Steady State Simulation of Plastic Pyrolysis Process using Aspen Hysys V9 Simulator

Selvaganapathy.T, Muthuvelayudham R, Jeya Kumar M.

Abstract: The present study was carrying out the simulation of plastic pyrolysis process modelled for the conversion of petroleum product from plastic wastes such as Poly-Styrene (PS), Poly-Ethylene (PE), Poly-Propylene (PP) and Poly-Styrene (PS) with the aid of Aspen Hysys V9 simulator. Aspen Hysys simulator was used to develop the steady state model and to simulate the pyrolysis process with the above mentioned plastic wastes. Peng-Robinson thermodynamics model was employed as a fluid package of this simulation. The process converts waste plastic to fuel, which was taking places in two stages in an Aspen Hysys Simulation Environment such as i) A conversion of plastic wastes into Vapour-Liquid Fraction (VLF) with small quantity of char residue using conversion reactor (Pyrolytic Reactor) and ii) Separation of produced Vapour-Liquid Fraction to pyro gases and liquid fuel with the help of water tube Condenser. The obtained results demonstrated that, a conversion of Poly-Styrene (PS) into liquid fuel is up to 88.7% was optimum than other plastics Poly-Ethylene (PE) 81.95% and Poly-Propylene (PP) 83.54 %. The simulated model can help an interested to researcher in knowing expected products and their individual component for better understanding and scale-up studies.

Keywords: Aspen Hysys V9simulator, Peng-Robinson, Pyrolysis process, Steady state model

I. INTRODUCTION

Plastic products have now become an integral part in our day by day life as an essential need and the demand is expanding due totheir high adaptability, moderately ease and attractive applications in agriculture [1], households [2], automobiles [3], packing materials [4], and variety of their other applications [5].Mostly, thermoplastics polymers makeup a high proportion of waste, and their generation has consistently expanding around the worldwide. It delivered on a monstrous scale worldwide and its generation crosses the 150 million tons for consistently comprehensive. In India approximately 8.33 Metric tons of plastic items are consumed every year.Considering, 70% of plastic utilization is changed over as waste, approximately 5.6 million tons per annum (TPA) plastic waste is produced in India,

which equivalents to 15342 tons per day (TPD). According to the Central Pollution Control Board (CPCB) survey, plastic contributes to 8% of the total solid waste, with Delhi delivering the maximum quantity followed by Kolkata and Ahmedabad [6].

Plastic solid wastes consist of polyethylene, polypropylene, polystyrene, vinyl, and polyethylene terephthalate [7]. Overall, about 50-70% of the total plastic waste is packaging materials derived from polyethylene, polypropylene, polystyrene, and polyvinyl chloride [8]. On average, polyethylene makes up the greatest fraction of all plastic wastes (69%), especially plastic bags and polyethylene comprises 63% of the total packaging waste [8].Hence, plastic solid waste become a very critical environmental issue because of their huge quantity and disposal problem as thermoplastic do not bio-degrade for quite a while.

Recycling is the best possible way/solution for environment, there are categorized into primary (re-extrusion), secondary (mechanical recycling), tertiary (chemical recycling) and quaternary recycling (incineration- restricted in India). Chemical recycling method also termed as pyrolysis is one of the most efficient and effective method of recycling of plastics simultaneously it converts waste plastic into fuel. Most of the recycling processes are expensive, energy intensive and end up producing low-grade products. Pyrolysis is a sustainable waste management process and Eco-Friendly approach to treat plastic solid waste containing carbonaceous materials like plastics and biomass [9].Pyrolysis also termed thermolysis derived from Greek (pur = fire; thermos = warm; luo = loosen) is a process which thermally breaks down higher molecular carbonaceous compound to produce lower molecular compounds in an oxygen-devoid environment at considerably high temperature [10]. The products of pyrolysis are condensable gases, char residue and non-condensable gases. The vapour consists of condensable gases that transform into liquid (pyrolytic fuel) after condensation while the non-condensable are collected or vented as gases [11]. Pyrolysis can be conducted at various variables temperature levels, reaction times, pressures, and in the presence or absence of catalysts. Plastics pyrolysis proceeds at low temperature (<400°C), medium temperature (400–600°C) or high temperature (>600°C) [12].

However the optimum temperature range (450°C) was predicted in our previous paper [13].

The purpose of steady state simulation is to imitate the performance of any chemical process. The process characteristics (e.g. flow rates, compositions, temperatures, pressures, properties, equipment sizes, etc.) are anticipated using analysis techniques. These techniques include mathematical models, empirical correlations and computer-

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aided process simulation tools (like Aspen Hysys). It is a computer-aided software which uses the underlying physical relationships (e.g., material and energy balances, thermodynamic equilibrium (Fluid Package) and rate equations) to predict process performance (e.g., stream properties and operating conditions. Therefore, in process simulation, we are given the process inputs and flow sheet and are required to predict process outputs [14]. Simulation of pyrolysis process is picking up attention because of the growing interest in pyrolysis of plastic wastes for the production of fossil fuels.
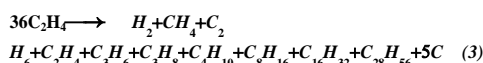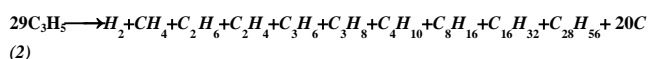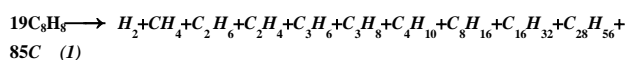
Few literatures [15, 16] having as far as I could possibly know reported a model set to give estimates of actual compositions of products obtainable from plastic solid wastes. In this present study, the simulation of different plastic wastes such as poly ethylene, polypropylene and polystyrene were carried out in Aspen Hysys V9 simulator. Aspen Hysys V9 simulator was chosen of this work because this simulator is able to perform and handled the feedstock conversion. The study will give an idea of compositions of various products expected from pyrolysis of the plastic wastes, which will help an interested to researcher in knowing the expected products and their individual compositions.

II.   SIMULATION OF PLASTIC PYROLYSIS PROCESS

The procedures are employed to accomplished the simulation of pyrolysis process with the aid of Aspen Hysys V9 are as outlined below.

A.   Component Selection

The components of both reactant and products stream, which were selected from the pure components of the component list section and added to the components in component list based on below depicted reactions.

$$19C_8H_8 \longrightarrow H_2+CH_4+C_2H_6+C_2H_4+C_3H_6+C_3H_8+C_4H_{10}+C_8H_{16}+C_{16}H_{32}+C_{28}H_{56}+85C \quad (1)$$

$$29C_3H_5 \longrightarrow H_2+CH_4+C_2H_6+C_2H_4+C_3H_6+C_3H_8+C_4H_{10}+C_8H_{16}+C_{16}H_{32}+C_{28}H_{56}+20C \quad (2)$$

$$36C_2H_4 \longrightarrow H_2+CH_4+C_2H_6+C_2H_4+C_3H_6+C_3H_8+C_4H_{10}+C_8H_{16}+C_{16}H_{32}+C_{28}H_{56}+5C \quad (3)$$

Reaction (1), (2) & (3) represents the thermal cracking reactions of poly-styrene, poly-propylene and poly-ethylene respectively [15].

B.   Selection of Fluid Package

After the selected of components list, the fluid package that was used to estimate the physical properties of thecomponents was also been chosen from property environment. The Fluid Package used in this work was selected to be Peng-Robinson model [16].

C. Development of the Pyrolysis Reaction

After selecting the fluid package for the process, the reactions involved in the process were developed based on reaction (1), (2) & (3). The developed reaction set were attached to the selected Fluid Package, which was Peng-

Robinson before being used in the simulation environment of the Aspen Hysys.

C. Simulation Environment

After every one of the steps had been preceded, then the simulation environment of the Aspen Hysys was entered. The development of the process flow diagram was accomplished by picking the parts of equipment from the palette (f$_4$ key) of the Aspen Hysys and connecting them together properly. The pyrolytic reactor which was conversion reactor where picked from the column section of the palette while the condenser was taken from the common section of the palette. After developing the flow sheet as described above, it was simulated using mass flow rate at 100 kg/hr of waste plastics such as PP,PE,PS at optimum temperature of 450 ^{o}C and a pressure of 1 atm as the feed to the Pyrolytic reactor. The vapour-liquid fraction was leaving from the top of the pyrolytic reactor, which was containing petroleum product whereas; char residue was leaved from bottom. The resulting vapour-liquid fraction was then fed into the condenser so as to obtain high purity of the desired product, which was liquid fuel .The desired product was observed to leave as liquid from the condenser, and it was stored in storage tank like silos and hopper. The results of this simulation can be viewed in workbook containing each of the equipment available in simulation environment.

III.   RESULT AND DISCUSSION

In the end of pyrolysis process, Large size waste plastic(PE, PP, PS) molecules are breakdown into smaller molecules which are Hydrogen, Methane, Ethane, Ethylene, Propene, Propane, n-butane, 1-octane, Cyclo-octane, 1-octocosene and Carbon. The simulation environments of different plastic pyrolysis process (PE, PP and PS) are shown in fig 1, 2 &3. The process which converts waste plastic into petroleum products, which was taking places in two several stages in Simulation Environment:(1)Conversion stage using Conversion reactor (Pyrolytic Reactor) and (2) condensing stage using water tube Condenser.
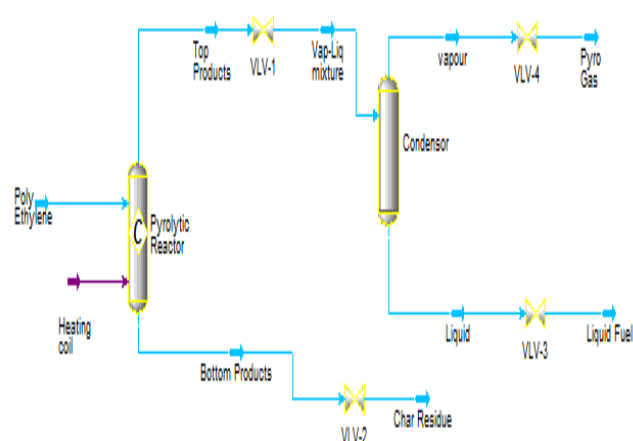

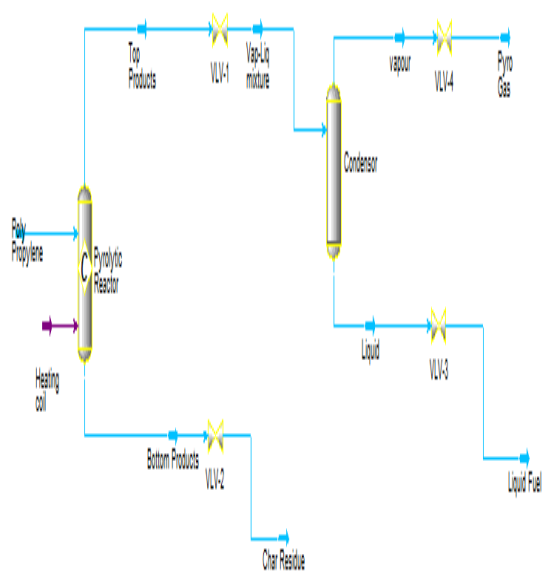**Fig 1 Poly-Ethylene thermal cracking**
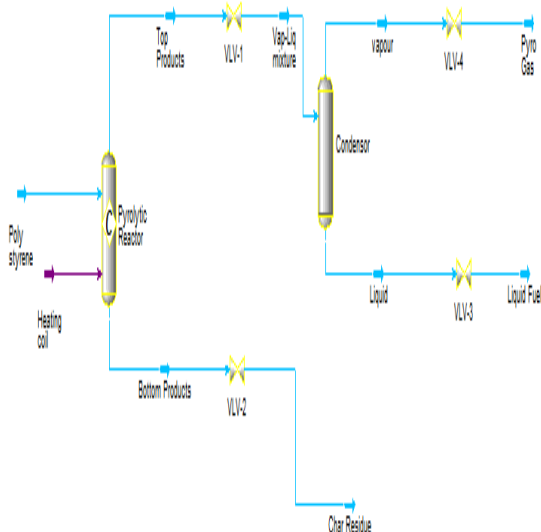
Fig 2 Poly-Propylene thermal cracking

Fig 3 Poly-Styrene thermal cracking

A. Overall Material and Energy balances around the Pyrolytic reactor

As can be seen Table-I, II and IIIrepresents the feedstock condition of different waste plastic pyrolysis and energy flow of the pyrolytic reactor in which the conversion of Vapour-Liquid Fraction from waste plastics was takes place.

Table-I Feedstock conditions and energy flow of the pyrolytic reactor with PE

Name	PE Fed	Vap-liq fraction	Char residue
Vapor Fraction	0	1.0	0
Temperature [ºC]	450	440	32
Pressure [atm]	1	1	1
Mass Flow [kg/hr]	100	96.63	3.37
Heat Flow	454.52	323.2	131.32

[kJ/hr]			

Table-II Feedstock conditions and energy flow of the pyrolytic reactor with PP

Name	PP Fed	Vap-liq fraction	Char residue
Vapor Fraction	0	1.0	0
Temperature [ºC]	450	440	32
Pressure [atm]	1	1	1
Mass Flow [kg/hr]	100	97.44	2.56
Heat Flow [kJ/hr]	454.46	342.2	112.26

Table-III Feedstock conditions and energy flow of the pyrolytic reactor with PS

Name	PS Fed	Vap-liq fraction	Char residue
Vapor Fraction	0	1.0	0
Temperature [ºC]	450	440	32
Pressure [atm]	1	1	1
Mass Flow [kg/hr]	100	97.67	2.33
Heat Flow [kJ/hr]	454.4	386.08	68.32

From the results in Table-I, II & III, the material stream which was plastic wastes (PE, PP&PS) fed into the pyrolytic reactor, was solid and its vapor fraction was zero. Also, char residue and vapor-liquid fraction existing at different temperature in all the cases. However, the amount of vapour-liquid fraction was more than that of the char residue. Also, it was observed from results, that the heat flow in feed is almost balances to their product, although the total heat loss around the pyrolytic reactor was found to be 0 kJ/hr. Furthermore, the reaction was endothermic reaction because its heat of reaction at 25℃ was estimated to be -2.7×10^5 kJ/kmol.

Table-IV Mass flow rates of the components around the pyrolytic reactor.

Components	PE Fed (kg/hr)	Vap-liq fraction (kg/hr)	Char residue (kg/hr)
Poly Ethylene	100	0	0
Hydrogen	0	8.68	0
Methane	0	4.34	0

Ethane	0	2.27	0
Ethylene	0	0.668	0
Propene	0	0.006	0
Propane	0	0.074	0
n-butane	0	0.042	0
1-octane	0	31.8	0
Cyclo octane	0	40.2	0
1-octocosene	0	8.55	0
Carbon	0	0	3.37

Table-V Mass flow rates of the components around the pyrolytic reactor.

Components	PP Fed (kg/hr)	Vap-liq fraction (kg/hr)	Char residue (kg/hr)
Polypropylene	100	0	0
Hydrogen	0	8.49	0
Methane	0	3.24	0
Ethane	0	1.52	0
Ethylene	0	0.999	0
Propene	0	0.0022	0
Propane	0	0.083	0
n-butane	0	0.0352	0
1-octane	0	32.14	0
Cyclo octane	0	42.25	0
1-octocosene	0	8.68	0
Carbon	0	0	2.56

Table-VI Mass flow rate of the components around the pyrolytic reactor.

Components	PS Fed (kg/hr)	Vap-liq fraction (kg/hr)	Char residue (kg/hr)
Poly-Styrene	100	0	0
Hydrogen	0	4.769	0
Methane	0	2.31	0
Ethane	0	1.06	0
Ethylene	0	0.792	0
Propene	0	0.0025	0
Propane	0	0.079	0
n-butane	0	0.036	0
1-octane	0	32.08	0
Cyclo-octane	0	47.64	0
1-octocosene	0	8.90	0
Carbon	0	0	2.33

Tables IV, V & VI revealed that,the mass flow rate of the individual components after thermal cracking in pyrolytic reactor. According to the results, the amount of waste plastic entering is almost same as the amount of leaving the product due to the occurrence of the reaction.

B. Overall Material and Energy balances around the Condenser

The feedstock condition and energy flow around the condenser during the pyrolysis process were revealed in Tables VII, VIII & IX. It expresses that, Vapor-liquid fraction entering the condenser as it is vapor fraction is 1 while leaving stream vapor fraction of pyro gas is 1 and 0 of liquid fuel. Also observed from the results, that as the temperature of the pyro gas and liquid fuel was less than that of the Vapor-liquid fraction of the condenser due to the basic principle of the condensation.

Table-VII Feedstock conditions and energy flow of the condenser.

Name	Vap-liq fraction	Pyro gas	Liquid fuel
Vapor Fraction	1	1	0
Temperature [°C]	440	32	36
Pressure [atm]	1	1	1
Mass Flow [kg/hr]	96.63	14.68	81.95
Heat Flow [kJ/hr]	286.08	27.86	258.19

Table-VIII Feedstock conditions and energy flow of the condenser.

Name	Vap-liq fraction	Pyro gas	Liquid fuel
Vapor Fraction	1	1	0
Temperature [°C]	450	32	36
Pressure [atm]	1	1	1
Mass Flow [kg/hr]	97.54	8.96	83.54
Heat Flow [kJ/hr]	342.2	27.86	258.19

Table-IX Feedstock conditions and energy flow of the condenser.

Name	Vap-liq fraction	Pyro gas	Liquid fuel
Vapor Fraction	1	1	0
Temperature [°C]	440	32	36

Pressure [atm]	1	1	1
Mass Flow [kg/hr]	97.67	8.963	88.7
Heat Flow [kJ/hr]	386.08	27.89	358.19

Table-X Mass flow rates of the components around the condenser.

Components	Vap-liq fraction (kg/hr)	Pyro gas (kg/hr)	Liquid fuel (kg/hr)
Poly Ethylene	0	0	0
Hydrogen	8.68	8.42	0
Methane	4.34	4.12	0
Ethane	2.27	1.354	0
Ethylene	0.668	0.666	0
Propene	0.006	0.006	0
Propane	0.074	0.072	0
n-butane	0.042	0.042	0
1-octane	31.8	0	32.3
Cyclo octane	40.2	0	40.78
1-octocosene	8.55	0	8.87
Carbon	0	0	0

Table-XI Mass flow rates of the components around the condenser.

Components	Vap-liq fraction (kg/hr)	Pyro gas (kg/h)	Liquid fuel (kg/hr)
Poly propylene	0	0	0
Hydrogen	8.49	8.224	0
Methane	3.24	3.0306	0
Ethane	1.52	1.526	0
Ethylene	0.999	0.999	0
Propene	0.0022	0.0022	0
Propane	0.083	0.083	0
n-butane	0.0352	0.0352	0
1-octane	32.14	0	32.19
Cyclo octane	42.25	0	42.93
1-octocosene	8.68	0	8.42
Carbon	0	0	0

Table-XII Mass flow rates of the components around the condenser.

Components	Vap-liq fraction (kg/hr)	Pyro gas (kg/hr)	Liquid fuel (kg/hr)
Poly Styrene	0	0	0
Hydrogen	4.769	4.74	0
Methane	2.31	2.26	0
Ethane	1.06	1.057	0
Ethylene	0.792	0.791	0
Propene	0.0025	0.0025	0
Propane	0.079	0.079	0
n-butane	0.036	0.034	0
1-octane	32.08	0	32.2
Cyclo octane	47.64	0	47.63
1-octocosene	8.90	0	8.87
Carbon	0	0	0

Tables X, XI &XII revealed that the mass flow rates of the each component areseparated from the condenser. As the condenser was only change the phase of the material and not for any mass changes. The amount of vapour-liquid fraction entering in the condenser was found to be equal to the amount of pyro gas and liquid fuel leavingit. Also it was resulting that the simulated model is a substantial one in terms liquid fuel conversion and possible condensation. Also the obtained results showed that, the conversion of liquid fuel (1-octane, Cyclo octane and 1-octocosene) in Poly-Styrene is maximum than the other plastic wastes that produced 88.7% of liquid fuel whereas, 81.95% of Poly-Ethylene and 83.54 % of Poly-Propylene.

Among all the pyrolysis process, the conversion of Poly-Styrene was optimized than the Poly-Ethylene and Poly-Propylene polymers. The results showed that the pyrolysis in Aspen Hysys V9 was substantial one in terms of conversion.

IV. CONCLUSIONS

The developed simulated model for the process which converting waste plastics to useful petroleum fuel was carried out with the aid of Aspen Hysys V9 simulator showed that the model was a substantial one because the results were found to be in good association with the hypothetical standards of the feedstock in each part of equipment used. In addition, it was demonstrated from the simulations that, the material balance around each parts of the equipment were balanced due to the conservation law of mass and reaction occurrence. Furthermore, the energy balances revealed that the pyrolytic reactor having heat duties of 0 kJ/h and its heat of reaction at 25 ℃ was found to be -2.7×10^5 kJ/kmol.The overall results obtained from this study, conclusively revealed that, the liquid fuel could be used as an alternative fossil fuels, which can reduces the negative impact to the environment.

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Retrieval Number: D7885118419/2019©BEIESP
DOI:10.35940/ijrte.D7885.118419
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