

Modeling Biomass Gasification in a Fluidized Bed Reactor

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Abstract

Utilization of biomass as energy source by gasification is preferred because it uses relatively low amounts of oxygen as compared to combustion; also, the synthesis gas produced is at a higher temperature than flue gas. Biomass as a feed can constantly change since its source can vary from time to time, a fluidized bed reactor should be used in order to have the flexibility of handling different feeds. The objective of the work presented in this paper is to model a biomass gasification process in ASPEN Plus. This was done by splitting the gasification process into five different sub processes, starting with pyrolysis or decomposition of the feed, volatile and non-volatile component separation, volatile reactions, char gasification and finally solid gas separation. The reaction kinetics of the model, boiled down to two first order differential equations, one for conversion through combustion and the second for conversion through steam gasification. These were solved in MATLAB using the reaction kinetic constants provided by Nikoo et al. Overall, the APSEN Simulation designed in this work can be used as a tool to test other biomass feeds for a gasification process by simply changing the feed composition and flow rates of biomass, steam and air.

Keywords

Biomass gasification, gasification in fluidized bed reactor, gasification modeling.

1. Introduction

1.1. Biomass Gasification

According to Stats Canada, roughly 562 MW of power was produced from biomass in the province on Ontario in 2005. In the same year, 18% of the total power generation of the province from coal-fired power plants. This shows that Ontario still heavily relies on coal to meet energy demands for the province. With increasing energy demands and the polluting nature of the current fossil fuels, there is strong drive to find alternative non-polluting renewable sources of energy. One such alternative is biomass, which is said to be one of the largest sources of energy, third from oil and coal (Werther et al, 1999). Also it has been estimated that, “in all its forms biomass currently provides about 1250 million ton oil equivalent [of energy] which is about 14% of the world’s annual energy consumption” (Nikoo, 2007).

Gasification of biomass can be comparatively more efficient than coal gasification, since biomass has a higher volatile content than coal. Also, biomass contains its own oxygen and water that are important for when forming gaseous molecules from hydrocarbon base materials, this is particularly important for the gasification process. Another parameter that can be used for comparison is the ash content; biomass has less than 2% ash, while coal is typically 5% to 20%. In addition, sulfur content in biomass is less than 0.1% compared to 2% to 4% in coal. Therefore, biomass can be a good alternative for coal in a gasification process (Nikoo, 2007).

There are several biomass gasification installations already in operation at pilot scale in research centres. The units mostly operate with air, or air mixed with steam. Also, “biomass gasification is still in its early stages of industrial applications and a lot more work is needed to build confidence in this technology, particularly with respect to tar reduction, ash behaviour, gas cleaning, the use of gas in different types of prime movers, relative independence of process with regard to the nature of biomass, etc.” (Franco et al, 2003).

1.2. Gasification Process

Hydrocarbons can be gasified with one fifth to one third the theoretical amount of oxygen required for complete combustion. The product is a mixture of combustible gases that can be burned in a gas turbine to produce electricity. Another use for this gas mixture is for synthetic natural gas production. During the gasification process, only pure oxygen can be used, this process is called oxygen-gasification. In addition, air gasification can be used, where the product gas will also contain nitrogen gas. Steam gasification uses a mixture of air and steam, this type of gasification produces more hydrogen gas and is the reason why steam gasification has become an area of growing interest. Furthermore, steam gasification, has other advantages because it produces a gas with higher heating value. Also, it reduces the diluting effect of N₂ from air and eliminates the need for an expensive oxygen plant when both air and oxygen are used as gasification mediums. However, steam gasification is a more complex process, as the heat necessary to the process is not supplied directly by the partial combustion of the feedstock during the gasification process, as it happens when air or oxygen is used (Franco et al, 2003).

Overall gasification process can be split up into two sub processes namely, pyrolysis and char gasification. Pyrolysis is a process where a substance is heated enough that it decomposes into its elements. It is a type of burning but without the presence of oxygen source. Pyrolysis extracts the volatile components from the fuel source and leaves the solid residue with rich carbon source. These steps of the process have a strong effect on the internal surface, reactivity and elemental composition of the char produced. Studies have also found that increasing the residence time, heating rate and particle temperature increases the release of volatiles and the restructuring of aromatic clusters. This results in a higher surface area on the microscopic level. On the other hand, low particle temperatures and heating rates favor cross-linking reactions; this reaction can solidify the reacting material (Nikoo, 2007).

In char gasification, the gaseous reactants have to move into the porous char particles for the reaction to take place. The overall process can be characterized by the several inter connected steps. First, the reactant has to transfer from the main gas stream to the char particle surface (mass transfer). Second, these gases have to diffuse into the pores of the char particles. This is followed by a surface chemical reaction, along with the adsorption of reactants and desorption of the products. The product gases formed have to diffuse through the pores of char particles. Finally, mass transfer of these product gases has to take place to get the products back into main gas stream from the surface of the particles.

1.3. Biomass characteristics

Ash Content: is the inorganic content of the fuel source, it can be measured on both a dry basis and wet basis. This is an important characteristic to measure since the composition of ash affects its behavior under high temperature gasification and combustion. Since melted ash would physically damage the reactor by clogging, this would also have significant effects on the performance of a fluidized bed reactor (Quaak et al, 1999).

Moisture Content: this measures the amount of water present in the material, expressed as a percentage of the materials total weight. As the moisture content of a material increases more energy is absorbed by the material to vaporize this moisture. Also means that there is lower content of the combustible material present (Quaak et al, 1999).

Volatile component: is the percentage of the biomass that is released when it is heated. During the heating process, the biomass decomposes into volatile gases and solid char (Quaak et al, 1999).

Elemental Composition: it is the amount of organic ash free components of the material, namely oxygen, hydrogen, sulfur, and sometimes nitrogen. These are reported as weight percents (Quaak et al, 1999).

Bulk Density: it is the weight of material per unit volume. This value together with the heating value of the material are used determine energy densities that is the potential energy available per unit volume of the material (Quaak et al, 1999).

Heating Value: the energy chemically bound to a fuel is given by the heating value of the fuel in energy per amount of matter. This value is not measured directly but with respect to a reference state (Quaak et al, 1999).

1.4. Fluidization

Fluidization is a phenomenon by which the solid particles behave like a fluid when a gas or liquid at high velocity is passed upwards through the bed of solid particles. A fluidized bed can be characterized by its minimum fluidization velocity, the velocity of the fluid or gas at which the particles start to move is called the minimum fluidization velocity, u_{mf} . The weight of the particles is counterbalanced by the frictional force between the particle and the fluid at minimum fluidization velocity. Also, the pressure drop in a section of the bed equals the weight of the particles and the fluid present in that section. At this point, the compressive force in the vertical direction between

adjacent particles also does not exist (Kunii et al, 1991). Another important parameter of the fluidized bed system is the superficial velocity can be defined as the upward velocity of gas flowing through the empty vessel.

In liquid-solid systems, if the flow rate is increased above the minimum fluidization velocity, it results in a smooth and progressive expansion of the bed. Such a bed is called a smoothly fluidized bed or homogeneously fluidized bed (Kunii et al, 1991).

In gas-solid systems, when the flow rate is increased above the minimum fluidization velocity, it results in large instabilities with bubbling and channeling of gas. If the flow rate is further increased, agitation becomes much violent, resulting in vigorous movement of solids. The bed is then called bubbling fluidized bed or heterogeneous fluidized bed (Kunii et al, 1991). In such a system as the gas bubbles rise, they coalesce. If the bed is deep enough with a small diameter, the bubbles may become very large and spread across the vessel. Fine particles smoothly flow down the wall around the rising void of gas; this is known as slugging (Kunii et al, 1991).

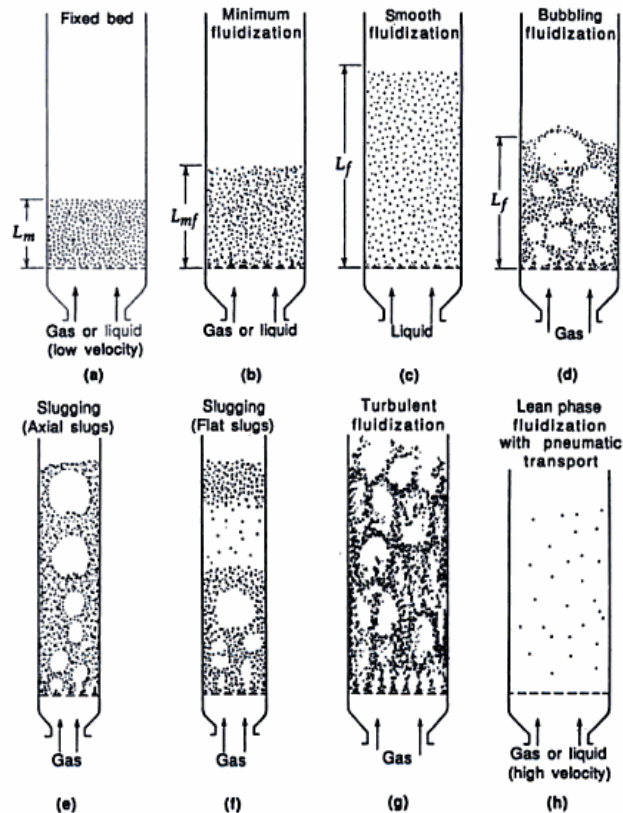


Figure 1: Various forms of solid-fluid contact (Kunii et al, 1991).

2. The Model

2.1. Reaction Kinetics:

The assumptions that were made while modeling the gasification unit are as follows (Nikoo et al, 2008):

- The process is at steady state
- The process is isothermal in nature
- All the gases are distributed uniformly in the emulsion phase
- Instantaneous devolatilization of biomass takes place
- The main components of volatile products are only hydrogen, carbon monoxide, carbon dioxide, methane and water
- Particles are of uniform size and are spherically shaped
- The diameter of the particles remains constant during the gasification process
- Char consists of only carbon (organic solid) and ash (inorganic solid)
- The gasification of char starts in the bed and completes in the freeboard

The process of gasification begins with pyrolysis, followed by combustion and steam gasification. The reactions involved in this process are as follows:

- Combustion reaction:



In the reaction above, α is a mechanism factor and ranges from 0.5-1. The mechanism factor is a function of the diameter of the char particles and the temperature (Nikoo et al, 2008). For the model proposed here, the value of α is 0.9 (Nikoo et al, 2008). Therefore, the above reaction can be rewritten as follows:



- Steam-Gasification reaction:



The value of β can be determined experimentally and ranges between 1.1-1.5 at 750-900°C (Nikoo et al, 2008). For the model proposed here, the value of β is 1.4. Therefore, the above reaction can be rewritten as follows:



The reaction rate equation for the above mentioned combustion and steam gasification reactions can be defined as follows:

- Reaction rate for combustion reaction:

$$\frac{dX_{CO}}{dt} = k_{CO} \exp\left(\frac{-E_{CO}}{RT}\right) P_{O_2}^n (1 - X_{CO})^{2/3} \quad (8)$$

- Reaction rate for steam gasification reaction:

$$\frac{dX_{SG}}{dt} = k_{SG} \exp\left(\frac{-E_{SG}}{RT}\right) P_{H_2O}^n (1 - X_{SG})^{2/3} \quad (9)$$

Kinetic parameters for reaction rates, can be determined experimentally to estimate the conversion of carbon by steam gasification and combustion.

2.2. Hydrodynamics

The assumptions that were made while modeling the hydrodynamics (Nikoo et al, 2008):

- There is perfect mixing of solid particles that consists of ash, char particles, and bed material.
- Any variations that occur in the conditions are considered to be in the axial direction because the fluidized bed is assumed to be one-dimensional.
- As height increases, the volumetric flow rate of the gas increases, corresponding to the production of gaseous products.
- Fluidized bed is divided into two regions: the bed and freeboard.
- Bubbling regime is maintained in the bed during fluidization
- The fluidized bed reactor is divided into finite number of equal elements with constant hydrodynamic parameters.
- The volume fraction of the solids decreases as the height increases, corresponding to the coalescence of the bubbles in the bed.

The minimum fluidization velocity can be calculated using:

$$u_{mf} = \frac{33.7\mu}{\rho_g d_p} \left(\sqrt{1 + 3.59 \times 10^{-5} Ar} - 1 \right) \quad (10)$$

$$Ar = \frac{d_p^3 \rho_g (\rho_s - \rho_g) g}{\mu^2} \quad (11)$$

Where,

μ = viscosity of the gas, Poise

ρ_g = density of gas, Kg/m³

ρ_s = density of solids, Kg/m³

d_p = particle diameter, m

Following equation can be used in order to determine the volume fraction by the bubbles:

$$\varepsilon_b = 1 - 1/B \quad (12)$$

$$B = 1 + \frac{10.978(u - u_{mf})^{0.738} \rho_s^{0.376} d_p^{1.006}}{u_{mf}^{0.937} \rho_g^{0.126}} \quad (13)$$

Where u = superficial velocity of the gas, m/s

The void fraction of the bed can be determined by:

$$\varepsilon_f = \varepsilon_b + (1 - \varepsilon_b)\varepsilon_{mf} \quad (14)$$

Where $\varepsilon_{mf} = 0.4$

In order to calculate freeboard void fraction, a graph is plotted using the equation below:

$$1 - \varepsilon_{fb} = (1 - \varepsilon_f)\exp(-az) \quad (15)$$

This graph can only be used when values of u and d_p fall in the following range:

$$u \leq 1.25 \text{ m/s}$$

$$d_p \leq 800 \mu\text{m}$$

Therefore, 'a' can be defined as:

$$a = 1.8 / u \quad (16)$$

The equations specified above can be used to effectively model the gasification process in ASPEN Plus, this will form the foundation for the simulation designed in the report.

3. APSEN Simulation

Gasification can be split into three different processes pyrolysis, combustion and steam gasification and the final product produced is called syngas. ASPEN Plus does not have a pre-defined unit that can be solely used to model the gasification process. Therefore, in order to simulate biomass gasification different pre-defined units within ASPEN will be used to simulate the different stages if the process. In ASPEN, a non-convectonal solid component will be defined that will have the properties and composition of biomass. The overall gasification flow sheet was divided into four sections: decomposition of the feed, volatile reactions, char gasification and then solid separation from the gas. The flow sheet is shown below:

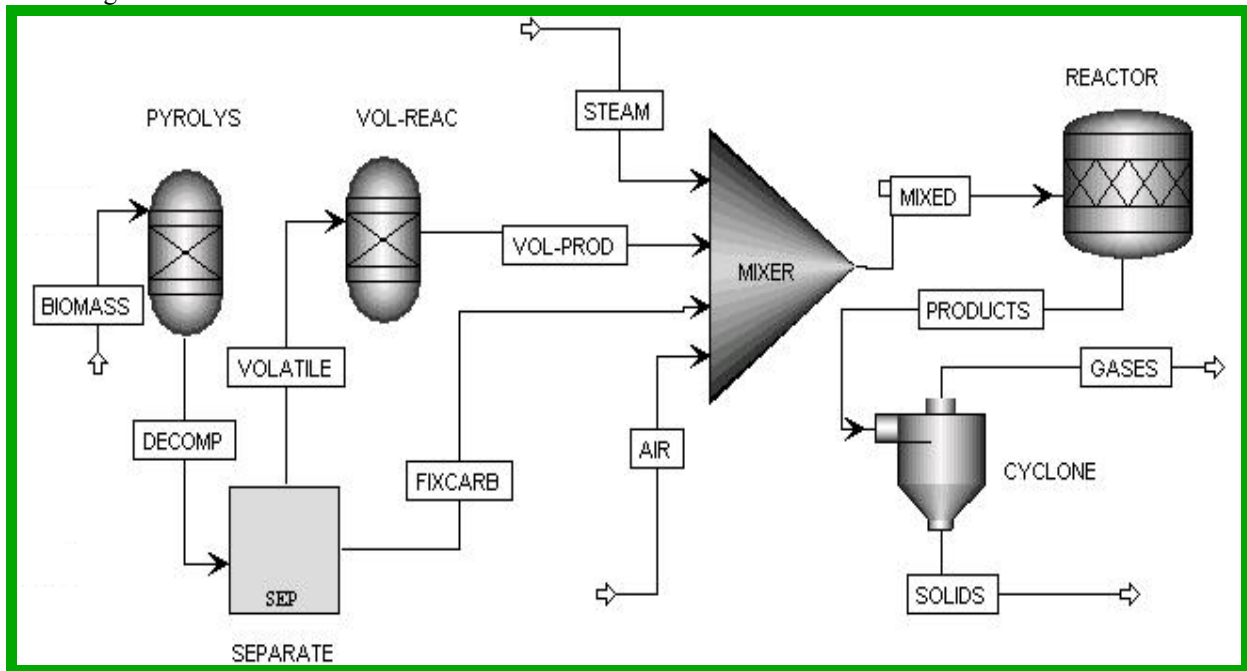


Figure 2: ASPEN flow sheet

3.1. Decomposition of the Feed

In Aspen, the decomposition of the feed will be performed using a RYIELD reactor. In this unit, the biomass will split into its volatile and non-volatile components. This split is called pyrolysis, where a substance is heated enough that it decomposes into its elements. It is a type of burning but without the presence of oxygen source and extracts the volatile components from the fuel source and leaving behind a solid residue, which is a rich carbon source. Since RYIELD was used, ASPEN needed to know the specific compounds that are being formed in the reactor so that a mass balance calculation can be conducted to quantify the products coming out of this reactor. The components specified for the volatile product stream are carbon, hydrogen, oxygen, sulfur, nitrogen as volatile components. On the other hand, solid carbon and ash are present in the non-volatile stream. This stream is where char formation is most likely along with other high carbon source solids. Since ASPEN does not have a conventional solid specified for ash and biomass, a two non-conventional components were created to model biomass and ash. In order to characterize the enthalpies of these solids, a pre-specified coal model called HCOALGEN was used. Similarly, the densities of these solids were specified using another pre-specified coal model called, DCOALIGT. For each non-conventional solid, PROXANAL, ULTANAL and SULFANAL analysis were entered to specify the elemental composition of the solids. Proxanal is the proximate analysis of the component where moisture, fixed carbon, volatile matter and ash are specified. This data helps ASPEN determine the amount of potential volatile and non-volatile matter present in the solid. Ultanal is the ultimate analysis of the biomass and contains the composition of the biomass/ash, for example, how much weight percentage of carbon is present in the biomass and what is the ash content of material. Sulfanal analysis differentiates between various forms of sulfur that is present in the non-conventional item. The table shown below summarizes the compositions of the biomass feed.

Table 1. Composition of Biomass (Nikoo et al, 2008)

Characteristics	Pine Dust	Wood Pellets
Moisture content (wt %)	8	4.87
Proximate analysis (wt % dry basis)		
Volatile matter	82.29	50
Fixed carbon	17.16	49.7
Ash	0.55	0.3
Ultimate analysis (wt % dry basis)		
Carbon	50.54	50.14
Hydrogen	7.08	6.14
Oxygen	41.11	43.33
Nitrogen	0.15	0.08
Sulfur	0.57	0.01
Average particle size (mm)	0.25-0.75	
Particle density (kg/m ³)	1300	

3.2. Volatile Reactions

Once the biomass has been decomposed into volatile and non-volatile components, a separating unit is needed to separate volatile gases from non-volatiles. After the volatiles are separated, they are passed through RGIBBS reactor which will be used for volatile combustion assuming that the volatiles reaction follow the Gibbs equilibrium conditions. Since the volatile components consist of hydrogen, nitrogen, oxygen, sulfur and water. The separation column was specified such that these components will come out in the volatile stream. Also, the biomass has 82% of carbon as volatile matter, therefore the volatiles will have 82% carbon in them and only 18% will be present in the non-volatile and ash stream. This volatile stream will then be fed into the RGIBBS unit which will be operated at 1 atm and 660 C and will produce H₂, CO, CO₂, CH₄ and H₂O. These products along with the solid components will be mixed with air and steam and fed into the char gasification section.

3.3. Char Gasification

This gasification reaction needs to include hydrodynamics and reaction kinetics. The rate laws for the reactions were first order differential equations; these were solved in MATLAB using the ODE45 function. The rate constants and activation energies were necessary to calculate the conversions, these constants were determined experimentally and were presented in the paper by Nikoo and Mahinpey, and these are shown below:

Table 2. Reaction Kinetic Parameters (Nikoo et al, 2008)

Kinetic Parameters	E/R (K)	k (s ⁻¹ atm ⁻¹)
Combustion	13,523	0.046
Steam Gasification	19,544	6474.7

In theory, the conversion through the steam gasification process is more desirable for this model than conversion through the combustion reaction. This was reflected in the results obtained from MATLAB, and primary conversion of the carbon to syn-gas was through steam gasification. The ASPEN unit used to simulate this part of the process is called RSTOIC, this type of reactor requires the specific reactions be inputted with their subsequent conversions.

Following this unit a cyclone was added to the flow sheet to separate the syn-gas from the solid mixture of carbon and ash. The carbon solid is assumed to be left over char that could not be reacted due to the reaction kinetic limitations. The cyclone was designed as a high efficiency cyclone since majority of the solid particulates need to be removed before the syngas can be used in run a gas turbine to produce power. The separation of the particles may also present an opportunity to recycle the left over solids; however, this can be done only after these particles have been analyzed to present potential to be gasified again.

4. Results and Discussion

4.1. MATLAB Results

MATLAB was used to solve the first order differential equations to obtain the conversion of carbon. While solving for the conversions it was validated that the dominant process for carbon conversion was steam gasification and not combustion. The boundary conditions used to solve the differential equation was that there is zero carbon conversion when time equals zero. The results of the differential equations were plotted against time to find a reasonable residence time for biomass. The plots of the results are shown below; these are calculated at a temperature of 900°C, the conversion for steam gasification was 94.82% and 0.004% conversion by combustion.

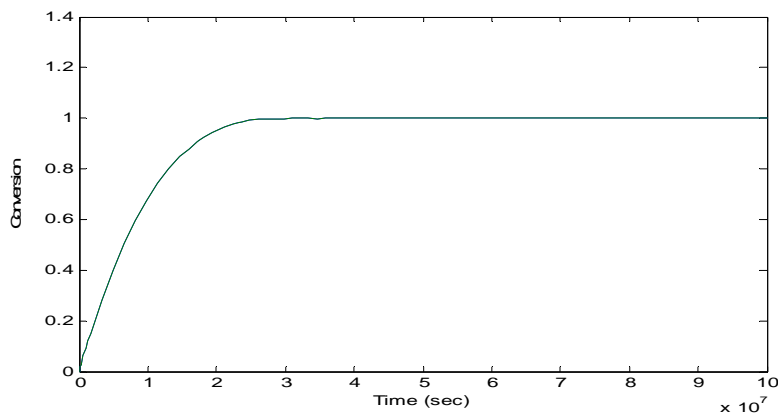


Figure 3: Conversion vs. time for the combustion process

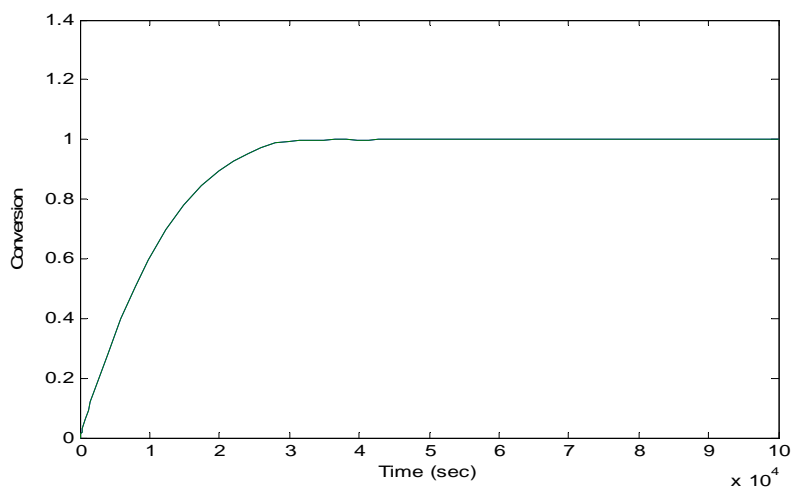


Figure 4: Conversion vs. Time for the steam gasification process

It can be seen from the plots that the combustion process takes a lot longer to reach 100% conversion of biomass to products, compared to steam gasification. These were then used in ASPEN plus to simulate the reaction kinetics for the gasification process.

The temperature of 900°C was selected because it was observed that the temperature had a significant effect on the residence time in the reactor. Since the reaction rate constants were provided for a temperature range of 700°C - 900°C, residence times were calculated at the temperature within this range. The plot can be shown in the Figure 4 below. At the lower point of 700°C, it found that the same conversion of 94.82% for the steam gasification reaction was reached but the time taken to reach this conversion was roughly 44 hours, as compared to 1.4 hours at 900°C. Therefore, it will be worthwhile to operate at a higher temperature to reach the same final conversion in a shorter period of time. Another benefit of operating at 900°C, was that the conversion of biomass by combustion was significantly lower 0.004% at 900°C, than 0.14% at 700°C. The temperature of 900°C would lower the formation of the combustion products keeping the gasification results the same.

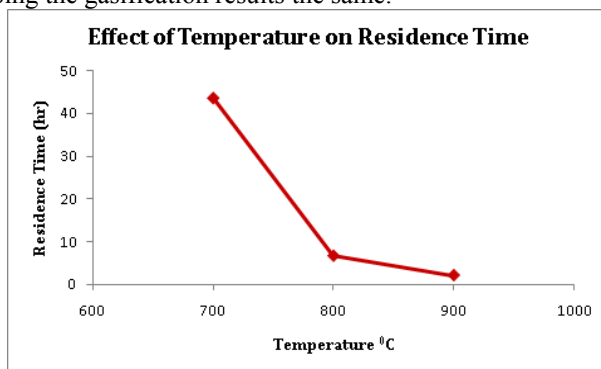


Figure 5: Effect of temperature on the residence time in the reactor.

4.2. ASPEN Results

The overall ASPEN flow sheet can be found in figure 2. The simulation takes in a feed of 1.669 tonnes/day of biomass, with the composition specified in Table 1, with 0.5341 tonnes/day of steam and 1.786 tonnes/day of air. The composition of the final products produced is shown below:

Table 3. Product gas composition from ASPEN

Temperature	1652 °F								
Pressure	1 atm								
Volumetric flow	26915.82 ft ³ /hr								
Component	H2	O2	N2	CO	CO2	CH4	H2O	H2S	NH3
Mole Percent	25.45	6.84	25.78	21.26	5.47	7.14	7.91	0.14	trace

4.3. Hydrodynamic Results

The minimum fluidization velocity of the particle is found to be 0.0588 m/s. The bed material used is silica sand with an average particle size of 0.275 mm. The bed diameter is equal to the freeboard diameter of 0.8 m and height is 3.19 m. Other hydrodynamic results of the fluidized bed reactor are summarized below:

Table 4. Hydrodynamic results

Bed		
	Fraction occupied by bubble	0.064
	Average bed voidage	0.439
	Voidage in emulsion at minimum fluidization	0.4
	Bed height	0.189 m
Free Board		
	Fraction occupied by bubble	0.569
	Average bed voidage	0.741
	Average voidage of freeboard	0.999

5. Economic Analysis

5.1. Gasifier

Low Pressure indirectly heated gasification unit

Fixed Capital Investment (FCI) = *capital cost x location ratio x inflation ratio x currency ratio*

$$FCI_{\text{gasifier}} = 14,185,000_{\text{USD 1988}} * \frac{1.15_{\text{ON}}}{1_{\text{USD}}} * \frac{1000_{\text{USD 2009}}}{918_{\text{USD 1988}}} * \frac{1.22_{\text{CAD}}}{1.00_{\text{USD}}} = 21,750,333.33_{\text{CAD 2009}}$$

5.2. Cyclone

Taken from Cooper et al. (2002):

$$P_c = 6520 A^{0.903}$$

Area for cyclone was obtained from ASPEN simulation: 0.269098 ft²

$$P_c = 6520 * 0.269098^{0.903} = 1,992.77_{\text{USD 1988}}$$

$$FCI_{\text{cyc}} = 1,992.77_{\text{USD 1988}} * \frac{1.15_{\text{ON}}}{1_{\text{USD}}} * \frac{1000_{\text{USD 2009}}}{852_{\text{USD 1988}}} * \frac{1.22_{\text{CAD}}}{1.00_{\text{USD}}} = 3,281.52_{\text{CAD 2009}}$$

5.3. Total Costs

Therefore, the total capital equipment cost is:

$$21,750,333.33 \text{ CAD}_{2009} + 3,281.52 \text{ CAD}_{2009} = 21,753,614.85 \text{ CAD}_{2009}$$

The following table shows the factors that were used to calculate other associated costs with the gasifier and cyclone.

Table 5. Cost Factors

Cost factors use to calculate the total cost	
Installation	15% of FCI
Maintenance	7% of FCI
Instrumentation	10% of FCI

Table 6. Total cost for Gasifier and Cyclone in Canadian dollars for 2009

Description	Gasifier	Cyclone	Total Cost
Installation	\$ 3,262,550.00	\$ 492.23	\$ 3,263,042.23
Maintenance cost	\$ 1,522,523.33	\$ 229.71	\$ 1,522,753.04
Instrumentation	\$ 2,175,033.33	\$ 328.15	\$ 2,175,361.49
Total Cost	\$ 6,960,106.67	\$ 1,050.09	\$ 6,961,156.75

Therefore the total costs of the gasification unit is,

$$\text{Total Cost: } 21,753,614.85 \text{ CAD}_{2009} + 6,961,156.75 \text{ CAD}_{2009} = 28,714,771.60 \text{ CAD}_{2009}$$

6. Conclusion

Overall, the model developed for gasification is a good model that can be used as a basis for further studies. The ASPEN simulation developed in this project is a flexible tool; since it is capable of handling different types of biomass feed streams. As long as the composition of the solid is known, the simulation is capable of handling different feed streams to produce syngas provided the same reaction kinetics are valid. Incorporation of tar reformation would further improve the quality of the model. Also, the area of biomass gasification is fairly novel and there is a lot work that still needs to be done in this field to propose the use of biomass gasification as an alternative fuel source.

7. Recommendations

The model presented in this report does not incorporate the effects of tar reforming, the lack of this step in the process may limit the applications of this model. Therefore, it is recommended to add this aspect of gasification to the model to improve its performance. In addition, the results obtained from the simulation should be validated

against experimental data, lab scale experiments should be carried out to measure the actual performance of the gasification process. Based on the actual results obtained a rigorous error analysis should be conducted. These results will help improve the accuracy of the simulation and provide a clearer perspective in terms of how well it matches up to the physical process.

Another improvement to the simulation would be to program the reaction kinetics and the hydrodynamics within ASPEN through FORTRAN coding. This would improve the quality of the results and will eliminate the use of MATLAB or other programs making it a self-sufficient model of gasification. Therefore, the model presented in this report can be used as a basis for future work in this area.

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Biography

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