

# Simulation and optimization of the steam gasification process using CPFDF

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## Abstract

Steam gasification is a well-known technology, which is used to produce a high quality product of gas, especially for power generation applications. The gas composition, gas quality and the purity has a great role to play depending on the end application. Hence the bio mass steam gasification process was studied using the Computational Particle Fluid Dynamics (CPFDF) simulation tool, 'Barracuda VRTM'. The software is well suited for simulating dense particle laden fluids due to its numerical solving methods for both the particles and the fluid.

Both the experiments and simulations were carried out for a cylindrical isothermal fluidized bed reactor without chemistry, to compare the deviations of simulation results from the experimental results. The simulation results were agreed with the experimental results and they confirmed the same minimum fluidization velocity.

Three dimensional simulations were carried out for a cylindrical geometry to study energy, and momentum transport within a simplified dual fluidized bed steam gasification reactor and the important chemistry were included. According to the simulation results, the product gas mainly consisted of CO and the amount of H<sub>2</sub> was less in comparison to the higher amounts of CH<sub>4</sub>. The cumulative production of combustible gasses (CO, CH<sub>4</sub> and H<sub>2</sub>) was estimated as 280 Sm<sup>3</sup>/day based on the simulation results.

*Keywords: bio mass steam gasification, Barracuda, CPFDF, product gas.*

## 1 Introduction

There is a growing demand for renewable energy options in the world due to the negative environmental impacts of fossil fuels, also in terms of energy security. Biomass is a choice for many nations when they set their renewable energy



targets due to its lesser environmental impacts. There are many types of biomass resources including wood and wood wastes, agricultural crops and their waste byproducts, municipal solid waste, animal wastes, waste from food processing, aquatic plants and algae [1]. But it is important that the harnessing of chemical energy stored in biomass should be environmentally and economically sustainable.

Biomass steam gasification is a promising technology which has the ability to produce a quality product gas which comprises of  $H_2$ ,  $CO$ ,  $CO_2$ ,  $CH_4$  and  $H_2O$  with a negligible amount of  $N_2$  and heavy hydrocarbons. This product gas has a medium calorific value, which ranges from 12–14 MJ/Nm<sup>3</sup> and this is far better than the low calorific product gas resulting from air gasification [2]. The steam gasification process is involved with a number of endothermic reactions and demands for energy. Being an allothermal process, steam gasification requires energy to be supplied externally [3]. Hence dual fluidized beds have been developed as a solution to overcome this challenge by providing the required heat energy in to the gasification reactor [4].

The dual fluidized bed (DFB) technology enables the separation of the combustion zone from the gasification zone. In this process the biomass gasification occurs in the gasifier and the non-converted char is sent into the combustor with circulated bed materials, where the combustion reactions take place amongst remaining char and air. This produces the necessary heat energy to supply the gasifier in the form of recirculated hot bed materials [5]. The temperature in a fluidized bed gasification zone is typically around 850°C (1123K) [6].

The gasification process in fluidized bed gasifiers consists of initial drying; fast pyrolysis of solid fuel and gasification of resultant chars [7]. Due to the proper mixing, fluidized beds provide enhanced gas solid contact which ultimately leads to high reaction rates and conversion efficiencies [8]. In fluidized bed gasifiers, the pyrolysis step is a short process that generates basically solid char and volatile gases. But during the gasification stage it involves a series of heterogeneous reactions that occurs between gasification agent and reactants as well as resultant gases and reactants [7]. It is possible to have homogeneous reactions among the generated gas species too. Hence gasification is a much slower process in comparison to the initial pyrolysis and it is dominant throughout the whole gasification process [9]. For a successful design and operation of a gasification reactor it is important to have a thorough knowledge regarding to the influence of fuel and operating parameters on the process [8]. The fuel composition, size of feed biomass, operating temperature, steam flow rate and temperature, bed material, use of catalysts and change of many other variables might affect the gasification process significantly.

Biomass steam gasification involves particulate multiphase flows and different methods have been used to model such cases. The CPFD approach is suitable for modeling reacting, thermal, particle laden fluid flows regardless of the solid volume fraction in the fluid [10]. It incorporates the numerical methodology called ‘multi-phase-particle-in-cell’ (MP-PIC) [11]. This is a hybrid numerical method that uses Eulerian computational grid for solving the



fluid phase and Lagrangian computational particles for modeling the solid phase [10]. The CPFD approach enables to solve the fluid and particle equations in three dimensions. Averaged Navier-Stokes equations which are strongly coupled with particle phase are used to describe the fluid dynamics while particle momentum equations follow the MP-PIC formulation [11]. The averaged form of the detailed mass and momentum equations are used to deduct the fluid phase mass and momentum equations, while in the MP-PIC method, the dynamics of the particle phase is predicted by solving a transport equation on the particle distribution function [10]. Barracuda VR<sup>TM</sup>, the commercial software used in this study, includes the CPFD approach for solving particle laden fluid flows. This study focuses on the simulation of biomass steam gasification using Barracuda software and the reader is referred to the study done by Snider *et al.* [10] for more details regarding to the model equations and the numerical solution.

## 2 Experiments and simulations

### 2.1 Experimental verification of simulation results

An experiment was performed to check for the deviation of simulation results from the reality. The test rig of a fluidized bed was used for the experiment. Glass beads were the bed material and air was the fluidizing agent. There were pressure sensors placed in the bed and six pressure sensors were considered from 3 cm, 13 cm, 23 cm, 33 cm, 43 cm and 53 cm away from the air distributor respectively. The height of the bed material was 52.5 cm. The bed material particle distribution was known to be 300–400  $\mu\text{m}$  and got confirmed by sieve analysis.

The air flow was adjusted to give the required air velocity into the bed and the pressure sensors were connected to a “LabVIEW” program for data acquisition. The pressure readings were recorded by the pressure sensors corresponding to each air flow rate.

The simulations were run under the same conditions as in the experiment (same geometry, same size range of bed materials, same inlet velocities, isothermal and without chemical reactions) using ‘Barracuda’.

### 2.2 Simulation of cellulosic biomass gasification

#### 2.2.1 Geometry and Mesh

A cylindrical geometry of 8.4 cm diameter and 140 cm height was considered for the gasification reactor. The geometry was drawn using ‘Solid works’ software, imported to ‘Barracuda’ as ‘.STL’ file and meshed so that it has 4408 total number of real cells. Five streams were considered as steam input, biomass input, hot bed material recycle, char and bed material out and product gas out from the top surface. The geometry and the input output streams are shown in Figure 1.



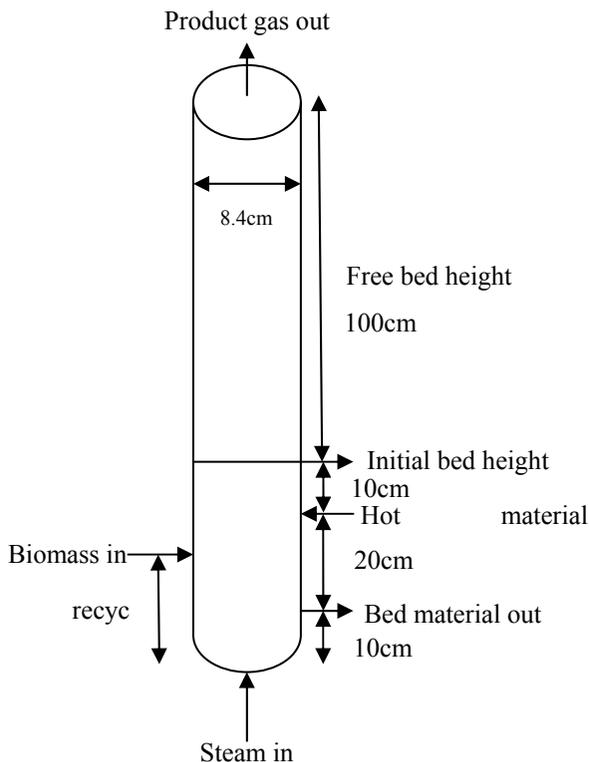


Figure 1: The simulation setup.

### 2.2.2 Assumptions

The simulations are based on the following assumptions:

- Concerning the absence of air in the reactor, combustion reactions are neglected.
- Biomass is broken in to 65% volatile gases and 35% char in the pyrolysis stage [12].
- Biomass is well dried and the water content is negligible.
- There's negligible Sulfur and Nitrogen content in the biomass fuel.
- Biomass char is considered as mainly the pure carbon [13, 14].
- The biomass particles become 1/10th of their size when it becomes char after releasing its volatile compounds.
- According to Stefan Kern *et al.* [3], for a circulated fluidized bed steam gasification reactor, the carbon conversion is typically higher than 99% for the whole system, when the char present in the product gas stream is neglected.
- Gasification occurs at the temperature of 850°C (1123K) [6].
- Product gas mainly contains CO, CO<sub>2</sub>, H<sub>2</sub>, CH<sub>4</sub> and H<sub>2</sub>O gases only.

### 2.2.3 Input data

The input data for the simulation case is shown in Table 1.

Table 1: Input data for the simulation.

Steam temperature(K)	900
Steam pressure(Pa)	$1 \cdot 10^5$
Steam inlet velocity at the bottom of reactor(m/s)	0.1
Feed biomass flow rate (kg/h)	36
Steam flow rate at biomass inlet(kg/h)	10
Particle size of feed biomass( $\mu\text{m}$ )	1000
Bulk Density of biomass( $\text{kg}/\text{m}^3$ )	180
Bulk Density of bed material( $\text{SiO}_2/\text{C}$ ) ( $\text{kg}/\text{m}^3$ )	2190
Size of bed materials ( $\mu\text{m}$ )	500
Steam flow rate at bed material recycle (kg/h)	10
Hot bed material recycle(kg/hr)	36
Temperature of recycle materials ( $^{\circ}\text{C}$ )	1200
Allowed steam leakage at char out let(kg/h)	$3.6 \cdot 10^{-17}$
Close pack volume fraction of particles	0.6
Particle/ fluid slip ratio	0.5

### 2.2.4 Chemistry

Pyrolysis occurs at the initial stage prior to the gasification stage and the released gas composition of volatile gases was recalculated from the data taken from literature [15]. These pyrolysis data had been found for Birch wood with nearly 30% char generation and tar released conditions. Hence the recalculated data are approximations and mentioned in the Table 2.

Four equilibrium chemical reactions were considered to occur within the gasification reactor. The equations are presented in Table 3.

Table 2: Pyrolysis gas compositions.

Gas component	Mass fraction (wt %)
CO	0.48
CO <sub>2</sub>	0.343
H <sub>2</sub>	0.011
CH <sub>4</sub>	0.166

Table 3: Chemical reactions and reaction rate data [10].

Reaction	Reaction rate
$C(s) + H_2O \xrightleftharpoons[r_{1b}]{r_{1f}} CO + H_2$	$r_{1f} = 1.372m_s T \exp\left(\frac{-22645}{T}\right) [H_2O]$
	$r_{1b} = 1.044 \times 10^{-4} m_s T^2 \exp\left(\frac{-6319}{T} - 17.29\right) [H_2][CO]$
$C(s) + CO_2 \xrightleftharpoons[r_{2b}]{r_{2f}} 2CO$	$r_{2f} = 1.272m_s T \exp\left(\frac{-22645}{T}\right) [CO_2]$
	$r_{2b} = 1.044 \times 10^{-4} m_s T^2 \exp\left(\frac{-2363}{T} - 20.92\right) [CO]^2$
$0.5C(s) + H_2 \xrightleftharpoons[r_{3b}]{r_{3f}} 0.5CH_4$	$r_{3f} = 1.368 \times 10^{-3} m_s T \exp\left(\frac{-8078}{T} - 7.087\right) [H_2]$
	$r_{3b} = 0.151m_s T^{0.5} \exp\left(\frac{-13578}{T} - 0.372\right) [CH_4]^{0.5}$
$CO + H_2O \xrightleftharpoons[r_{4b}]{r_{4f}} CO_2 + H_2$	$r_{4f} = 7.68 \times 10^{10} m_s T \exp\left(\frac{-36640}{T}\right) [CO]^{0.5} [H_2O]$
	$r_{4b} = 6.4 \times 10^9 m_s T \exp\left(\frac{-39260}{T}\right) [H_2]^{0.5} [CO_2]$

### 2.2.5 Boundary conditions and initial conditions

The steam input, biomass input, recycle input and the bed material output points were defined as ‘Flow boundary conditions’. The product gas outlet surface was defined as ‘Pressure boundary conditions’. Initially the tube was defined to be filled with N<sub>2</sub> and initial particles were considered as 20% Carbon and 80% SiO<sub>2</sub>. The initial bed material height was 40 cm.

## 3 Results and discussion

### 3.1 Experimental validation of simulation results

The experimental and the simulation results are plotted in Figure 2 and the results are agreed together. Both the experimental and the simulation results highlight a same minimum fluidization velocity of 0.14 m/s. This result proves that the simulation results are acceptable and the model is used in the future work.

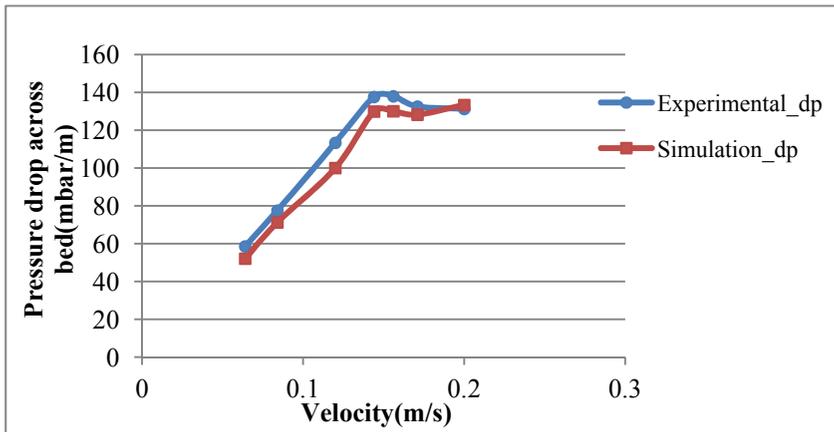


Figure 2: Pressure drop vs. velocity.

### 3.2 Simulation of cellulosic biomass gasification

Simulations were performed by subjecting the cellulosic biomass for steam gasification. The geometry and the input output streams were shown in Figure 1 and the results are discussed.

#### 3.2.1 Gas production

The gas composition of the product gas at the outlet of the reactor during a 20 s time period is shown in Figure 3. The highest fraction of gases was consisted of CO (~40%vol) and the mole fraction of H<sub>2</sub> (~15%vol) was quite less than expected and the CH<sub>4</sub> (~25%vol) was significant. This could be due to the contribution of pyrolysis gasses to generate more CH<sub>4</sub>. On the other hand the available H<sub>2</sub> could have been favorably spent for hydrogenating gasification. The bed material used in the simulations was non catalytic SiO<sub>2</sub> and according to some previous studies [16], the yield of combustible gasses and especially the yield of H<sub>2</sub> could have been enhanced by using other types of catalytic bed materials. In that case the simulation stage would require the specific kinetic data regarding to the specific catalytic material.

As shown in Figure 4, the cumulative gas production of combustible gasses (CO, CH<sub>2</sub>, and H<sub>2</sub>) is around  $65 \times 10^{-3}$  Sm<sup>3</sup> (standard cubic meter). This can be estimated as 280 Sm<sup>3</sup> of combustible gasses per day for a 24hr operating plant.

Average mass fractions of CO, H<sub>2</sub> and the mass fraction of H<sub>2</sub>O across the cross sectional area after 10 seconds of simulation is shown in Figure 5. The mass of the product gas was comprised of nearly 70% H<sub>2</sub>O and the rest was CO, CH<sub>4</sub>, CO<sub>2</sub> and H<sub>2</sub> gasses.

### 3.2.2 Temperature, pressure and velocity

Figure 6(a) shows the temperature distribution across the reactor after 10 seconds of the simulation. The gasification was considered to occur at 850°C (1123K) and the reactor temperature is around this temperature. The cold spots can be seen probably in the areas of endothermic reactions and the point of biomass feed while the hot spot is seen around the point of hot bed material recycle stream. Typically, the recycle stream of the dual fluidized bed gasifiers have a maximum temperature of 100°C above the reactor temperature. Hence some fraction of the products gas is combusted to supply adequate amount of heat energy in to the reactor. But in the simulations it was only the recycling hot bed materials coming from the combustor that supplied the heat energy for the endothermic gasification reactions. Hence the hot bed material recycle stream was assumed to have a temperature of 1200°C (1473K). Figure 6(b) illustrates the pressure distribution and Figure 6(c) shows the velocity vectors across the reactor cross sectional area. The fluid velocity is higher at the feed stream points and across the mid-way of the reactor where the product gas and the extra steam are transported towards the outlet.

### 3.2.3 Reactor mass

The mass of the bed material within the reactor is shown in Figure 7 and there is a gradual decrement of the reactor mass over the time. But this is insignificant in comparison to the simulation time and can be considered as more or less steady over the time. This steady system mass depicts the steady production of combustible gasses.

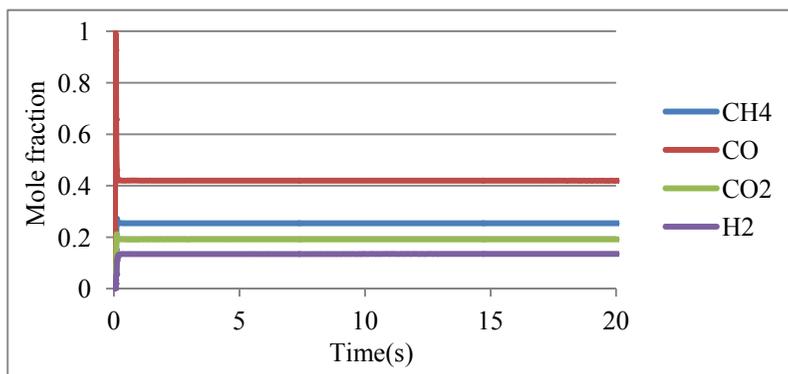


Figure 3: Molar composition of product gas.

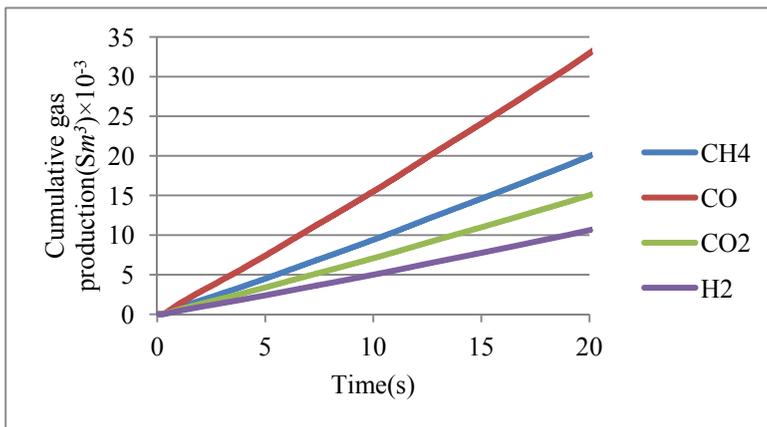


Figure 4: Cumulative gas production.

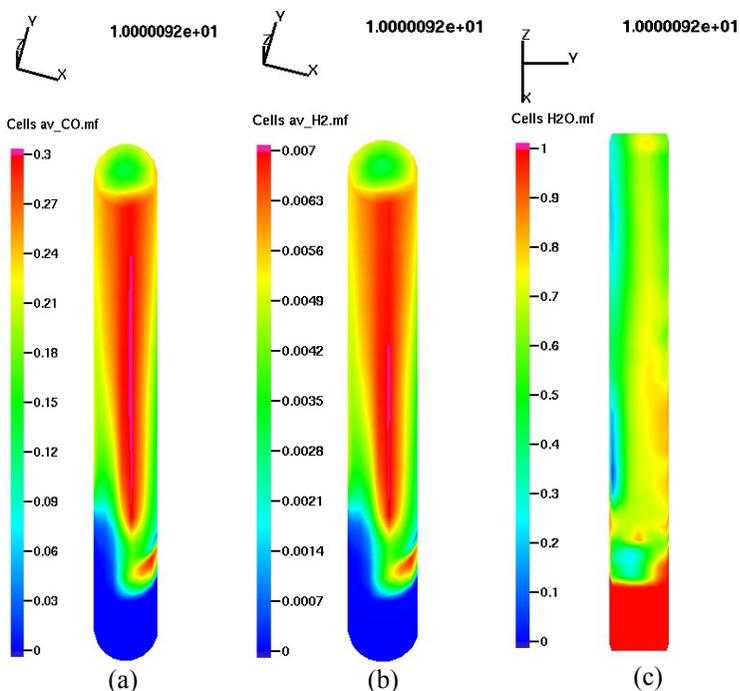


Figure 5: Mass fraction of (a) CO (b) H<sub>2</sub> (c) H<sub>2</sub>O at 10s.

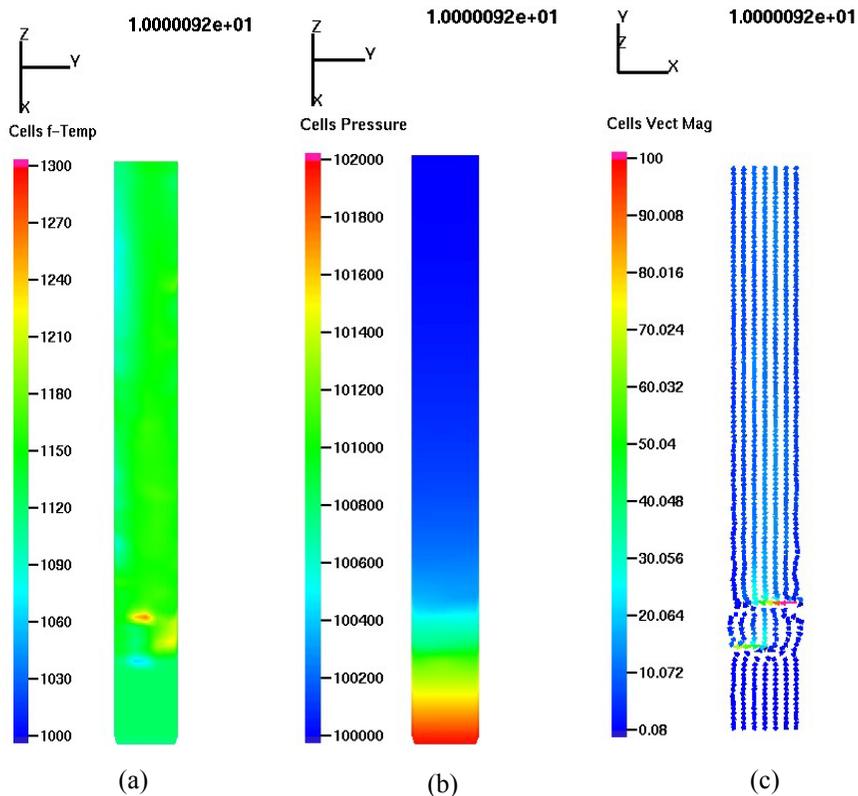


Figure 6: (a) Fluid temperature [K]; (b) pressure [Pa]; (c) velocity vectors within the reactor at 10 s.

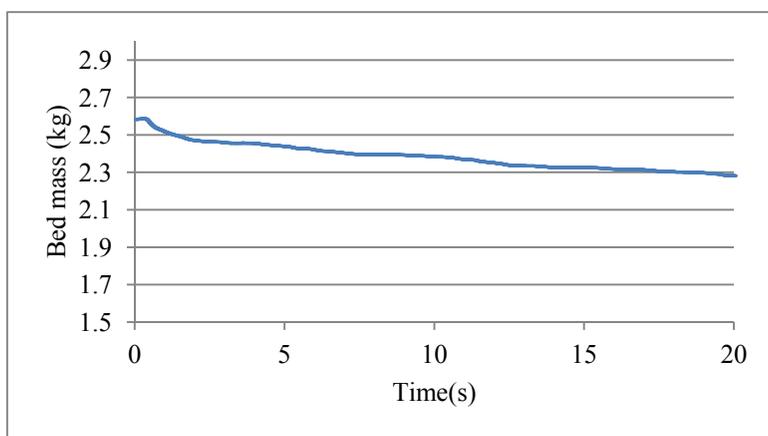


Figure 7: Particle mass within the reactor.

## 4 Conclusion

Biomass steam gasification in a simplified dual fluidized bed gasification reactor was simulated using the CFPD software ‘Barracuda VR<sup>TM</sup>’. Simulation results of glass bead fluidization under isothermal non reacting conditions were compared with real experimental data, prior to the simulations and same minimum fluidization velocity was confirmed.

Cellulosic biomass steam gasification was simulated under thermal and reacting conditions by including relevant chemistry. The reactor temperature was maintained around the desired gasification temperature of 850°C using a hot bed material recycle stream. The highest molar fraction of the product gas was mainly CO (~40%) whereas H<sub>2</sub> (~15%) content was less than expected. The simulations were resulted with considerable volume of combustible gases extrapolated around 280 Sm<sup>3</sup> per day.

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