivity factor was selected and a temperature range of 1000-2000 K was defined. Substitution of all the parameters in the model equations and subsequently simulating them using Runge-Kutta method in MATLAB-7 facilitated the evaluation of producer gas composition. The inlet composition of synthesis gas was zero. The final compositions of CO and H₂ were obtained for time range of 10 seconds, from the composition data. Using these values, rate of formation of producer gas was calculated at different temperature. The optimum temperature was selected as that temperature where the maximum production of CO and H₂ was obtained. The simulation of models was performed for the optimum value of temperature to get final producer gas composition and final reduction time.

Composition curves obtained for all three materials; *Wheat Straw*, *Rice Husk* and *Corn Stover*, for isothermal conditions are shown in Fig. 5. It was observed from Fig 5 that the rate of formation of CO sharply increased in the temperature range of 1000-1200K, after which, the increase was trivial. After 1400K, there was no effect of temperature on the production of CO. For H₂, the production was high in the range of 1000-1100K, after which, the increase was trivial from 1100 – 1300 K. The overall optimum temperature was taken to be 1400K since after this temperature, increasing the temperature of the reduction zone had no substantial effect on the composition of CO and H₂ in producer gas.

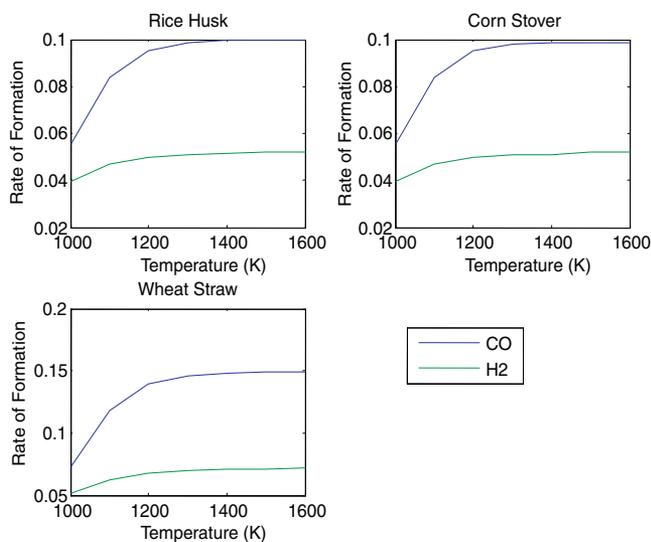


Figure 5: Rate of formation of CO and H₂ vs. temperature for different biomass materials under isothermal conditions

The kinetic models were again simulated at the optimum temperature of 1400 K and the final producer gas compositions were calculated for the three biomass materials. The plots of these compositions are shown in the Fig. 6.

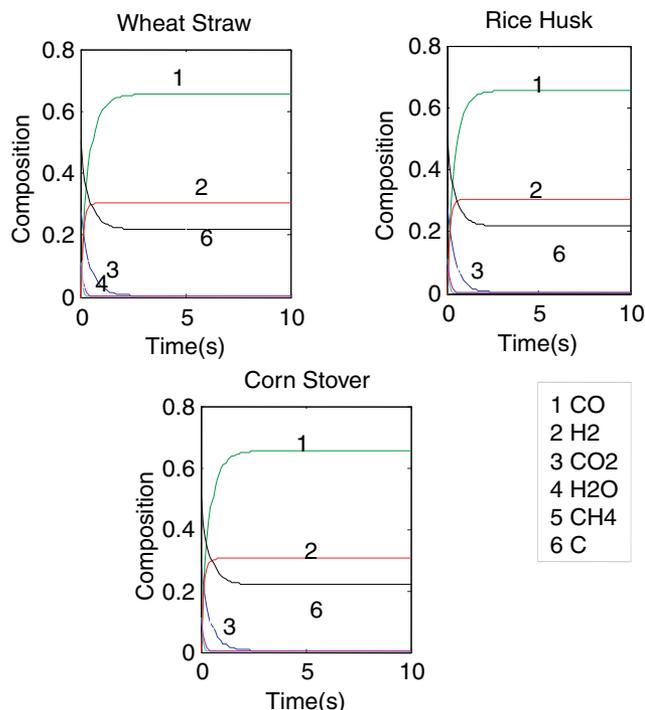


Figure 6: Composition curves for the three Biomass materials under isothermal condition, at optimum temperature of 1400K

All the parameter including optimum temperature, final reduction time and the final composition of producer gas components, obtained as a result of the simulation of kinetic models, are summarized in Table 2.

Table 2: Optimum values of different parameters as a result of Reduction of different biomass under Isothermal conditions

Optimum Parameters	Wheat Straw	Corn Stover	Rice Husk
Optimum Temperature, K	1400.0	1400.0	1400.0
Final Reduction Time, sec	4.000	4.000	4.000
Final Composition of CO ₂	0.0039	0.0017	0.0033
Final Composition of CO	0.7079	0.6433	0.5491
Final Composition of H ₂	0.3121	0.3320	0.2567
Final Composition of H ₂ O	0.0040	0.0019	0.0048
Final Composition of CH ₄	0.0021	0.0011	0.0036
Final Composition of Char (C)	0.0184	0.0125	0.1995

A comparison of the final composition of the producer gas at the end of reduction zone is provided in Fig. 7. It was seen that the composition of CO and H₂ was high as they were produced in the reduction zone, while the composition of CO₂, H₂O and CH₄ had reduced. It was also observed that the composition of char (C) was different for different biomass materials and was highest in the case of rice husk. It is also evident from Fig. 7 that the maximum H₂ and CO content and minimum char production was achieved in the case of wheat straw.

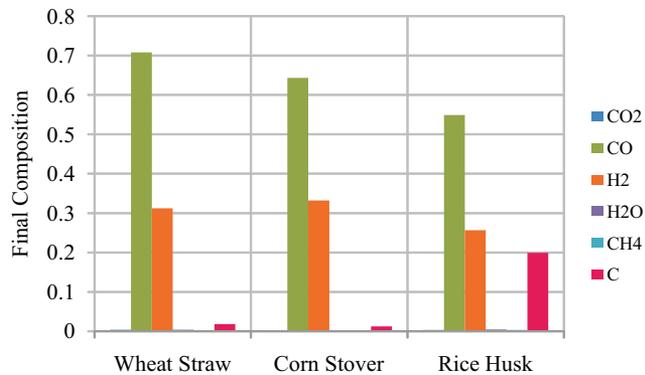


Figure 7: Comparison of final composition of the producer gas for different biomass materials under isothermal conditions at optimum temperature $T=1400$ K

Conclusions

Kinetic models were selected as rate equations for the modeling of different reactions taking place in the reduction zone of downdraft biomass gasifier. After specifying the initial temperature and compositions, the kinetic models were solved under isothermal conditions for three different biomass materials, wheat straw, rice husk and Corn Stover. The trends obtained for the equilibrium and rate constants were in well agreement with the previously reported data, the small differences occurred due to different range of temperature and different finishing criteria. The composition curves obtained were optimized on the basis of the maximum contents of CO and H₂ in producer gas. For isothermal conditions, the kinetic models of reduction reactions were simulated over the temperature range of 1000-2000K by taking a step size 100 K. Maximum producer gas composition was obtained at a temperature of 1400 K under isothermal conditions all three biomass materials. The CO and H₂ in producer gas were at maximum and char production was at a minimum in the case of wheat straw.

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