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Optimization of Waste Plastics Gasification Process Using Aspen-Plus

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1. Introduction

In this era of plastics dominated world, it remains a fact that there exists an ever-increasing margin between the volume of waste plastics generated and the volume recycled [1]. Of the total plastic waste, recyclable thermoplastics like polyethylene, polystyrene, polypropylene and PVC account for nearly 78% of the total and the rest is composed of the non-recyclable thermosets like epoxy resins and polyurethane [2]. Typically, plastics waste management is practiced according to the following hierarchical order: Reduction, Reuse, Recycling, and finally energy recovery. Although reuse of plastics seems to be best option to reduce plastic wastes, it becomes unsuitable beyond certain cycles due to the degradation of plastic. Mechanical recycling of plastics involves significant costs related to collection and segregation, and is not recommended for food and pharmaceutical industries. While chemical recycling focuses on converting waste plastics into other gaseous or liquid chemicals that act as a feedstock for many petrochemical processes, energy recovery utilizes the stored calorific value of the plastics to generate heat energy to be used in various plant operations. Moreover, since plastic wastes always consist of a mixture of various polymeric substances, chemical recycling and energy recovery seems to be best possible solution, both in terms of economic and technological considerations.

One of the major processes of chemical recycling involves thermal treatment of the waste plastics. The inevitable shift in world's energy paradigm from a carbon based to hydrogen based economy has revolutionized the capabilities of thermal treatment processes, viz. combustion, gasification and pyrolysis, in particular on the latter two techniques. In fact, recent technical investigations on the novel municipal solid waste (MSW) management methods reveal that a combined gasification and pyrolysis technique is more energy efficient and environmentally friendly than other processes [3].

In general the process of gasification for energy extraction from solid carbon source involves three simultaneous or competing reactions namely combustion, pyrolysis and gasification. The partial combustion of solid fuel creates an oxygen devoid, high temperature condition within the reactor which promotes the pyrolysis reaction, breaking the fuel into products that are a mixture of char and volatiles containing small and long chain hydrocarbons. The presence of gasifying agent (steam) drives the water shift reaction converting the carbon sources in to a mixture of valuable chemicals, tar, fuel gases and some residual particulate matter. The products undergo various downstream operations in order to separate and purify the valuable gaseous products that are later utilized for energy generation. This auto thermal feature makes the gasification process an economically viable and efficient technique for recovery of energy from waste plastics.

Gasification in commercial scale is practiced based on batch, semi batch and continuous modes of operation depending upon the processing capacity of the plant. Typically a plant processing large throughput utilizes fluidized beds due to the advantages such as enhanced gas-solid contact, excellent mixing characteristics [4], operating flexibility [5], and ease of solids handling [6] that lead to a better overall gasification efficiency. Fluid beds are preferred as it offers high heat and mass transfer rate and a constant reaction temperature which results in a uniform spectrum of product in a short residence time. It is important to keep the good fluidization characteristics of the bed, since introduction of material with different properties than the original components of the bed affect the quality of fluidization. Introduction of plastic material in fluidized beds demand additional attention due to its softening nature and possibility of blocking the feeding line. As soon as the plastic enters the hot reaction zone, it thermally gets cracked and undergoes a continuous structural change until it is eliminated from the bed. The sequence of interaction between the inert particle in the fluidized bed and the plastic material has been narrated by Mastellone et al., [7].

Gas-solid fluidization is the operation by which a bed of solid particles is led into a fluid-like state through suspension in a gas. Large scale gasifiers employ one of the two types of fluidized bed configurations: bubbling fluidized bed and circulating fluidized bed. A bubbling fluidized bed (BFB) consists of fine, inert particles of sand or alumina, which are selected based on their suitability of physical properties such as size, density and thermal characteristics. The fluidizing medium, typically a combination of air/nitrogen and steam, is introduced from the bottom of the reactor at a specified flow rate so as to maintain the bed in a fluidization condition. The dimension of the reactor section between the bed and the freeboard is designed to progressively expand so as to reduce the superficial gas velocity which prevents solid entrainment, and to act as a disengaging zone. A cyclone is provided at the end of the fluidized bed either to return fines to the bed or to remove fines from the system. The plastic waste is introduced into the fluidized bed at a specified location, either *over-bed* or *in-bed* using an appropriately designed feeding system. Pyrolysis experiments by Mastellone et al. [7] has shown that when the feed is introduced over the bed (from the freeboard region), it results in uniform surface contact with the bed material, thus enhancing transfer properties. The bed is generally pre-heated to the startup temperature either by direct or indirect heating. After the bed reaches the ignition temperature, plastic wastes are slowly introduced into the bed to

raise the bed temperature to the desired operating temperature which is normally in the range of 700-900 °C. The plastic wastes are simultaneously pyrolyzed as well as partially combusted. The exothermic combustion reaction provides the energy to sustain the bed temperature to promote the pyrolysis reactions.

One of the main disadvantages of fluidized bed is the formation of large bubbles at higher gas velocities that bypass the bed reducing transfer rates significantly. If the gas flow of a bubbling fluidized bed is increased, the gas bubbles become larger forming large voids in the bed entraining substantial amounts of solids. The bubbles basically disappear in a circulating fluidized bed (CFB) and CFB the solids are separated from the gas using a cyclone and returned back to the bed forming a solids circulation loop. A CFB can be differentiated from a BFB in that there is no distinct separation between the dense solids zone and the dilute solids zone. The residence time of the solids in the circulating fluid bed is determined by the solids circulation rate, attrition of the solids and the collection efficiency of the solids in the cyclones. The advantages of the circulating fluidized bed gasifiers are that they are suitable for rapid reactions resulting in high conversion. The disadvantage being, i) temperature gradients in the direction of the solid flow, ii) limitation on the size of fuel particles iii) high velocities resulting in equipment erosion. Although there are many different types of fluidized beds available for gasification and combustion, bubbling fluidized type is the most preferred type whenever steam is used as a gasifying medium [8]. The advantages of steam gasification have been well addressed in the literature [9].

A wide variety of plastics are in use depending upon the type of application, of which the most widely utilized are polyethylene (PE), Polypropylene (PP), Polyvinyl chloride (PVC), Polystyrene (PS) and Polyethylene terephthalate (PET). Each type differs in physical and chemical properties, and so do their applications. In general, the combustion of most of the plastics is considered safe with the exception of PVC that generates dioxins due to the presence of chlorine compound in its structure. In contrast with combustion, pyrolysis and gasification are endothermic process which require substantial amount of energy to promote the reactions. The pyrolysis process generally produces gas, liquid and solid products, the proportions of which depends on the operating conditions, while the gasification is predominantly reactions involving carbon or carbon-based species and steam, producing syngas (CO and H₂) and minor higher molecular weight hydrocarbons [6].

Cracking of PE either into its constituent monomer or other low molecular weight hydrocarbons has become a vital process due to the increased amounts of polyethylene wastes in the present world. Pyrolysis and/or gasification of PE serve as an appropriate tool for the recovery of energy and for waste plastic disposal simultaneously. Compared with other alternative feedstock like biomass and coal, PE possesses relatively higher heating value, and is much cleaner in terms of fuel quality attributing to lesser fuel pre-processing costs. Pyrolysis or gasification of PE results in a product stream rich in hydrogen and minimal CO or CO₂ content as compared to cellulose based wastes that yields relatively higher carbon monoxide and lower hydrogen product composition mainly due to the presence of oxygen in cellulose based feedstock.

Irrespective of the type of reactor and type of waste being handled, the key operating parameters that play a vital role in the gasification process are the equivalence ratio, reactor temperature, steam to fuel ratio, gasifying medium and residence time. In order to exert better reliability of the system, the operating variables have to be optimized and controlled with significant accuracy. The cheapest and most effective technique to qualitatively understand the effect of each operating variable and to identify possible optimal conditions is through process simulation. Such attempts to develop simulation models for process optimization has been reported in open literature of fuel sources such as, tyre [6], coal [10-13], and biomass [8, 14-16] using various computer simulation packages. However, the utility of any process simulation tool has not been well explored or recorded in the literature for modeling plastics gasification.

This chapter discusses recent work by the authors on Aspen Plus based process model to analyze the performance of a plastics gasification process under equilibrium conditions. The primary goal of this work is to successfully test and demonstrate the applicability of Aspen Plus to simulate the gasification process for one of the most abundantly used plastic, polyethylene (PE). This study will serve some preliminary qualitative and quantitative information on the overall behavior of the gasification process including the sensitivity of process parameters.

2. Model development

2.1. Modeling the gasification process

The gasification process models available in literature can be generally classified under steady state or quasi-steady state or transient state models. The steady state models do not consider the time derivatives and are further classified as kinetics *free* equilibrium models or kinetic rate models [17]. The following is a list of few researchers who have used the above-mentioned models for modeling the gasification process of various fuels; transient model for coals by Robinson [18], steady state kinetic model for biomass by Nikoo [14], steady state kinetic model for plastic wastes by Mastellone [7], kinetics *free* equilibrium model for biomass by Doherty [15], Paviet [17], and Shen [8], kinetics *free* equilibrium model for tyre by Mitta [6]. Of these, the kinetics *free* equilibrium steady state model is the most preferred for predicting the product gas composition and temperature, and more importantly for studying sensitivity analysis of the process parameters. Table 1 shows a summary of a few gasification simulation models developed in Aspen Plus for various materials.

The model used in this work to investigate the simulation of PE gasification in fluidized bed reactor is based on the model previously developed by Mitta et al. [6] for simulating tyre gasification. The *simplified* tyre gasification equilibrium model was simulated using Aspen Plus and it was successfully validated using the experimental data. Such an equilibrium type of approach considers only the equilibrium products, namely methane, hydrogen, carbon monoxide, carbon dioxide, water, sulphurous and nitrogen compounds formed

within the reactor. Any other high molecular weight hydrocarbons, such as tars and oils, are less likely to form under equilibrium conditions and hence are not included in the simulation. More importantly, the equilibrium condition facilitates an exhaustive optimization study focusing on key process parameters, including the gasification temperature, equivalence ratio, steam to fuel ratio, and gasifying medium, thereby neglecting the complexities of the gasifier hydrodynamics and reaction kinetics.

Material	Model	Process Variable	Range	Findings / Remarks	Ref.
Biomass	Equilibrium (<i>volatile rxns.</i>) & kinetic (<i>char gasification</i>)	Temperature (°C)	700-900	Higher temperature, lower ER and higher steam-to-fuel ratio favors hydrogen and CO production Boudouard and methanation reactions were not considered	[14]
		ER	0.19-0.27		
		Steam to fuel ratio	0-4		
Tyre	Equilibrium	Temperature (°C)	750 -1100	Higher temperature, higher fuel/air ratio and lower steam/fuel ratio favors hydrogen and CO production All components listed in gasification reactions, along with H ₂ S, are considered as possible products	[6]
		Fuel to air ratio	0.2-0.8		
		Steam to fuel ratio	1.25-5		
Biomass	Restricted Equilibrium	Temperature (°C) (achieved by changing ER between 0.29 - 0.45)	674-1195	Air preheating effective at ER's less than 0.35 Without air preheating, optimum conditions for ER is 0.34 and gasification temperature between 837 to 874 °C Only Reactions (1-8) along with reactions for the formation of H ₂ S and NH ₃ were considered for Gibbs free energy minimization	[15]
		Air Preheating Temperature (°C)	25-825		

Table 1. Summary of gasification simulation of various materials using Aspen Plus from literature.

The following assumptions are made in the current study for developing the process model.

1. All the chemical reactions were assumed to have reached equilibrium within the gasifier.
2. Only methane, hydrogen, carbon monoxide, carbon dioxide, oxygen, nitrogen, H₂S, and water were considered to be present in the product stream.
3. The primary components of char are only carbon and ash.

The entire gasification process was modeled using Aspen's *built-in* unit operation library in two stages; pre-processing and gasification. The two stages are discussed separately in the following sections.

2.1.1. Fuel pre-processing

Figure 1 illustrates the process flow sheet of the *simplified* PE gasification model. The first stage corresponds to fuel preprocessing where the polyethylene sample was processed or conditioned to remove any moisture present before the start of the gasification process. Drying and separation are the unit operations grouped in this stage and are represented by the respective modules in Aspen Plus. The fuel polyethylene stream labeled as "PE" was defined as a non-conventional stream and the ultimate and proximate analysis are provided as input to the model, refer Table II for parameter values. Polymer NRTL/Redlich-Kwong equation of state with Henry's law "POLYNRTL" and "POLYSRK" was chosen as parameter models to calculate the thermo physical properties of the components.

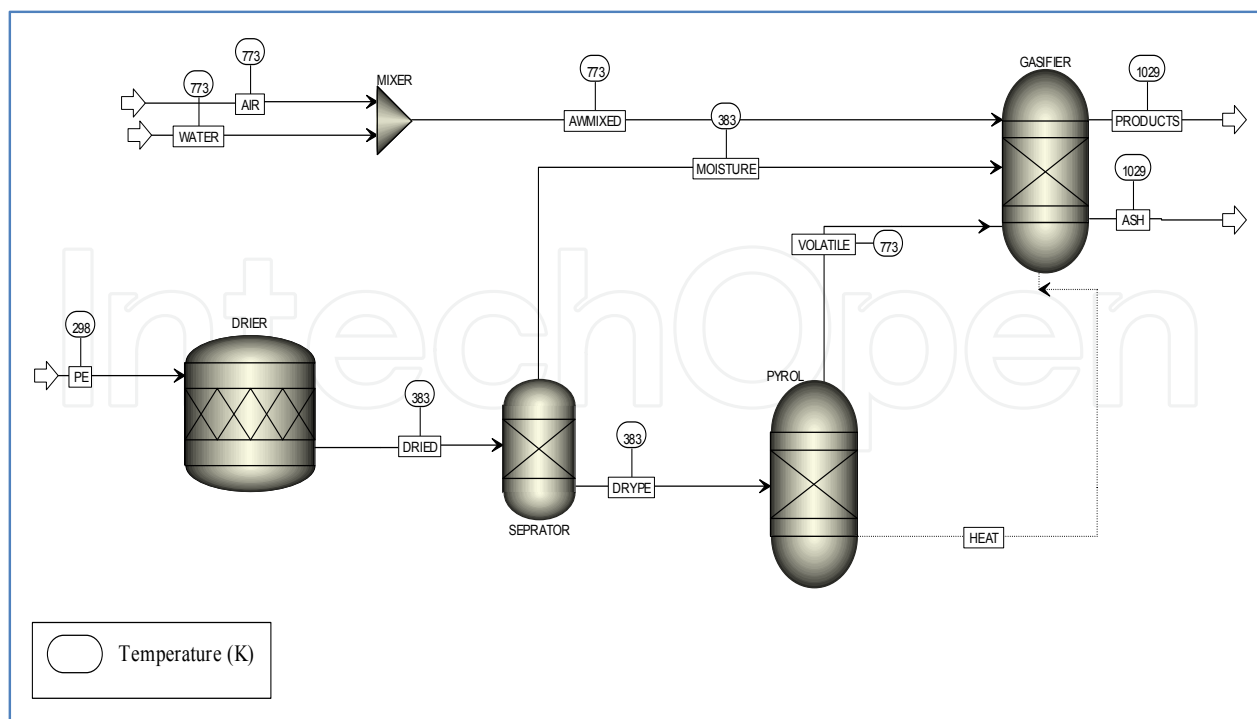


Figure 1. Process flow diagram of a PE gasification process in Aspen Plus

Sample	Proximate Analysis				Ultimate Analysis						
	Moisture	FC	VM	Ash	Ash	C	H	N ₂	Cl ₂	S	O ₂
PE	0.02	0	99.85	0.15	0.15	85.81	13.86	0.12	0	0.06	0
Tyre	0.94	31.14	65.03	3.83	3.83	85.65	8.26	0.43	0	1.43	0.4

Table 2. Proximate and Ultimate analysis of the fuels used in this study.

At first, the fuel stream was first introduced into a drying unit “DRIER”, which was modeled in Aspen Plus using an RSTOIC module. A temperature of 110 °C and a pressure of 1 atm were selected as drier operating conditions. The stream leaving the drier, labeled “DRIED” contains the dried PE in solid phase and the removed moisture in vapor phase. This stream was fed to a separation unit “SEPARATOR” that splits the feed stream into product streams, labeled as “DRYPE” and “MOISTURE”.

2.1.2. Volatiles and char gasification

In a typical gasification process, the fuel is first pyrolyzed by applying external heat where it breaks into simpler constituent components. These volatile components, along with char are then combusted, and the heat liberated from the combustion reactions would be used up by the subsequent endothermic gasification reactions. In the Aspen plus model, the dried portion of the fuel “DRYPE” exiting from the “DRIER” enters a pyrolyzer “PYROL” modeled as a RYIELD block in Aspen Plus. Based on the ultimate analysis of PE shown in Table II, the product yield distribution was calculated in the RYIELD module using Aspen Plus built-in calculator. An operating temperature of 500 °C and a pressure of 1 atm were chosen in order to set the exiting stream “VOLATILE” to a pre-heated temperature of 500 °C.

Parameter	Type	Value / Range
Fuel feed rate	constant	6 kg/h
Air flow rate	variable	5 – 30 kg/h
Steam flow rate	variable	0.3 – 30 kg/h
Air temperature	constant	773 K
Steam temperature	constant	773 K
Pyrolyzer temperature	constant	773 K
Drier temperature	constant	383 K

Table 3. List of process parameters provided as input to the model.

No.	Gasification Reactions	Heat of Reaction (kJ/mol) T =1000 K, P = P _o	Type
1	$C + \frac{1}{2} O_2 \leftrightarrow CO$	-112	Reactions with oxygen
2	$CO + \frac{1}{2} O_2 \leftrightarrow CO_2$	-283	
3	$H_2 + \frac{1}{2} O_2 \leftrightarrow H_2O$	-248	
4	$C + H_2O \leftrightarrow CO + H_2$	136	Reactions with water
5	$CO + H_2O \leftrightarrow CO_2 + H_2$	-35	
6	$CH_4 + H_2O \leftrightarrow CO + 3H_2$	206	
7	$C + CO_2 \leftrightarrow 2CO$	171	Boudouard reaction
8	$C + 2H_2 \leftrightarrow CH_4$	- 74.8	Methanation reactions
9	$CO + 3H_2 \leftrightarrow CH_4 + H_2O$	-225	
10	$CO_2 + 4H_2 \leftrightarrow CH_4 + 2H_2O$	-190	

Table 4. Summary of Gasification Reactions.

The volatiles stream, along with char was then passed to a gasifying unit "GASIFIER" that was modeled as a RGIBBS module. As it can be noticed in the model, the combustion and gasification reactions are allowed to take place within the "RGIBBS" module itself. The RGIBBS module calculates the equilibrium composition of the system using Gibbs free energy minimization technique. It provides an option to either consider all the components present in the system as equilibrium products or restrict the components based on some specific reactions or restrict it based on a temperature approach. In this study, all components from the gasification reactions, listed in Table IV, along with H₂S were included as possible fluid phase or solids products in the RGIBBS module. The gasifying mediums, air and steam, are preheated and mixed before it is sent to the gasifier. The outlet stream labeled as "PRODUCTS" contains product gases resulting from the gasification process while the "ASH" stream contains any residual solids.

The flow rate of fuel stream was held constant at 6 kg/h for all simulations. The two key parameters that influence the reactor temperature and the product distribution are equivalence ratio and the steam-fuel ratio, and hence were the only variables considered in the simulation. Equivalence ratio can be defined as the ratio of mass of oxygen/air supplied to the mass of oxygen/air necessary for complete combustion of all the carbon and hydrogen present in the feed to carbon dioxide and water respectively.

2.2. Model validation

The base case model for the gasification process was developed using Aspen plus built in modules based on the simulations popularly adopted in literature. In order to validate the appropriateness of the present model, simulations have been performed for gasification of

tyre and the results were compared with the work due to Mitta et al. [6]. The ultimate and proximate analysis data used for tyre simulation in this study has been listed in Table II. However since the simulation parameters were not fully detailed by the authors, the parameters utilized in the present simulation is not the same as reported by Mittal et al. Therefore, only a qualitative comparison of the effect of parameters on the product distribution was considered for comparison purposes. Results showed good agreement in terms of the trends of the composition *versus* temperature plots and that serves as a basis for model validation.

In this work, a similar kind of study was performed to investigate the performance characteristics of the PE gasification process. In the case of isothermal gasification studies, it is challenging to include the temperature variation effects resulting from the entering steam flow, and exclusion of which results in significant deviation in the simulation results [14]. Hence, in this work, an adiabatic type of gasification reactor was modeled to investigate the effects of two key parameters, namely the equivalence ratio and steam-to-fuel ratio. The response variables include the gas composition, Carbon monoxide efficiency, hydrogen efficiency, and combined CO and hydrogen efficiency.

The carbon monoxide efficiency measures the extent of conversion of carbon present in the fuel to carbon monoxide. The definition of hydrogen efficiency and the combined efficiency follows the same. Van den Bergh [18] has reported expressions to calculate the CO, H₂, and combined CO and H₂ efficiencies. A similar definition was introduced in this work to estimate carbon dioxide efficiency as shown below.

$$\text{CO efficiency} = \left[\frac{f_{CO} \times F}{V_m} \right] \times \frac{1}{r_C} \times 100\% \quad (1)$$

$$\text{CO}_2 \text{ efficiency} = \left[\frac{f_{CO_2} \times F}{V_m} \right] \times \frac{1}{r_C} \times 100\% \quad (2)$$

$$\text{Hydrogen efficiency} = \left[\frac{n_{H_2}^H \times f_{H_2} \times F}{V_m} \right] \times \frac{1}{r_H} \times 100\% \quad (3)$$

$$\text{Combined CO and H}_2 \text{ efficiency} = \frac{\left\{ \frac{(f_{CO} + f_H) \times F}{V_m} \right\}}{\left\{ \frac{r_H}{n_{H_2}^H} + r_C \right\}} \times 100\% \quad (4)$$

where, f_{CO} and f_{CO_2} represents the volume fraction of CO and CO₂ in the product gas respectively, r_C is the rate of carbon feeding [moles of carbon/min], F is the total gas flow rate [L/min], V_m is the standard molar volume [24.1 L/mol at 293 K and 1 atm], r_H is the rate of elemental hydrogen feeding [moles of elemental H/min], $n_{H_2}^H$ is the number of H atoms in PE monomer, and f_{H_2} is the volume fraction of hydrogen in the gas. The combined efficiency represents the fraction of the maximum possible conversion or production achievable by the system. This maximum limit is considered when all the available carbon and hydrogen present in the fuel is converted to CO and H₂ [18]. The performance of the gasifier is also analyzed in terms of cold gas efficiency (CGE) that is defined as:

$$\text{CGE} = \frac{V_g Q_g}{M_b C_b} \quad (5)$$

Where

V_g = Gas generation rate (m^3/sec)

Q_g = heating value of the gas (kJ/m^3)

M_b = fuel consumption rate (kg/sec)

C_b = heating value of the fuel (kJ/m^3)

3. Results and discussion

3.1. Effect of steam-to-PE ratio

The effect of steam-to-PE mass ratio on PE gasification process was investigated in the range of 0.05 to 5 (corresponding to a mole ratio of 0.04 to 3.9) with a constant PE feed rate of 6 kg/h and an equivalence ratio of 0.15 (air flow rate of 15 kg/h). It can be expected that at low concentrations of water, oxidation reactions *via* Reactions (1-3) would dominate resulting in a higher temperature. The resulting temperature rise in turn would propel Reactions (4 and 6), which according to chemical equilibrium principle would shift forward, resulting in formation of CO and hydrogen. When the partial pressure of the reactant steam was increased, Reactions (4-6) would exhibit a tendency to shift forward, thus leading to a higher CO₂ and hydrogen content with simultaneous drop in CO molar composition. Due to the participation of the endothermic reactions at higher steam composition, the overall equilibrium temperature would show a decreasing trend. At some point, when there is enough hydrogen available to react with the carbon, the formation of methane would be favored as per Reactions (8–10). Subsequently, the methane formed would react with the excess steam to form back CO and hydrogen, as depicted by reaction (6). Overall, at any steam-to-PE ratio, the equilibrium system temperature and product composition would be a result of the competing simultaneous endothermic and exothermic reactions.

Figure 2 illustrates the variation of product molar composition and the equilibrium reactor temperature as a function of steam-to-PE mass ratio. The simulation *predicted* equilibrium temperature resulting from the gasification process helps to deduce certain qualitative conclusions on the overall gasification reaction and thus validate the theoretical explanations. From the simulation results, it can be noticed that when steam content is much less than the stoichiometric amount required for Reaction (4), which is equivalent to a steam-to-PE mass ratio of 1.33, the composition of hydrogen displays a sharp increasing trend while that of methane decreases. The high temperature and high methane content at lower steam-to-PE ratios are a result of the methanation and oxidation reactions. Above the stoichiometric point, hydrogen along with carbon monoxide shows a gradual decreasing tendency with a simultaneous increase in CO₂ content. This is in agreement with the theoretical explanation, wherein it was predicted that an increase in the amount of steam would strongly favor the forward endothermic reaction forming carbon monoxide and hydrogen. With higher steam content, the oxidation of CO is favored resulting in a steady

increase of carbon dioxide during the gasification process. The steam composition in the product stream is a result of the excess and unreacted steam entering and exiting the reactor. As expected, above the stoichiometric point, the temperature of the reactor remains constant at around 850 K, possibly balanced by the complicated endothermic and exothermic gasification reactions.

Figure 3 shows the effect of the steam-to-PE ratio on the fractional efficiency of CO, CO₂ and H₂. It is evident that at around a steam-to-PE ratio of 0.4, the production of CO and hydrogen peaks while that of carbon dioxide is at a minimum. This is a favorable condition for any waste gasification process where it is desired to minimize as much as carbon dioxide as possible. Hence, it can be concurred that the favorable steam-to-PE mass ratio for the gasification process should be between 0.4 and 0.6, where the combined as well as the individual compositions of CO and H₂ are at a maximum. Furthermore, the cold gas efficiency (CGE) of the process seems to be affected only at lower steam-to-PE ratio. The predicted CGE values are much higher than those obtained in typical waste gasification process which is about 60%. It can be expected that under equilibrium conditions, as considered in this study, the gas yield is significantly higher than real process which directly contributes to increased efficiency.

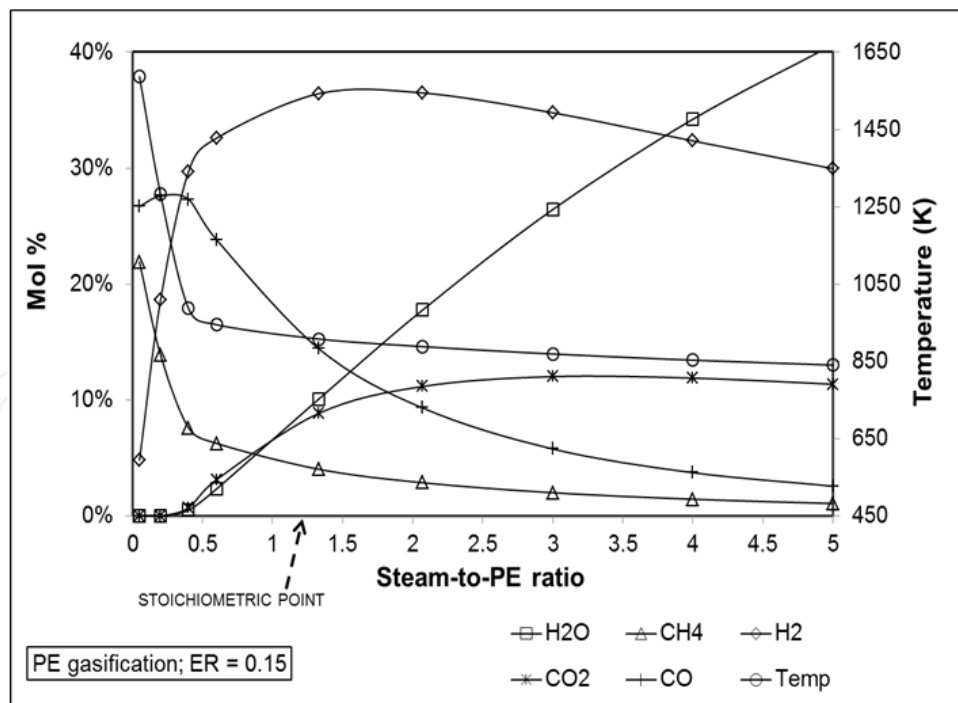


Figure 2. Product molar composition and temperature at various steam-to-PE ratios.

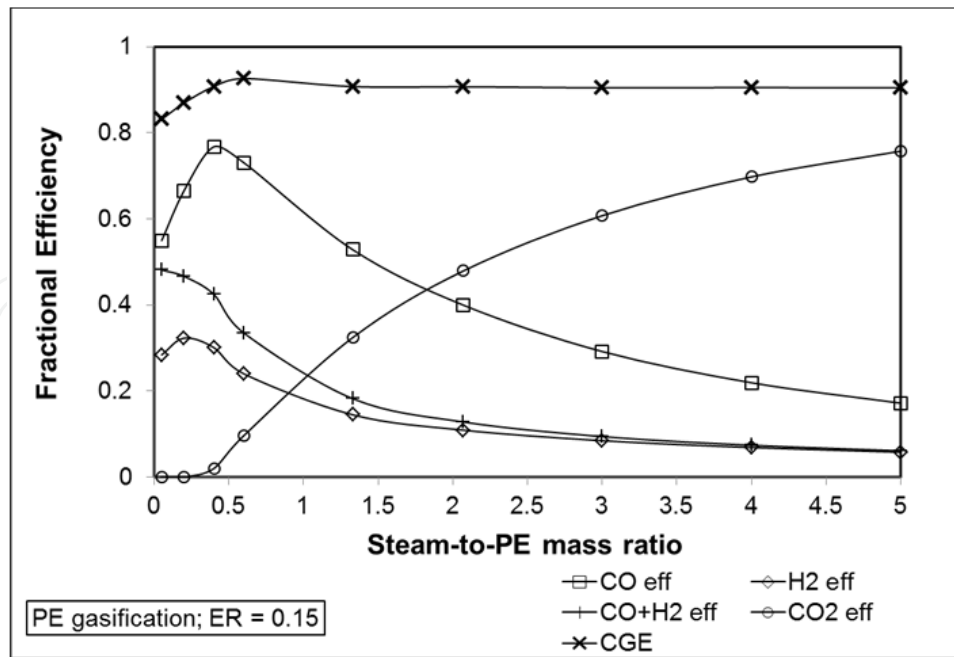


Figure 3. Fractional efficiencies at various steam-to-PE ratios.

3.2. Effect of equivalence ratio

The effect of equivalence ratio on the overall gasification efficiency was studied at two different steam-to-PE ratios. Typically, a commercial biomass gasifier is operated at an ER value of 0.25 in order to maintain auto thermal conditions (van den Bergh, 2005). Hence, a range of 0.05 to 0.3 was selected for this study in order to determine the optimum ER for PE gasification process. The cases for the two different steam-to-PE ratios have been presented and discussed separately below.

The oxidation reactions of carbon, CO and hydrogen, depicted by Reactions (1-3) are spontaneous and exothermic, resulting in release of significant amount of heat energy. It can be expected through Reaction (1) that at low values of ER (low values of stoichiometric air), only incomplete combustion of carbon would take place leading to the formation of CO with release of heat. Therefore, for the range of ER considered in this study, only Reactions (1) and (3) are the possible oxidation reactions, and thus any heat released during the combustion process will be directly attributed to these two reactions.

In general, at any fixed steam-to-PE ratio, the other parameters that drive the gasification process would be the ER and consequently the heat released from the combustion reactions. The intensity of the heat released controls the temperature, which in turn affects the directional shift in equilibrium of the gasification reactions. For example, the endothermic reactions (4, 6, and 7) would tend to shift in the forward direction with an increase in temperature and *vice versa*. Hence with increasing ER, it can be expected that the conversion of carbon to CO and hydrogen would be highly favored to other products such as carbon dioxide and methane.

Case 1: Steam-to-PE ratio 0.6

At low ER and low steam content, Reactions (4, 5 and 7) would be possibly controlled by the temperature and the partial pressure of steam. At such conditions, it could be expected that Reaction (5) would not be driven forward resulting in lower carbon dioxide formation. Furthermore, at low ER values, reactions with water would significantly compete with the oxidation reactions, thus limiting the resulting equilibrium temperature. At high ER and low steam content, this effect would be compounded such that temperature would be the primary variable that would determine the direction of the gasification reactions. In addition, at higher ER the composition trend of CO could be expected to fall down due to the subsequent combustion and methanation reactions of CO.

Figure 4 illustrates the variation of product gas composition and temperature as a function of various equivalence ratios. Between ER values of 0.05 and 0.2, reactor temperature, CO content, and hydrogen content increases steadily while the composition of methane decreases very sharply. In addition, the composition of carbon dioxide shows a steady decrease whereas the molar composition of water remains a constant. At ER values higher than 0.2, it can be observed that the temperature increases very sharply along with a steady decrease of hydrogen and carbon monoxide. It can also be noticed that beyond this point, only hydrogen, CO, and water are the major components of the product stream. The low values of carbon dioxide predicted throughout the range can be explained by the fact that at such low ER and steam-to-PE ratios considered in this study, neither complete oxidation nor steam gasification of carbonaceous components, depicted by reactions (2) and (5) respectively, proceeds at any significant rate. The sharp increase in the temperature beyond ER = 0.2 is due to the domination of the exothermic combustion reactions over others. The simulation results are very much in agreement with the theoretical expectations discussed earlier in this section.

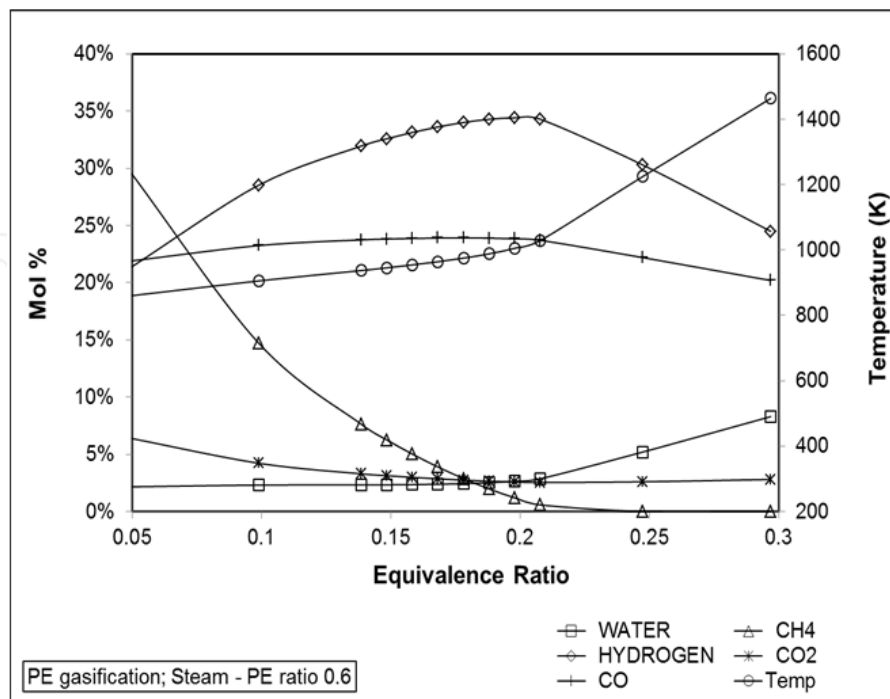


Figure 4. Illustration of the effect of equivalence ratio on product composition and temperature.

Figure 5 illustrates the variation of the fractional efficiencies with the equivalence ratios. It is clear that the efficiency of the conversion proceeds rapidly at lower ER's and reaches a maximum at ER of 0.2 and at a fixed steam-to-PE ratio of 0.6. The effect of ER on CGE is not significant at lower values since the composition of CO, hydrogen and methane that directly contribute to the heating value of the product gas increases until ER = 0.2. Beyond this point, since the yield of the above products decreases, CGE follows a decreasing trend and records a value of about 75% at an ER value of 0.3.

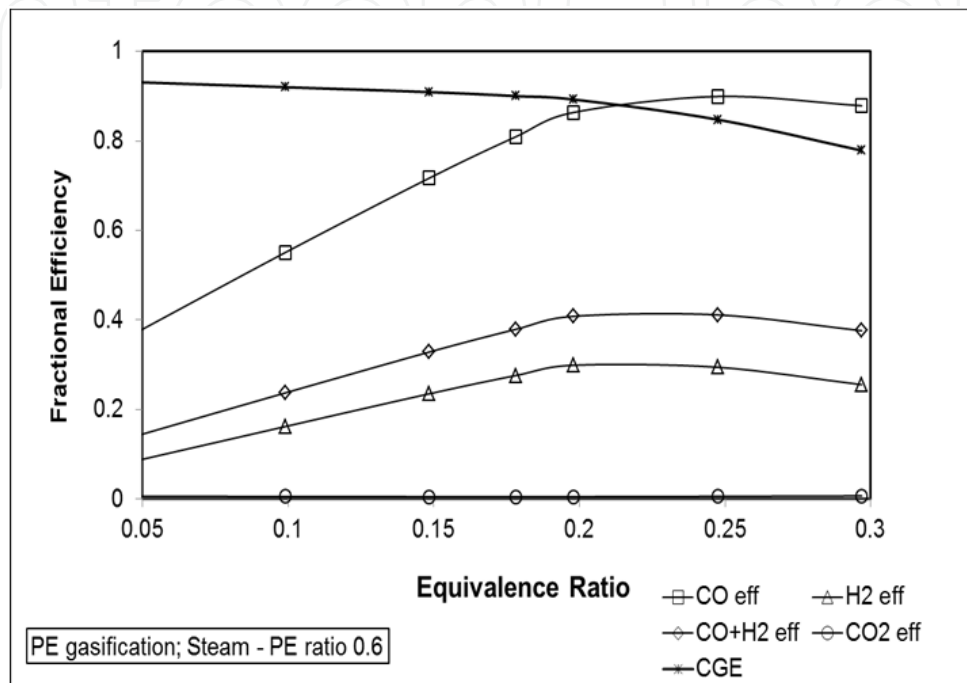


Figure 5. Illustration of the effect of equivalence ratio on gasification efficiency at a fixed steam-to-PE ratio of 0.6.

Case 2: Steam-to-PE ratio 4

An additional study of the effect of ER on the gasification process at a higher steam-to-PE ratio was included to provide better and comprehensive understanding of the sensitivity of equivalence ratio. In this case, the gasification reactions would not only be driven by the heat released by the preceding combustion reactions, but also by the partial pressure of steam. At a higher steam-to-PE ratio, it could be expected that Reaction (4) would significantly compete with Reaction (1) to consume the carbon present in the feed. Hence, the absolute value of the equilibrium temperature would be lower when compared to the previous case, steam-to-PE ratio of 0.6. Although high ER values would restrict the forward shift of the exothermic Reaction (5), the presence of higher steam content would favor the equilibrium to shift in the forward direction resulting in higher net carbon dioxide content.

Referring to Figures 4 and 6, it is evident that the trends of composition and temperature follow the same as case 1, but with different absolute values. It should be noted that the simulations predicted a temperature of about 800 K at an ER of 0.1 for case 2 compared to a value of ca. 850 K for case 1. It can also be observed that the composition of carbon dioxide

was slightly higher and that of carbon monoxide was significantly lower than the results reported earlier in Case 1.

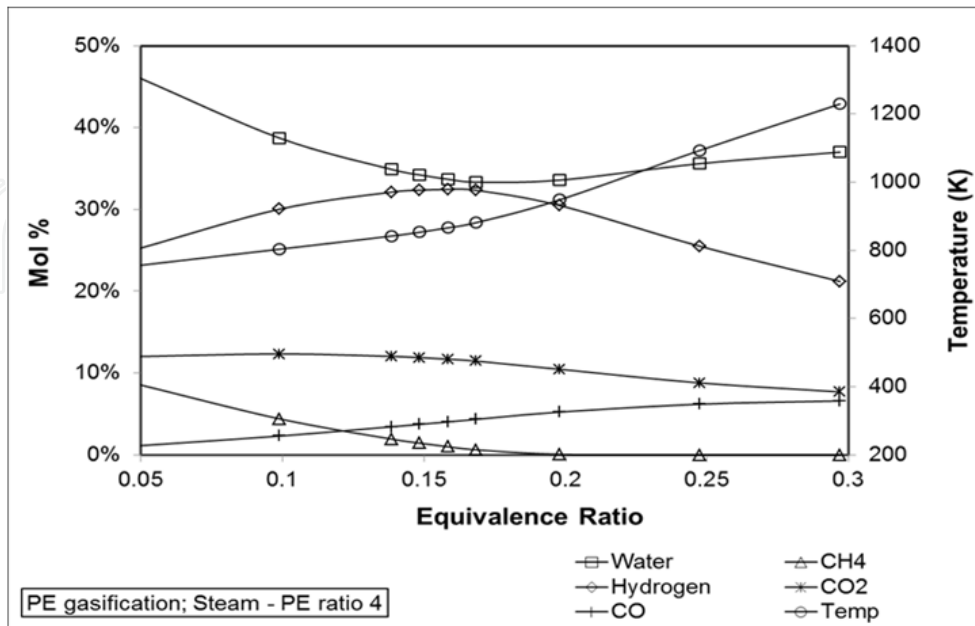


Figure 6. Illustration of the effect of equivalence ratio on product composition and temperature at a fixed steam-to-PE ratio of 4.

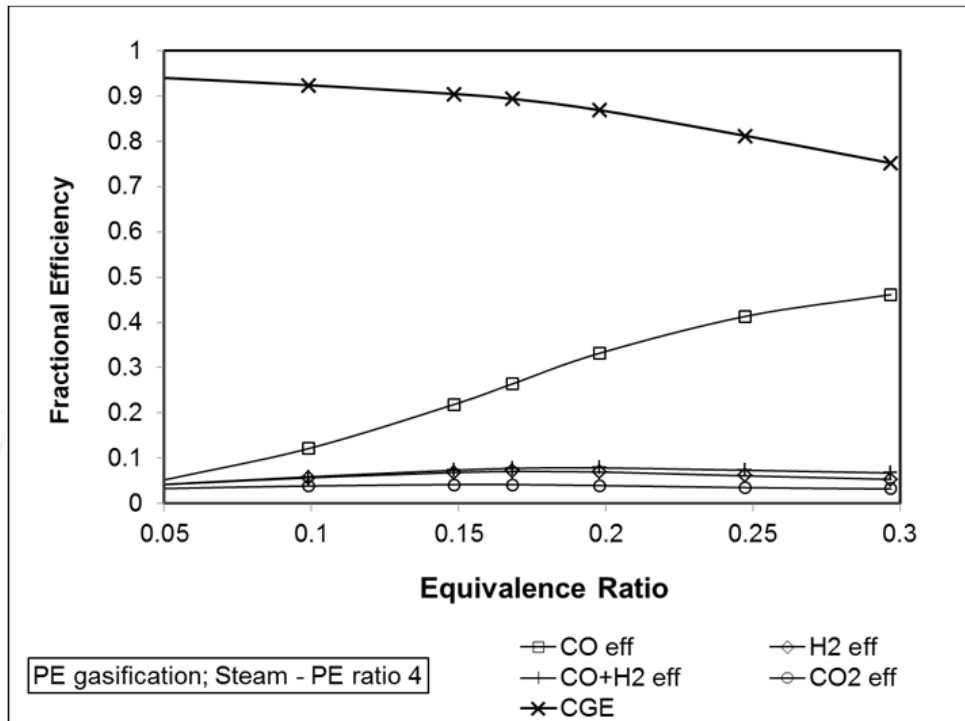


Figure 7. Illustration of the effect of equivalence ratio on gasification efficiency at a fixed steam-to-PE ratio of 4.

It can also be noticed from Figures 5 and 7 that the absolute maximum value of the combined CO and H₂ efficiency is significantly different among the two cases, which are

predicted as 40% for case 1 and 7% for case 2. The composition of carbon dioxide in the product gases is very negligible at lower steam content, while it reaches about 4% for the case of higher steam content. Nevertheless, in both the cases, the maximum fractional efficiency of all the components occurs at an ER value of ca. 0.2. Furthermore, as discussed earlier in section 3.1, the effect of steam-to-PE ratio on CGE is remarkable only until 0.6. Thus, the trend of CGE in Figure 7 for the case of higher steam-to-PE ratio resembles the same as that of Figure 5.

Hence, it can be concluded that an ER value of 0.2 and steam-to-PE ratio of 0.4 to 0.6 would yield a product stream containing 35% hydrogen, 25% CO, and negligible CO₂ at a temperature of 1000 K. These values seem acceptable for all practical purposes and are very much in agreement with the literature data, where a value steam-to-fuel value of 0.42 and an ER value of 0.15 were reported as the optimum parameters for co-gasification of wood and polyethylene [18].

4. Conclusions

The gasification process of waste polyethylene was successfully modeled using a combination of various unit operation modules available in Aspen Plus simulation package. The model used in this work to investigate the simulation of PE gasification in fluidized bed reactor is based on the model previously reported in literature for simulating waste tyre gasification. The equilibrium model developed in this study enables one to predict the behavior of PE gasification process under various operating conditions. Moreover, the results obtained are easy to interpret and thus could be directly corroborated with actual plant data.

Although temperature plays a vital role in controlling the conversion and product composition, it has been treated as a *free* variable in this study. Other process conditions were optimized in order to attain the appropriate temperature suitable for different applications that ideally lies between high temperature low calorific value and low temperature high calorific value product gas. The product distribution was the result of many competing simultaneous reactions mainly dictated by the temperature and the steam flow. The effect of the equivalence ratio and steam-to-PE ratio on the gasification efficiency was investigated in the range of 0.05 to 0.3 and 0.05 to 5 respectively. Based on the simulation results, the behavior of the conversion process was characterized and the values of the combined and individual fractional efficiencies have been presented. The following results summarize the findings from this study:

- Optimum steam-to-PE ratio was determined to be between 0.4 and 0.6 for low temperature applications. Under this condition, the yield of syngas and cold gas efficiency reaches a maximum.
- Product gas temperatures as high as 1273 K could be attained at higher steam-to-PE ratio at the expense of decrease in calorific value
- Sensitivity analysis on ER proposes an optimum value of about 0.2. Both CGE and syngas efficiency reaches a maximum at this point.

Due to the lack of detailed experimental data on waste PE gasification for various process conditions, the predicted data could not be validated. Although the results from this work heavily depend on the assumption made, i.e. thermodynamic equilibrium, significant qualitative results were deduced that would help to establish a sound reference for any detailed process optimization studies. Furthermore, this model can be used to estimate the final gas composition and other parameters, including gas yield and temperature for other solid waste fuels and mixtures. Upon including the hydrodynamics and gasification kinetics, this model could be used to evaluate the performance and behavior of many types of gasifiers under different process conditions.

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