RESEARCH ARTICLE

Simulation of waste medical plastic pyrolysis process using aspen plus V8.8

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ABSTRACT

The generation of plastic waste has global concern due to its negative effects on the environment. So, plastic waste (PW) management has emerged as a significantly challenges now global faced. Pyrolysis is a promising method to reduce pollution from plastic waste by converting waste plastic into char, pyrolytic oil and syngas. In this paper, we designed pyrolytic reactor to minimize medical plastic waste samples to pyrolytic product. This experiment also run through Aspen to compare the result with experimental value. Syringe and Glucose Bottle material was used for the experiment and simulation with the help of Redlich-Kwong model to simulate the thermal degradation process on LDPE and PP. It was found that solid, oil and Gases formation separate at first stage from the reactor and separation of gas and liquid from vapour formation with the aid of water tube condenser. The key pyrolysis conditions like temperature ranges (e.g., $3^{\circ}C - 400^{\circ}C$), operating pressure (e.g., 1.01bar to 10.13 bar) are added. The study results in the reduction in medical plastic waste collected from Medical Waste Collection centre and which we can use 15 % oil to produce Energy as a fuel in Vehicles. We can use 2% solid char for construction material and also use of 80% gas for as a fuel for burners. The work aims to optimize the pyrolysis of medical plastics for sustainable waste management, energy recovery, and safe disposal of hazardous materials. obtained results demonstrated that a conversion of Low-density polyethylene into liquid fuel up to 15% has been optimum value.

Keywords: aspen plus V8.8; Redlich-Kwong; LDPE; PP; steady state model

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1. Introduction

Medical care sector produces large Polyethylene Terephthalate (PET) and Polystyrene (PS) plastic waste for which Hospitals can use better Segregation, Medical Management and Life Cycle Assessment (LCA) to reduce effect of the incineration method for medical plastic waste treatment.^[1]. Most of medical plastic waste have use incineration method but it releases harmful toxins and sustainable solution is to use as a recycling medical plastic as a new feedstock material as well as fuel.^[2] Low recycling rate of medical plastic waste generate challenge to ecology and Health risk produces due to improper disposal of Medical waste such as Syringe, Intraverous bag and infusion set have high potential for recycling which is checked by field visit, testing and data analysis.^[3] Due to inadequate training and inadequate segregation, nations are unable to establish the necessary framework for processing medical waste. Regenerative healing is possible for medical plastic waste.^[4] The paper emphasizes requirement of Automatic waste treatment system in Covid 19 and also suggest that Biodegradable plastic serve as one of the options to handle situation of use of single use plastic in addition to that Government regulation and Widespread knowledge among people.^[5] Plastic Waste Pyrolysis provide solution by 60 to 80% generation of Valuable products with added advantage to handle different feedstock PE, PP, PS and mixed plastic waste. Improvement in 15% Oil yield possible with catalysts like zeolite in this process although scope of work in High Energy demand with reactor limitation to attend Energy efficiency, and policy support for broad implementation.^[6]



Figure 1. Waste to energy approach for medical plastic waste.

For Waste plastic pyrolysis provide competent solution as a method for WTE (Wate to Energy generation) like a valuable conversion of liquid and Syn gas up to 60 to 85 % which reduce greenhouse gas omission up to 40%. Revenue generation scope up to \$900/ton and 800 kWh of energy on the other hand favourable policy design for broad acceptance there is a scope of work in reactor efficiency, renewable integration and Catalyst Development.^[6] Pyrolysis of Plastic waste depends on temperature, heating rate, residence time, pressure, feedstock blend, and reactor design although less work on optimization of this factors and in this research to upgrade biochar efficiency and it's scale up to lab scale set up.^[7] This findings highlights gasification and pyrolysis as a good options due to lower emissions with benefit in the form of Capital cost and high feedstock quality tolerance and effective power generation. Both methods positioned as competitive and sustainable Waste to Energy option by study, which also highlights the significance of reference plant availability and assesses each technology according to capacity, energy output, environmental impact, and operating costs.^[10] Global waste is vanquished with the manoeuvre of conversion method from diagnostic plastic waste to be separated by the ordinance of Gujarat Pollution Control Board (GPCB) under which a global waste to Energy conversion goal can be achieved. All recyclable medical plastic waste gathered from the health care facility must sterilized using Autoclave /microwaving / hydro-calving followed by shredding or mutilation or combination of sterilization and shredding. Recyclable waste must never be disposed of along with general waste in dry stream and same is required to be disposed of only through registered or authorized vendors or to waste to energy plants or plastics to diesel or fuel oil or for road making, whichever is possible. One of the solutions for Single used plastic is with the Pyrolysis method shown in Figure 1. Oil generated from process work similar to Diesel as a fuel alternative to fulfil the green energy conditions. As a part of Source for the energy generation some drawbacks like production of hazardous gases as well as the increased percentage of carbon monoxide etc. ^[16] Regretfully, plastics are not biodegradable; it takes over a century for them to break down. Plastic garbage is currently disposed of in landfills or burned. Plastic incineration releases harmful emissions that are bad for the environment. However, over time, disposing of waste plastics in landfills might reduce the fertility of the soil. Due to the increasing volume of plastic waste and its harmful environmental impact, various technologies have been developed to convert waste plastics into sustainable fuel. Pyrolysis, a

method that safely decomposes plastics in the absence of oxygen, has been identified as a key solution for turning waste plastic into liquid fuel.^[8] Pyrolysis's economic feasibility depends on factors like plastic type, operating conditions, and product yields. Studies using experimental methods and simulation models provide valuable insights into these factors.^[9] compared the properties of waste HDPE-derived pyrolysis oil to those of regular diesel fuel. The pyrolysis procedure was carried out by the researchers with a range from 400 °C to 900°C with selectable set up for output in the form. The scientists hypothesized that the pyrolysis oil made from waste plastic might make a good blend ingredient for normal diesel fuel. Plastic pyrolysis from landfills yielding approximately 50% oil with 4 ppm chlorine. Remaining PVC in waste plastics contributed to the chlorine content. The author recommends 1% chlorine content for high-quality oil production.^[11] Compared to experimental research, simulation models have a number of benefits, such as the capacity to examine a broad waste materials, reduced expenses, and quicker findings.^[8] Numerous academics have employed various methodologies to replicate the process of pyrolysis. Of these methods, the simulation program Aspen Plus is thought to be one of the most widely used for simulating various forms of waste plastic pyrolysis. For instance, used the Aspen Plus program to model the pyrolysis of leftover low-density polyethylene. According to their research, increasing the pyrolysis temperature from 300 to 600 °C led to a decrease in the yield of char (11% to 4%), while the yield of syngas increased from 69% to 84%. ^[12] Aspen Plus was selected for its advanced thermodynamic modeling and superior handling of complex chemical and multiphase processes. It offers greater flexibility and accuracy compared to Aspen HYSYS, RESPONSEYS, or costly experimental methods.^[17] Used Aspen Plus to study the pyrolysis of PET waste, with an emphasis on optimizing process variables like temperature and residence time to increase the output of liquid oil.^[11] Their research made clear how important reaction temperature is in managing the quality and distribution of products. Similarly, the study used Aspen Plus to model the pyrolysis of mixed plastics, achieving the highest conversion rate of 96.36% at 500°C and 30 min retention time. The process's profitability and payback period were found to be 1.42 years, with a 35.97% return rate. It also addresses limitations by considering diverse plastic types and operating conditions, offering a more comprehensive evaluation of process performance. This approach enhances understanding and implementation of WTE related work. The Redlich-Kwong equation of state was chosen for modelling medical plastics due to its reliable prediction of vapor-liquid equilibrium in moderately nonideal systems and its computational efficiency for hydrocarbons and light gases, which are often involved in polymerization and processing. It strikes a good balance between accuracy and simplicity for thermodynamic calculations in medical plastic production.^[18] The syringes and glucose bottles were used as feedstock for most consumable items in medical sectors.^[19] Aspen plus software and minimized the waste generation by formation of pyrolytic oil.^[20] The objective of this research paper is to get the optimized result with the help of Aspen plus software and minimized the waste generation by formation of pyrolytic oil.

2.Materials and methods for testing of raw material

To get results of Elemental analysis based on Pregi & Dumas's conventional method. A Pressurized Oxygen Injection System (TurboFlash Technology) is part of the system to provide optimal combustion in a wide range of sample matrices. As a result, nitrogen, water, and carbon dioxide are released.

Proximate Analysis can be possible with ASTM D 5630 standard using Muffle furnace. It is advised to assess the inorganic residues from plastic ash using the ASTM 5630 test technique, which is crucial to understand for the manufacturing process. By means of the destructive ashing process, the test method ascertains the inorganic content of polymers. A 0.01 percent ash level is part of the test procedure. To determine Vinyl Chloride monomer (VCM) content in PVC resin as per IS: 10151. This method involves gas chromatography using a capillary column (e.g., HP-5 or equivalent) with a temperature program starting around 50°C and ramping up to ~280°C. Carrier gas (usually helium) flow rate, detector temperatures, and sample preparation steps should also be specified to ensure methodological clarity and reproducibility. The

volatiles are 'caught' at room temperature on an absorbent column, sometimes referred to as a concentrator or trap. Subsequently, the volatiles are guided into the carrier gas stream by heating the trap. The volatiles are 'caught' at room temperature on an absorbent column, sometimes referred to as a concentrator or trap. Subsequently, the volatiles are guided into the carrier gas stream by heating the trap. Such a system, which is often connected to the S/SL port, can be used to introduce samples that need to be purified or pre concentrated. ASTM D5630 for ash content analysis involves weighing a known sample mass (e.g., 1-10 g), placing it in a muffle furnace, and heating gradually to around 600°C at a controlled rate. The sample is held at this temperature for 2 hours until all combustible material is removed, and the remaining ash is weighed to calculate the content. Including these details ensures reproducibility and adherence to standard procedure.

2.1. Feedstock used and its characterization

Glucose Bottle and Syringe sample which is a Biomedical waste are the feedstocks used in the current study. The proximal and ultimate analyses that have been employed for this goal are documented in the literature. The proximate and ultimate analysis Glucose Bottle and Syringe sample was completed in a prior study, as shown in **Table 1**.



Figure 2. Gas chromatography setup.

| Table 1. | Physical | characteristic | of glucose | bottle and | syringe | sample. |
|----------|----------|----------------|------------|------------|---------|---------|
| | 2 | | 0 | | 2 0 | 1 |

| No. | Variables | Glucose Bottle(S1) | Syringe sample(S2) |
|-----|-----------------|--------------------|--------------------|
| 1 | Moisture | 0.05 % ±0.01% | 0.05% ±0.01% |
| 2 | Volatile matter | 98.62% ±0.02% | 98.62% ±0.02% |
| 3 | Fix Carbon | 0.44% ±0.02% | 0.28% ±0.02% |
| 4 | Ash | 1.05% ±0.01% | 1.1% ±0.01% |

2.2. Elemental analysis



Figure 3. CHNS analysis testing setup.

With the help of Pregi & Dumas which required Pressurized oxygen Injection system for combustion of a wide variety of sample Matrices. Sample Size less than 1 mg to 100 mg with Measuring range from 100 ppm to 100% Separation of combustion product can be possible using Thermal conductivity Detector. Detection ranges from 1 mg to 0.00001 mg for each element, run time is <10 minute with combustion temperature from 800 to 1800 °C. employ certified reference materials (CRMs) such as acetanilide, sulfanilamide, or benzoic acid. These standards are chosen for their known and stable compositions of carbon, hydrogen, nitrogen, and sulfur, ensuring accurate calibration of the instrument.

| | | | T |
|-----|---------|--------------------|--------------------|
| No. | Element | Glucose Bottle(S1) | Syringe sample(S2) |
| 1 | С | 86.037% | 86.867% |
| 2 | Н | 0% | 0% |
| 3 | Ν | 0% | 0.001% |
| 4 | S | 0% | 0.001% |
| 5 | CL | 0% | 0% |
| 6 | 0 | 11.31% | 11.85% |
| 7 | Ash | 1.05% | 1.1% |

Table 2. Elemental analysis of glucose bottle and syringe sample.

2.3. Process simulation approach

- Cubic equation of state for Redlich-Kwong-Soave (RKS) for all thermodynamic characteristics, with the exception of liquid molar volume.
- High temperature and high-pressure environments, such as those seen in supercritical extractions or hydrocarbon processing applications, are most suited for this property approach.
- At all pressures and temperatures, you can anticipate reasonable outcomes. In the critical region, the RK-SOAVE property technique is consistent.

3.Simulation process

The plastic pyrolysis process was simulated using the Aspen Plus V8.8 simulator using the following procedures.

3.1. Selection of component

The components which are a part of the property environment that are shown below. Thermal Cracking of Plastic materializes at 400° C with Distribution ratio for PE and PP is about 60%.



Figure 4. Thermal cracking pattern of plastic.

The mentioned details of (1) and (2) show the thermal cracking reaction of PE and PP, which is part of the selection in the simulator and was mentioned in **Figure. 4**

3.2. Fluid package selection

It determines the set of thermodynamic models and parameters used to calculate the properties of chemical compounds and mixtures. Here's why the selection of a fluid package is important, Aspen Plus is essential for ensuring the accuracy, reliability, and applicability of process simulations, which are crucial for process design, optimization, and analysis in various industries such as chemical engineering, petroleum refining, and pharmaceuticals. As follows the selection of the components list within the simulation software.

Specifying Components: Enter the used components in the simulation - Specification Selection sheet is used. The components in this simulation are CH4, C2H4, N2, H2O etc. We consider a conventional type as an automatic selection as participation of the same is as per phase Equilibrium. As plastic material like LDPE and PP considers as a non-conventional as standardize.

| Properties « Con | Properties < Components - Specifications + | | | | | | | | | | |
|--------------------------------|--|---|----------------------|-----------|--|--|--|--|--|--|--|
| All Items 🔹 🥥 | Selection OPetro | leum 🛛 🥝 Nonconventional 🗍 Enterprise Dat | tabase Information | | | | | | | | |
| Setup Setup Components | ect components | | | | | | | | | | |
| Specifications | Component ID | Туре | Component name | Alias | | | | | | | |
| Molecular Structure | METHANE | Conventional | METHANE | CH4 | | | | | | | |
| Signature Assay/Blend | BIOMASS | Nonconventional | | | | | | | | | |
| Petro Characterization | BIO-OIL | Pseudocomponent | | | | | | | | | |
| Pseudocomponents | ETHENE | Conventional | ETHYLENE | C2H4 | | | | | | | |
| Component Attributes | NITROGEN | Conventional | NITROGEN | N2 | | | | | | | |
| Henry Comps UNIFAC Groups | WATER | Conventional | WATER | H2O | | | | | | | |
| Polymers | HYDROGEN | Conventional | HYDROGEN | H2 | | | | | | | |
| Methods | PROPENE | Conventional | PROPYLENE | C3H6-2 | | | | | | | |
| Chemistry | BUTANE | Conventional | N-BUTANE | C4H10-1 = | | | | | | | |
| Data | 1-BUT-01 | Conventional | 1-BUTENE | C4H8-1 | | | | | | | |
| Estimation | 1-OCT-01 | Conventional | 1-OCTENE | C8H16-16 | | | | | | | |
| analysis | BENZE-01 | Conventional | BENZENE | С6Н6 | | | | | | | |
| Customize | ETHANE | Conventional | ETHANE | C2H6 | | | | | | | |
| Results | PROPANE | Conventional | PROPANE | СЗН8 | | | | | | | |
| | TOLUE-01 | Conventional | TOLUENE | С7Н8 | | | | | | | |
| | ETHYL-01 | Conventional | ETHYLBENZENE | C8H10-4 | | | | | | | |
| | 2-MET-01 | Conventional | 2-METHYL-1-PENTENE | C6H12-D2 | | | | | | | |
| □-{□ Simulation | 3-MET-01 | Conventional | 3-METHYLCYCLOPENTENE | C6H10-D2 | | | | | | | |
| Safety Analysis | STYRE-01 | Conventional | STYRENE | С8Н8 | | | | | | | |
| A Safety Analysis | 1-HEP-01 | Conventional | 1-HEPTENE | C7H14-7 | | | | | | | |
| 🚯 Energy Analysis | 1 DEC 01 | Conventional | | | | | | | | | |
| - E | Find Elec | Wizard User Defined Reorder | Review | | | | | | | | |

Figure 5. Selecting component list for pyrolysis of LDPE and polypropylene.

3.3. Pseudo-component

Based on reference data temperature 300 °Specific Gravity 0.7477 gm/cc and Molecular Weight 144.99 added for the petroleum fraction mixture which is considered for Pseudo component.

| roperties (Components - Pseudocomponents × + | | | | | | | | | | |
|--|------------------|----------------|-----------|---------------------------|------------------|---------------------|--|--|--|--|
| All Items 🔹 | Specifications | Vapor Pressure | Viscosity | Water Solubility | Petro Properties | | | | | |
| Setup Components Specifications | View Basic layou | t | • | | | | | | | |
| Specifications Molecular Structure Assay/Blend | Property metho | od ASPEN | Jata | • | | | | | | |
| ☑ Light End Properties ▷ ☑ Petro Characterization | Compor | nent Averag | ge NBP | Gravity ecific gravity | | Molecular weight | | | | |
| Pseudocomponents Component Attributes | | C | ▼ gn | n/cc | | | | | | |
| Henry Comps UNIFAC Groups | BIO-OIL | 350 | 0.7 | 477 | 1 | 44.99 | | | | |
| Delymers Methods | | | | | | | | | | |
| Chemistry Property Sets | | | | | | | | | | |
| Data | | | | | | | | | | |
| 🗀 Analysis 🕞 🤯 Customize | | | | | | | | | | |
| > 🔯 Results | | | | | | | | | | |

Figure 6. Pseudo components consider.

3.4. Methods

These derived reactions were then integrated with the chosen Fluid Package, initially RK-SOAVE. The Redlich-Kwong is effective for Vapor-liquid equilibrium in system for light hydro carbon and for moderately non ideal gas equation. Its computational efficiency and reasonable accuracy make it suitable for simulating processes like the pyrolysis of medical plastics, where such compounds are prevalent. The key pyrolysis conditions like temperature ranges (e.g., $40^{\circ}C$ – $500^{\circ}C$), operating pressure (e.g., 1.01325bar to 5.06625 bar) Specifically, the chosen fluid package for this investigation is the RK-SOAVE, Soave-Redlich-Kwong 1 equation of state is a modification of the original EOS. Compilation of fluid packages available in Aspen Plus V8.8 simulator is depicted in **Figure 7**.

| Pro | perties < | _ | Methods × | + | | | | | | |
|-----|---|---|-------------|---------------|--------------|------------|-------------------------------------|--------------|-----------|-----------|
| All | Items • | | 🥝 Global | Flowsheet | t Sections | Referenced | Information | | | |
| | 😺 Setup 🤯 Components | | Property m | nethods & c | options | | Method nar | ne | | |
| | Specifications | | Method filt | ter | COMMON | - | RK-SOAVE | | Methods | Assistant |
| | Molecular Structure | | Base methe | od | RK-SOAVE | - | | | | |
| | Assay/Blend | | Henry com | ponents | | ~ | Modify | / | | |
| | Light End Properties | | Petroleun | n calculatio | on ontions | | EOS | | ESRKSTD | - |
| | Petro Characterization Petro Characterization | | Free-wate | er method | STEAM-TA | - | Data set | | 1 | ** |
| | Component Attributes | | Water sol | lubility | 3 | | Liquid gar | mma | | - |
| | 🔚 Henry Comps | | | | | | Data set | | | |
| | UNIFAC Groups | | Electrolyt | te calculatio | on options - |] | Liquid mo | lar enthalov | HIMX107 | - |
| | Polymers | | Chemistry | y ID | | - | Liquid mo | lar volumo | VLMX20 | |
| | or Methods | | 🗸 Use tr | ue compor | nents | | | | V LIVIAZO | |
| 1 | Chemistry | | | | | | Heat of mixing | | | |
| | Property Sets | | | | | | Poynting correction | | | |
| | Estimation | | | | | | Use liquid reference state enthalpy | | | |
| | Analysis | | | | | | | | | |
| ⊳ [| Customize | | | | | | | | | |
| ⊳ [| log Results | | | | | | | | | |
| | | | | | | | | | | |
| Z | Properties | | | | | | | | | |

Figure 7. Selection of RK-SOAVE fluid package.

The SRK EOS model is defined by

$$p = \frac{RT}{\nu - b} - \frac{a}{\nu(\nu + b)} \tag{1}$$

Where a and b are the EOS model parameters^[15]. The pure component parameters (a and b) can be calculated by

$$a = \Omega_a \frac{R^2 T c^2}{P c} \alpha(T)$$
⁽²⁾

$$b = \Omega_b \frac{R.Tc}{Pc} \alpha(T) \tag{3}$$

$$\alpha(T) = \left[1 + m(\omega)\left(1 - \sqrt{\frac{T}{T_c}}\right)\right]^2 \tag{4}$$

Defining properties for defining variables like K values, Global units like METCBAR for defining units like pressure and temperature with steady state process. As we are using standard data for the analysis so it is highly recommended to use the Steady state mode as it is not suggesting the optimized behavior of the system and with Mixed Subroutine which mention that the mixture is of all solid, Liquid and Vapor phase. Selection of Ambient temperature mainly on the higher side consider for 10 bar.

| Simulation < | Economics | | Energy | | | EDR Exchang | jer Feasil | oility | |
|----------------------|-----------------------|----------------------------|-----------------|-----------------|--------------|----------------|------------|---------------|--------------|
| All Items * | Capital Cost | Utility Cost | Available En | ergy Savings | | Unknown | ОК | At Risk | |
| 🕨 🔽 Setup | | | | | | 0 | 0 | 0 | |
| Property Sets | USD | USD/Year Off | MW | % of Actual | off | | | | |
| 🗀 Analysis | Main Flowsheet × Con | trol Panel × Convergence × | Results Summary | - Streams × Res | sults Summar | v - Run Status | Setup × | SEP-2 (Elash2 | $n \times 1$ |
| Flowsheet | | i i i | ,, | | | , | | | |
| Streams | Global Description | Accounting Diagnostics | Information | | | | | | |
| Blocks | | | | | | | | | |
| REACTOR | Title | | | | | | | | |
| SEP-1 | | | | | | | | | |
| ▷ 🗔 SEP-2 | Global unit set METCB | AR - Global settings | | | | | | | |
| Utilities = | | Input mode | Steady-State | | | | | | |
| Reactions | | Stream class | MIXNC | - | | | | | |
| Convergence | | Flow basis | Mass | - | | | | | |
| Flowsheeting Options | | Ambient press | IFP 1.01325 | har - | | | | | |
| Model Analysis Tools | | Ambient press | | bui | | | | | |
| EO Configuration | | Ambient temp | 10 | C - | | | | | |
| Results Summary | | Valid phases | | - | | | | | |
| Charles Charles | | Free water | No | - | | | | | |
| Convergence | | Operational ve | ar 8766 | hr - | | | | | |
| Convergence | | , , , | | | | | | | |
| CO2 Emissions | | | | | | | | | |
| Strooms (Custom) | | | | | | | | | |
| | | | | | | | | | |
| | | | | | | | | | |
| 4D | Model Palette | | | | | | | | _ |

Figure 8. Assign steady- state process for set up.

3.5. Flow sheet

As we are considering plastic material which can a part of Non-conventional biomass to be added in the Reactor heated at sample temperature with a range from 300 °C to 500 °C with the gases as a Output is input for the separator 1 with Gas, Oil and Solid Char as a outcome can be considered from which oil and char can be used but the Gas outcome can be utilized and provided to separator 2 in which Gas can be released to atmosphere and Oil can be collected as a petroleum product mixture with potential to work as Fuel.



Figure 9. Process flow diagram in aspen plus V8.8.

3.6. Feed specification

Feed specification like temperature, pressure, mass/flow rate and total flow rate can be added for the condition like mixed specification. Biomass component specification for ULTANAL and SULFANAL using Proximate and Ultimate Analysis as per **Figure 10**.

| Simulation < | Economics | | Energy | EDR Exch | nanger Feasibility | |
|--------------------|------------------------------------|---|---------------------------------------|--------------------------|------------------------------|--|
| All Items * | Capital Cost | Utility Cost | Available Energy Savings | Unknown | n OK At Risk | |
| 🕨 🛃 Setup | | | | 0 | 0 0 | |
| Property Sets | USD | USD/Year Off | MW % of Actual 🌔 | off | • | |
| analysis | Main Flowshoot X | Control Panel X Convergence | Poculte Summany Streams V Pocu | Its Summany Run Status | × Strooms × SED 2 (Elash2) × | |
| Flowsheet | Widin Flowsneet A | Control Parlet X Convergence | Results Sulfillary - Streams A Resu | ins summary - num status | | |
| ▲ 🔯 Streams | Mixed CI Soli | id Solid Flash Options | EO Options Costing Information | | | |
| 🔺 🔯 FEED | | | | | | |
| 💽 Input 🗮 | Specifications | | | | | |
| Results | - State variables - | | Composition | | | |
| 🥺 EO Variables | Substream name | @ NC | ▼ Mass-Flow ▼ | ka/hr 🔹 | | |
| Gream Results (Cus | Terreture | 10 0 | | | | |
| GAS | Temperature | 40 L | Component | Value | | |
| GASES | Pressure | 1 atm | BIOMASS | 100 | | |
| LIQUID | Total flow basis | Marc | | | | |
| DIL | Total now busis | Muss | | | | |
| PRODUCT | Total flow rate | kg/hr | Total | 100 | | |
| SOLIDS | | | | | | |
| Blocks | Component | Attribute | | | | |
| REACTOR | Component ID | SIOMASS - | | | | |
| ▷ 🔯 SEP-1 | Attribute ID | ØPROXANAL - | | | | |
| ▷ 🗔 SEP-2 | Flement | Value | | | | |
| litilities | MOISTURE | Value | | | | |
| | WIOISTOKE | • | | | | |
| A Properties | FC | 0 | | | | |
| | ▶ VM | 99.3 | | | | |
| | ASH | 0.7 | | | | |
| | Destinte Cine Di | a de la calencia de l | | | | |
| Safety Analysis | Particle Size Dis | stribution | | | | |

Figure 10. Added feed specification for the reactor.

3.7. Reactor specification

Reactor specifications like temperature, Pressure and Process phased detail added in the Specification sheet like reactor will work at 500 $^{\circ}$ and working pressure is 1 atmospheric for the steady state Sequential process.

| Main Flowsheet × Control | Panel × Convergen | ce × Results Sumr | mary - Streams $	imes$ | Results Summary - Run | Status × | Setup × RE | ACTOR (RStoic) × + |
|--------------------------|-------------------|-------------------|------------------------|-----------------------|----------|-------------|--------------------|
| Specifications React | tions Combustion | Heat of Reaction | Selectivity PS | D 🛛 🖉 Component Attr. | Utility | Information | |
| Operating conditions | - | | | | | | |
| Flash Type | emperature 🔻 P | ressure 🔻 | | | | | |
| | · . | | | | | | |
| Temperature 50 | 00 C | • | | | | | |
| Pressure 1 | at | tm 🔻 | | | | | |
| Duty | CC | al/sec 🔹 | | | | | |
| Vapor fraction | | | | | | | |
| - Valid phases | | | | | | | |
| Vapor-Liquid | • | | | | | | |
| | | | | | | | |
| | | | | | | | |
| | | | | | | | |
| | | | | | | | |
| | | | | | | | |
| | | | | | | | |

Figure 11. RStoic reactor specification.

We can identify the stoichiometry of the element conversion from BIOMASS to the different output which is obtained like for BIO OIL conversion from the BIOMASS etc. Based on the conversion factor and relationship-based outcome added.

3.8. Separator-1 Specification

| \square | /lain | Flowsheet × Control | Panel × Convergence × | Results Summary - Stre | ams 🗙 🛛 Results Summ | nary - Run Status | × Setup × SEP-1 (Sep) × |
|-----------|-------------------|---|-------------------------|------------------------|----------------------|-------------------|-------------------------|
| | 🥑 S | pecifications Feed Flas | sh Outlet Flash Utility | Information | | | |
| | Out Out Sub | let stream conditions — let stream GASES stream MIXED | • | · · · | | | |
| | | Component ID | Specification | Basis | Value | Units | A |
| | ► | METHANE | Split fraction | | 1 | | |
| | | BIO-OIL | Split fraction | | 0 | | = |
| | | ETHENE | Split fraction | | 1 | | |
| | | NITROGEN | Split fraction | | 1 | | |
| | | WATER | Split fraction | | 1 | | |
| | | HYDROGEN | Split fraction | | 1 | | |
| | | PROPENE | Split fraction | | 1 | | |
| | | BUTANE | Split fraction | | 1 | | |
| | | 1-BUT-01 | Split fraction | | 1 | | |
| | | 1_OCT_01 | Colit fraction | | 1 | | T |

Figure 12. Process flow diagram in aspen plus V8.8.

For each component we can show the split fraction for each component for Separator 1 which specify the component concentration for the product. As per the availability and non-availability we can specify the fraction of the Component ID as 1 suggest availability and 0 indicate Non availability for the component.

| Mai | n Flowsheet × | Control Panel × Conve | ergence × | Results Summary - S | treams × Results | s Summary - Run Status | × Setup × | SEP-1 (Sep) × |
|-----|--------------------|------------------------|-----------|---------------------|------------------|------------------------|-----------|---------------|
| | Specifications | Feed Flash Outlet Flas | h Utility | Information | | | | |
| | itlet stream condi | tions | | | | | | |
| 0. | Itlet stream OIL | • | | | | | | |
| Su | bstream MIX | ED 🔻 | | | | | | |
| | | | | | | | | |
| | Componen | t ID Specific | ation | Basis | Value | Units | A | |
| ► | METHANE | Split fraction | | | 0 | | | |
| Þ | BIO-OIL | Split fraction | | | 1 | | = | |
| Þ | ETHENE | Split fraction | | | 0 | | | |
| Þ | NITROGEN | Split fraction | | | 0 | | | |
| Þ | WATER | Split fraction | | | 0 | | | |
| Þ | HYDROGEN | Split fraction | | | 0 | | | |
| Þ | PROPENE | Split fraction | | | 0 | | | |
| Þ | BUTANE | Split fraction | | | 0 | | | |
| Þ | 1-BUT-01 | Split fraction | | | 0 | | | |
| | 1_OCT_01 | Solit fraction | | | 0 | | Ŧ | |

Figure 13. Separator 1 oil based split fraction details.

Mixed stream oil component details can be considered like for Bio oil suggest availability with major fraction.

3.9. Separator-2 specification

| _ | Main Flowsheet $	imes$ | Control Panel > | Convergen | ce × / | Results Su | mmary - Strear | ns × | Results Summary | / - Run Status | × Setup × | SEP-2 (Flash2) × |
|---|------------------------|-----------------|-------------|---------|------------|----------------|------|-----------------|----------------|-----------|------------------|
| | Specifications | Flash Options | Entrainment | PSD | Utility | Information | | | | | |
| | - Flash specification | S | | | | | | | | | |
| | Flash Type | Tempera | ture 🔻 P | ressure | • | • | | | | | |
| | | | | | | | | | | | |
| | Temperature | 5 | C | | • | | | | | | |
| | Pressure | 1 | at | tm | • | | | | | | |
| | Duty | | cc | ıl/sec | Ŧ | | | | | | |
| | Vapor fraction | | | | | | | | | | |
| | Valid phases | | | | | | | | | | |
| | Vapor-Liquid | | - | | | | | | | | |
| | | | | | | | | | | | |
| | | | | | | | | | | | |
| | | | | | | | | | | | |
| | | | | | | | | | | | |
| | | | | | | | | | | | |
| | | | | | | | | | | | |

Figure 14. Separator 2 specification for vapor-liquid phase.

We have specified Flash specification for the SEP-2 with the pressure, temperature and phases details. Consider 5 $^{\circ}$ C and 1 atmospheric pressure for the Vapor and Liquid phase to be generated.

| Reactions | | | | |
|-----------|--------------------|----------------------------------|--|--|
| No. | Specification type | Stoichiometry | | |
| 1 | Frac. conversion | BIOMASS>0.00689703 BIO -OIL [23] | | |
| 2 | Frac. conversion | BIOMASS>0.0623334 METHANE | | |
| 3 | Frac. conversion | BIOMASS>0.0356458 ETHENE | | |
| 4 | Frac. conversion | BIOMASS>0.496061 HYDROGEN | | |
| 5 | Frac. conversion | BIOMASS>0.0237639 PROPENE | | |
| 6 | Frac. conversion | BIOMASS>0.0172048 BUTANE | | |
| 7 | Frac. conversion | BIOMASS>0.01782291-BUT -01 | | |
| 8 | Frac. conversion | BIOMASS> 0.00891146 1-OCT-01 | | |
| 9 | Frac. conversion | BIOMASS> 0.0128019 BENZE-01 | | |
| 10 | Frac. conversion | BIOMASS> 0.0332561 ETHANE | | |
| 11 | Frac. conversion | BIOMASS> 0.0226775 PROPANE | | |
| 12 | Frac. conversion | BIOMASS> 0.010853 TOLUE-01 | | |
| 13 | Frac. conversion | BIOMASS> 0.00941909 ETHYL-01 | | |
| 14 | Frac. conversion | BIOMASS> 0.0118819 2-MET-01 | | |
| 15 | Frac. conversion | BIOMASS> 0.0121735 3-MET-01 | | |
| 16 | Frac. conversion | BIOMASS> 0.0096014 STYRE-01 | | |
| 17 | Frac. conversion | BIOMASS> 0.0101845 1-HEP-01 | | |
| 18 | Frac. conversion | BIOMASS> 0.00712917 1-DEC-01 | | |
| 19 | Frac. conversion | BIOMASS> 0.00941909 O-XYL-01 | | |

4. Result and discussion



Figure 15. FTIR spectrum of syringe sample: PP- polypropylene.

In accordance with ASTM E1252 guidelines, the FTIR analysis employing ATR with ZnSe crystal produced trustworthy spectral data for the syringe sample. Through the use of a calibration curve, the generated spectra allowed for a quantitative assessment of the recycled material.

Figure 15 shows the spectrum of sample Syringe. It is possible to define this polymer as polypropylene. The FTIR spectrum of polypropylene presents a shoulder at 2948 cm⁻¹, and the asymmetric and symmetric inplane C–H (–CH3) at 1453 and a shoulder at 1375 cm⁻¹ confirms that it is a polypropylene. The peak at 1376 cm⁻¹ is assigned to –CH3 group.



Figure 16. FTIR spectrum of glucose bottle sample: LDPE -low density polyethylene.

Figure 16 shows the spectrum of sample Glucose Bottle. The main stretching vibrations for polyethylene appear at 2847 and 2914. The main bending mode of the –CH2 is located at 1462. As In case of LDPE these bans are located at 1462.

| Bond | Functional Group | Frequency in cm ⁻¹ | Graph no | |
|------|-------------------------|-------------------------------|--------------------------|--|
| С-Н | Alkane | 2916-2948 | Figure_02 (3353 syringe) | |
| С-Н | Alkane | 2847-2914 | Figure_03 (3354 Bottle) | |

Table 4. FTIR sample functional group.



Figure 18. TGA test (Bottle sample)

Test performed TGA analysis as per ASTM 1131 for the sample of Glucose bottle and Syringe sample also. Thermo gravimetric (TGA) analysis provides determination of endotherms, exotherms, and weight loss on heating, cooling, and more. Materials analyzed by TGA include Polymer samples. For **Figure 18** test sample weight 6.793 mg with heating from 50 °C to 850 °C at 20 °C/min. For Figure 17 test sample weight 8.292 mg with heating from 50 °C to 850 °C at 20 °C/min.

TGA uses heat to force reactions and physical changes in materials. TGA provides quantitative measurement of mass change in materials associated with transition and thermal degradation. TGA records change in mass from dehydration, decomposition, and oxidation of a sample with time and temperature. Characteristic thermo gravimetric curves are given for specific materials and chemical compounds due to

unique sequence from physicochemical reactions occurring over specific temperature ranges and heating rates. These unique characteristics are related to the molecular structure of the sample. Set the inert (usually N2) and oxidative (O2) gas flow rates to provide the appropriate environments for the test. Place the test material in the specimen holder and raise the furnace. Set the initial weight reading to 100%, and then initiate the heating program. The gas environment is preselected for either a thermal decomposition (inert - nitrogen gas), an oxidative decomposition (air or oxygen), or a thermal-oxidative combination.



Figure 19. Differential scanning calorimetry test (Syringe sample)

In a lab, testing was performed with a Differential scanning calorimetry on the samples in order to obtain the melting points of the different polymers that compose the plastic waste, a technique that is also widely used to complement the previous ones. The analysis was performed on Perkin Elmer thermal balance model STA 6000, in accordance with the standard ISO ASTM D 3418 used. In the case of the Syringe sample, DSC uses new technology which combines ultra-fast responsiveness with high stability. After the test piece is melted, cooled and reheated, only a single melting peak is obtained at 161.48°C for Figure 19 The heating of melting is 90.5 J/g, which yields a percent crystallinity of 43.7%.



Figure 20. Differential scanning calorimetry test (Bottle sample)

In order to determine the type of poly-amide the melting temperature was determined. From Figure 19. Maximum peak found at a melting temperature of 161.48 °C with e Area of 507.69 mj and delta H value 61.9146 J/g.From Figure 20. Maximum peak found at a melting temperature of 121.59 °C with Area of 690.76 mj and Delta H value 90.8897 J/g. Area under the curve indicate the latent heat of Melting and Delta H with positive value describes that Endothermic process.



Figure 21. Pressure and temperature diagram of pyrolytic oil formation.

The yield of oil percentage is increased from 0 to 15% with temperature range from $40^{\circ}C - 300^{\circ}C$ whereas temperature and pressure relationship understand form **Figure 19**. For example at 300 °C the oil fraction percent found Liquid fraction. Same way we have observed at lower temperature Oil has a higher Moisture content and Lower Viscosity. The output of bio-oil increases with the percentage of volatile components in biomass. Heat can be used to evaporate this volatile component, which condenses into bio-oil. Solid yield increases as per the High fixed carbon value which is 86.42 that can increase char production, whereas lower ash content which is 0.7 can decrease bio-oil yield. Mass balance result identified that 61.68 % Gas 15 % of oil with 5% char found which is considered Optimal operating condition of Plastic pyrolysis.



Figure 22. GC/MS chromatogram of LDPE waste plastic to diesel fuel



Figure 23. GC/MS chromatogram of PP waste plastic.

The LDPE waste GC-MS Spectra shows propane (C_3H_8) to octacosane ($C_{28}H_{58}$) indicates same spectrum used in fuel. Produce fuel could be use in internal combustion engine and feed for feed stock refinery or using diesel grade fuel could be generated electricity as well. The PP waste GC-MS Spectra shows that the carbon chain of the liquid fuel is in the range of C8-C12 contains hydro carbon which has potential to use as a fuel. [21,22]

5. Conclusion

The Aspen Plus V8.8 simulator was used to simulate the conversion of waste plastics into petroleum fuel. The model was found to be robust, with material balanced and pyrolytic reactors having a heat duty of 0 kJ/h and a reaction heat of 2.7×10^5 kJ/kmol. The study suggests liquid fuel could be an alternative fossil fuel, reducing environmental impact.

The model can be used to investigate the impact of different types of plastic waste feedstocks on pyrolysis outcomes, offering insights into feedstock selection like change of pressure and temperature did not show any change in the result. The simulation model presented in this work can only provide the scalability of the process in industries. Mass balance result identified that 61.68 % Gas 15 % of oil with 5% char found which is considered Optimal operating condition of Plastic pyrolysis. As In this work the specific heat value of pyrolysis oils is not generated via experiment. So, energy balance is not possible with this data.

Conflict of interest

The authors declare no conflict of interest.

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