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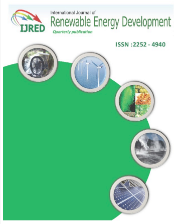

Research Article

An Experimental Investigation and Aspen HYSYS Simulation of Waste Polystyrene Catalytic Cracking Process for the Gasoline Fuel Production

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ABSTRACT. Plastic wastes are necessary to recycle due to their disposal issues around the world. They can be recycled through various techniques i.e., mechanical reprocessing, mechanical recycling, chemical recycling and incineration. Most recycling techniques are expensive and end up in producing low-grade products excluding chemical recycling; it is an eco-friendly way to deal with plastic waste. Catalytic cracking is one of the chemical recycling methods, for converting waste plastics into liquid fuel same as commercial fuels. An experimental investigation of polystyrene catalytic cracking process was conducted with impregnated fly ash catalyst and 88.4% of liquid product yield was found as a maximum at optimum operating conditions 425℃ and 60 min. The liquid fuel quality was analyzed using FTIR spectra analysis, GC/MS analysis and Physico-chemical property analysis. The GC/MS analysis shows that the fly ash cracking of polystyrene leads to the production of gasoline fuels within the hydrocarbon range of C3-C24, and the aliphatic and aromatic functional compounds were detected using FTIR analysis. Moreover, the Aspen Hysys simulation of polystyrene catalytic cracking was conducted in a pyrolytic reactor at 425℃ and at the end of the simulation, 93.6% of liquid fuel yield was predicted. It was inferred that the simulation model for the catalytic cracking is substantial to fit the experimental data in terms of liquid fuel conversion.

Keywords: Catalytic cracking; Polystyrene; Aspen Hysys simulation; Fly ash; Gasoline fuels; FTIR.

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1. Introduction

The recent research activity across the world focusing on plastic waste management. The generation of plastic in solid waste is a major environmental issue which exist in metric tons worldwide. Plastic waste has increased drastically due to its reliability and scope of applications in various sectors such as agriculture, construction, households, packaging, automobile, aerospace manufacturing, etc., (Amoodi *et al.* 2013). The generation of plastic waste has gone up exponentially on a worldwide scale since 1950 and has reached around 150 metric tons per annum all-inclusive (Cleetus *et al.,* 2013). In the upcoming decades, around 300 million tons of plastic waste would be emanated each year which corresponds to the equivalence of world human population (Saxena *et al.,* 2017). The plastic waste generation in India during 2018-2019 was estimated as 3360043 tons per annum (Annual Report-Ministry of Housing and Urban Affairs 2019). Around 50-70% of plastic wastes being packaging items mostly contained recyclable plastics such as polyethylene (PE), polypropylene (PP), polystyrene (PS), and polyvinyl chloride (PVC). Polystyrene is one of the components in municipal solid waste, which contributes 10% of total plastic wastes. The vast quantity of waste polystyrene is expected to expand even further due to the high demand for polystyrene products in our everyday life (Istadi *et al.* 2010). Polystyrene is a by-product of petrochemical industries, which is generally made up of styrene monomers. Commercially, it can be applied in households, packaging, constructions, computer cabinets and cold drink cups (Selvaganapathy *et al.* 2020).

Several disposal techniques can impel plastic waste generation, but they have some limitations. Still, plastic wastes are extensively being landfilled. These techniques have adverse effects on the environment and release harmful gases to the earth (Pinto *et al.* 1999). Recycling is the best solution to the environmental challenges in achieving sustainable manufacturing; this turns waste materials into financial, environmental and societal resources (Patni *et al.* 2013). The plastic waste can be recycled through different recycling techniques such as mechanical reprocessing, mechanical recycling, chemical recycling and incineration (Selvaganapathy & Muthuvelayudham 2019). Most recycling methods are expensive, energy-consuming and often end up in producing low-grade products excluding chemical recycling; it can significantly reduce disposal cost. Chemical recycling method is an eco-friendly approach to

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treat plastic waste containing carbonaceous materials (Patni *et al*. 2013).

The thermal and catalytic cracking's are the two different approaches of chemical recycling, which have been recognized as ideal approaches for converting waste feedstock to fuel (Lerici *et al*. 2015 and Sarker& Rashid 2013). Thermal cracking involves the decomposition of plastic wastes by applying heat (350-900℃) in an oxygen de-void condition. In contrast, catalytic cracking involves the presence of catalysts, which demonstrated as an effective conversion technique of waste plastic into useful fuel products at moderate temperatures and short retention time when compared with thermal cracking (Patni *et al*. 2013, Jouhara *et al*. 2018 and Garieb Alla & Alhag Ali 2014). FCC, fly ash, bentonites, dolomites, zeolites and silica alumina-based catalysts were extensively used in the catalytic cracking process (Miandad *et al*. 2016). However, the catalyst synthesis can enrich the catalyst's catalytic activity. Babajide et al. (2010) studied the fly ash catalyst impregnation with an aqueous KNO_3 solution and found the impregnated fly ash catalyst produced a maximum conversion than raw fly ash material. Hence, the investigated fly ash catalyst is synthesized with 20 wt.% of aqueous KNO_3; which could be a novel approach of this investigation.

Despite numerous researches being studied for the liquid fuel production from waste plastics through cracking but still, it remains inconclusive of the appropriate product composition of pyrolysis products. Only a few researchers have been focused on modeling and simulation studies by programming software such as Matlab, Pro Sim, Chem-Cadd, Aspen Hysys and Aspen Plus. The importance of this programming software like the Aspen Hysys is used to imitate the performance analysis of any chemical process. In the Aspen Hysys simulator, the product distribution of any chemical process was anticipated by operating parameters and chemical reactions. Aspen Hysys is a computer-based simulator, which relates to the physical correlations of any chemical unit process such as material and energy balances (Selvaganapathy *et al*. 2019). Based on these observations, a few investigations only have modelled the waste plastic thermal cracking process and no more research presented for catalytic cracking process (Adeniyi *et al*. 2018 and Moses *et al*. 2018). Hence, this research work is aimed to simulate the polystyrene catalytic cracking process using the Aspen Hysys simulator and. Also, the experimental investigation of polystyrene catalytic cracking process was performed with different ratios of impregnated fly ash and polystyrene materials. At the end of experiment, the produced liquid fuel was characterized using FTIR analysis, GC/MS analysis and physico-chemical property analysis.

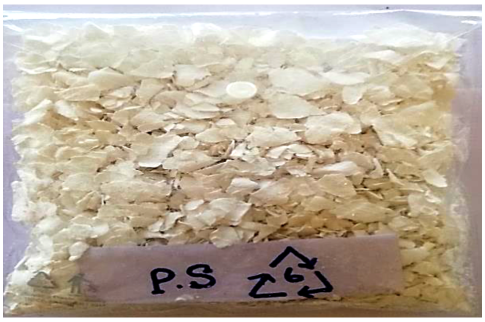


Fig.1 Polystyrene waste after shredding

2. Materials andMethods

2.1 Plastic Material

The polystyrene-type waste plastic was selected for the catalytic cracking experiments (Fig 1). Initially the raw polystyrene was shredded into a small size. The shredded polystyrene plastic was then appropriately cleaned and dried to remove unwanted dirties. The polystyrene degradation stages were assessed using a simultaneous Thermogravimetric with derivative thermogravimetric analysis (TGA-DTG).

2.2 Catalyst Material

The coal-fly ash material was selected and which is available in local markets. To promote raw catalyst's catalytic activity, incipient impregnation method was used for fly ash catalyst synthesis. Precisely, 10 g of fly ash (Fig 2) was added gradually with specified amount of aqueous KNO_3 (20 wt.%) and mixed until homogeneity. After the homogeneous reaction, the impregnate was dried in a hot air oven for 8 h at 100℃ and then cooled down to the ambient temperature. The final impregnate was again calcinated at 500℃ for 5 h. A grey coloured crystal form of the heterogeneous catalyst appeared after calcination (Fig 3). The raw and impregnated fly ash catalyst were characterized by a scanning electron microscopy (SEM) with energy dispersive spectroscopy (EDS) using an FEI-Quanta 250 analyzer. The morphological structure of the catalyst was performed using an SEM analysis, where the atomic composition was identified by EDS.

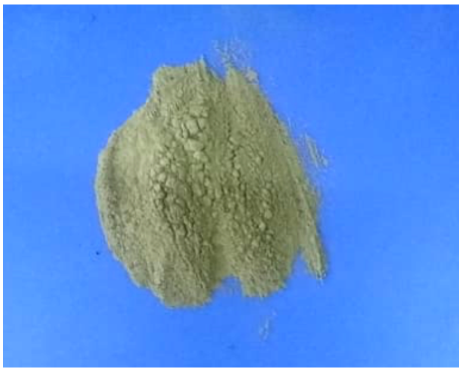


Fig.2 Raw fly ash before impregnations

Fig.3 Impregnated (20 wt.% KNO_3) fly ash catalyst

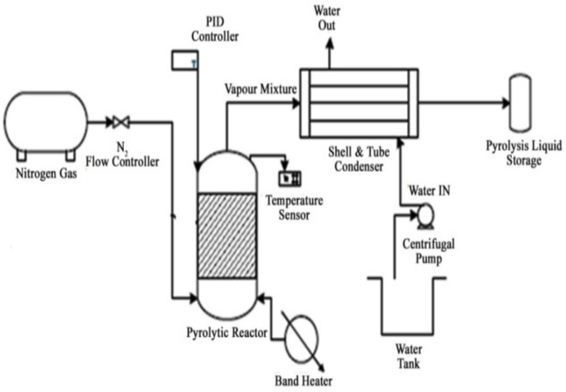


Fig.4 Experimental setup for the catalytic cracking of polystyrene

2.3 Experimental investigation of Polystyrene Catalytic cracking process

Pilot-scale equipment was used for the catalytic cracking of waste polystyrene (Fig.4). This set-up comprises the pyrolytic reactor, shell and tube condenser, band heater, PID (Proportional - Integral - Derivative) controller, temperature sensor, and purging gas (nitrogen) cylinder. The steps involved in catalytic cracking of waste polystyrene have described below;

The pyrolytic reactor with 2 kg capacity was employed for the polystyrene catalytic cracking process, and a PID controller controlled the reacting system. The nitrogen purging (10 mL/min) in the reactor prevents even the trace amount of oxygen gases. About 1:10 (0.2), 1:4 (0.25), 1:2 (0.50) and 3:4 (0.75) ratios of polystyrene with fly ash catalyst (Impregnated) were loaded to the reactor; the whole reacting system was heated at the temperatures between 400-500°C using a band heater. After the cracking reaction proceeded, the vapour mixtures coming from the reactor were then condensed through the shell and tube condenser. The liquid condensate was collected in the liquid collection point, while the condensed pyro gas was collected from the gas collector. At the end of cracking experiments, a mass balance of pyrolysis products could be made using standard mass balance analysis.

2.4 Characterization of liquid fuel

The liquid fuel obtained from the polystyrene catalytic cracking process was characterized by FT-IR spectra, GC/MS analyses and Physico-chemical property analysis. FT-IR analysis was carried out using a Perkin-Elmer spectrum (Agilent Technologies Cary-630 FTIR) in the spectral region between 400- 4000cm^{-1}. GC/MS (Agilent Technologies) analysis indicates hydrocarbons present in a liquid sample with respect to different retention times. The capillary column was fused with a capillary tube having dimensions of 30 m of length, 0.25 mm of inner diameter and film thickness of about 0.5 μm. He_2 gas was used as a carrier gas and its flow rate was maintained at 1.5 mL/min. The column oven temperature was maintained at 40℃ for 5 min, and then increased to 325℃ at a heating rate of 10℃/min, held for 10 min. The mass spectra and the data samples were interpreted and matched with standard MS programs with mass scan 35-528 EI+ data format centroid, scanning time 0.25 s. Gas chromatography with mass spectrometry (GC/MS) analysis indicates different hydrocarbon chain compounds with a different retention time of pyrolysis liquid fuel. The Physico-chemical properties of liquid fuel were analyzed using ASTM standards.

2.5 Development of simulation model for the polystyrene catalytic cracking process

The assumption to make the most feasible model for the polystyrene catalytic cracking are;

- The model is a steady-state model.
- Isobaric process and Isothermal conditions.
- The solid char residue contains carbon contents only.

Aspen Hysys V9 simulator employed the simulation of catalytic cracking of polystyrene to value-added products. In this Simulink tool contains property and simulation environments. The components used for the polystyrene catalytic cracking process were chosen from the property environment, as tabulated in Table 1. The thermodynamic model (fluid package) was also chosen from the property environment and which is used to evaluate the stoichiometric coefficient and other physical parameters of all components. Peng-Robinson's model was chosen for the thermodynamic model which is expressed in Eq. (1) (Adeniyi *et al.* 2018 and Moses *et al.* 2018). The heterogeneous catalytic reaction was chosen as a reaction set and the developed reaction set was attached to the developed fluid package. Once the reaction set was agreed, the simulation environment was moved. Unit operation blocks were picked from the palette section of the simulation environment.

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

$$19\,C_8H_8 \xrightarrow{\Delta} H_2 + CH_4 + C_2H_6 + C_2H_4 + C_3H_6 + C_3H_8 + C_4H_{10} + C_8H_{16} + C_{16}H_{32} + C_{28}H_{56} + 85C \tag{2}$$

In the Aspen Hysys, the model was developed based on the process flow sheet of Adeniyi *et al.* (2018). The reactor block was chosen from the column section and the condenser was selected from the common section in the palette. A brief description of unit operations used for catalytic cracking of polystyrene along with their section containing in the palette is described in Table 2.

Table 1
Component selection in component list environment (GariebAlla& Ali. 2014)

Component	Chemical formula	CAS number
Styrene	C_8H_8	100-42-5
Hydrogen	H_2	1333-74-0
Methane	CH_4	74-82-8
Ethane	C_2H_6	74-84-0
Ethylene	C_2H_4	74-85-1
Propene	C_3H_6	115-07-1
Propane	C_3H_8	74-98-6
n-butane	C_4H_{10}	106-97-8
Cyclo-octane	C_8H_{16}	292-64-8
1-Hexadecene	$C_{16}H_{32}$	629-73-2
1-Octocosene	$C_{28}H_{56}$	18835-34-2
Carbon	C	7440-44-0

Table 2
Brief description of blocks used catalytic cracking of polystyrene along with their section containing in the palette

Block Name	Section in palette	Description
Heating Element	Common	To heat the reactor for the burning waste plastics.
Pyrolysis reactor	Column	Simulates the pyrolysis process of waste plastic.
Condenser	Common	To convert vapour into gas and liquid.

3. Results and discussions

3.1 Thermal analysis of polystyrene

Fig.5 shows the polystyrene thermal degradation at various heating rates viz., 5, 10, 15 and 20℃/ min. With an increase in the heating rate 5 to 20 ℃ /min, the degradation temperature increases from 355.24 to 474.98 ℃. The DTG curve infers that 18% weight loss was recorded at 370.14℃ and 99.99% degradation occurred at 474.98℃. The degradation pattern is seen as single stage process from the single peak for the polystyrene wastes, which observation is also reported in several researches (Phetyim & Art 2018 and Nisar *et al.,* 2019). Further no significant variations were observed in the regime < 350℃ and >480 ℃. Nisar *et al.* (2019) reported that the polystyrene degradation occurred in the temperature between 387-428℃at various heating rates.

3.2 Catalyst Characterization

The synthesis of the raw catalyst is required to enhance the catalytic activity by increasing pore size, pore-volume and surface area (Adil, 2013). Fig.6 shows the morphological structure of the raw fly ash, which is observed as smooth with larger spherical shapes and irregular. The structure of 20 wt.% KNO_3 impregnated fly ash looks like a micro-sphere, typically between 2-10 µm, can be represented as a hollow cenosphere. The impregnation effect on fly ash catalyst destructed the structural morphology and removed the undesirable earth materials. Olivia *et al.* (2019) reported the impregnation effect on fly ash has destructed their physical structure and eliminated the unwanted impurities.

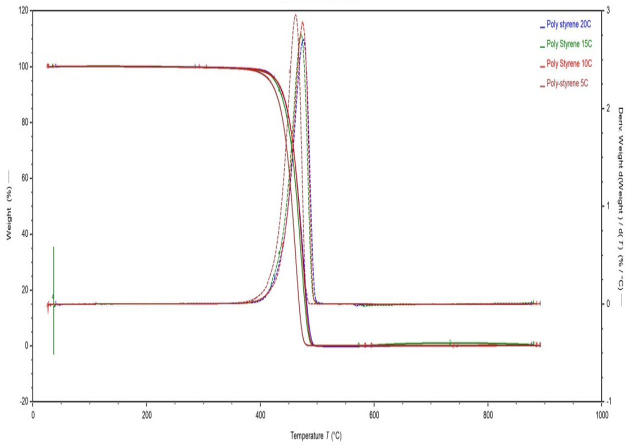


Fig. 5 TGA-DTG curves of polystyrene degradation at 5, 10, 15 and 20 °C/min

Table 3
The elemental composition of raw and impregnated fly ash catalysts

Elements	Raw fly ash	20 wt.% impregnated fly ash
O, K	50.76	56.91
Na, K	0.92	0
Mg, K	1.59	1.55
Al, K	12.70	9.72
Si, K	20.07	13.79
S, K	1.37	0
K, K	0.63	8.47
Ca, K	7.32	6.56
Fe, K	4.63	2.99

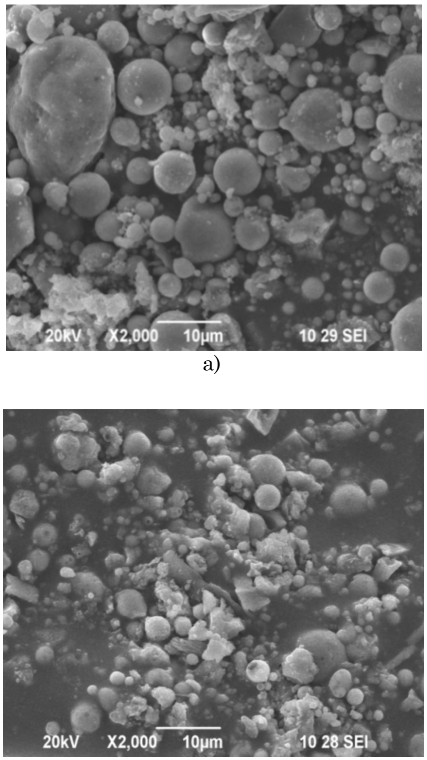
The Energy Dispersive Spectrometer (EDS) analyses used to compare the both the raw and synthesized catalyst's elemental compositions. The elemental composition of the raw and impregnated fly ash catalysts are given in Table 3 and their spectral regions are shown in Fig.7 respectively. The raw fly ash has numerous earth metals such as Ca, Fe, Na, Mg, and K. The weight percentages of the major component in raw fly ash were found to be 50.76% of O, 12.70% of Al, 20.07% of Si, 7.32% of Ca, and 4.63% of Fe with a minor component of 0.92% of Na, 1.59% of Mg, 1.375 of S and 0.63% of K. The impregnated fly ash with 20 wt.% KNO_3 catalysts had the elemental composition - 56.91% of O, 1.55% of Mg, 9.72% of Al, 13.79% of Si, 6.56% of Ca, and 2.99% of Fe. Further, it was observed that the pre-treatment has improved the number of essential elements such as Si (SiO_2), Al (Al_2O_3), Mg (MgO), Ca and K by eliminating undesirable sulfur and sodium. Olivia *et al.,* (2017) observed the impregnation effect on fly ash has enhanced the desirable Si, Al, Mg, Ca and K compositions with undesirable S and Na reductions

3.3 Factors influencing the polystyrene catalytic cracking process

In order to optimize the operating conditions, the waste polystyrene were catalytically cracked with impregnated fly ash catalyst by varying the reaction temperature from 400 to 500°C and reaction time from 45-90 min under nitrogen atmosphere. The major influencing parameters were discussed as follows;

3.3.1 Effect of Catalyst to feedstock ratio on Liquid Yield

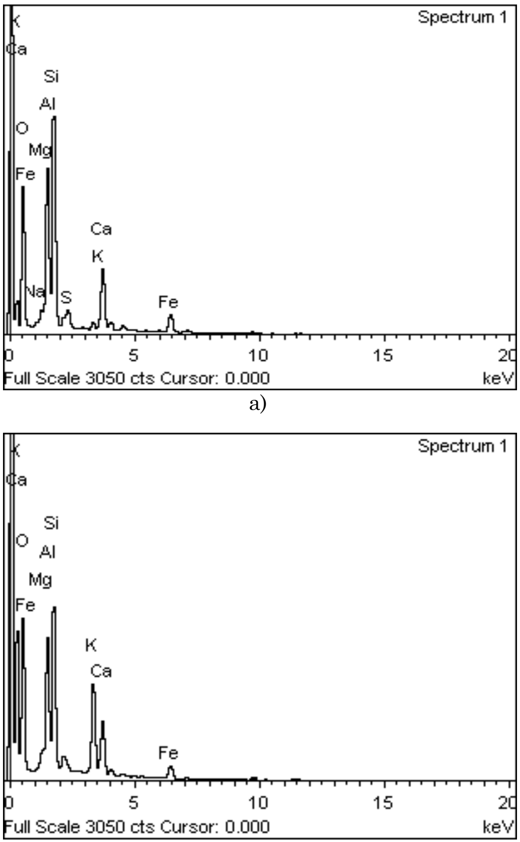
To know the appropriate quantity of catalyst for maximizing the liquid yield, the fly ash catalyst and polystyrene plastics were cracked in various ratios, viz., 1:10, 1:4, 1:2 and 3:4 under optimum conditions. The resultant plot is presented in Fig.8 and the maximum liquid yield (88.4%) was obtained at 1: 4 ratios. The liquid product yield was decreased with an increase in the fly ash amount 1:10, 1:2 and 3:4 ratios and thus ratios are not significant for the polystyrene catalytic cracking process, which is coincidence with many researchers (Cleetus *et al.*, 2013 and Panda and Singh, 2013). Panda and Singh (2013) performed thermo-catalytic process and the maximum liquid yield (87.5%) was observed at 1: 3 ratios. However, Cleetus *et al.* (2013) were found the 1:4 ratios as an optimum condition of producing maximum liquid fuel.



a)

b)

Fig.6 SEM images of a) raw fly ash catalyst andb) impregnated fly ash catalyst



a)

b)

Fig.7 EDS analysis of a) raw fly ash catalyst and b) impregnated fly ash catalysts

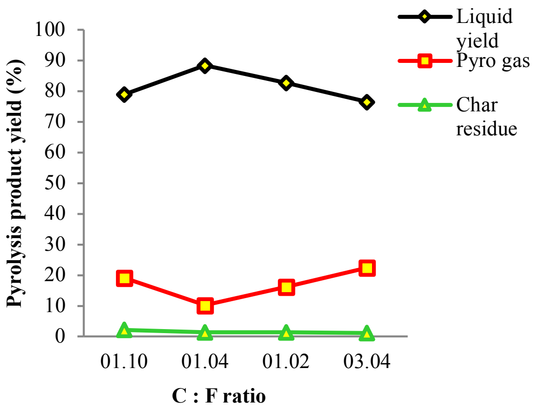


Fig.8 Effect of C: F ratio on polystyrene catalytic cracking process

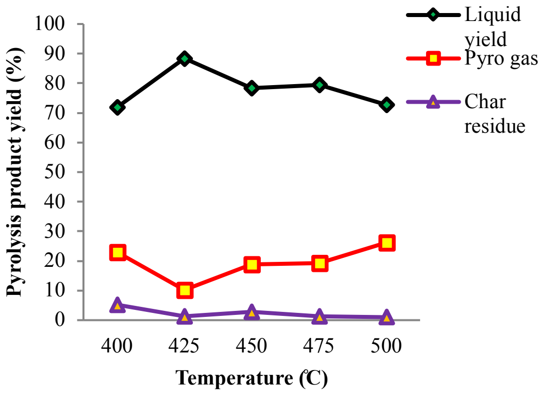


Fig.9 Effect of temperature on polystyrene catalytic cracking process

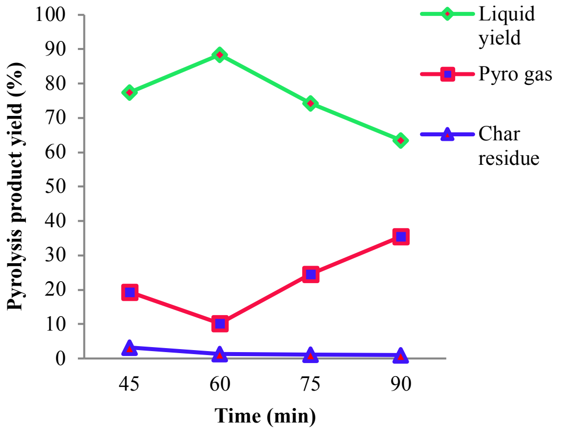


Fig.10 Effect of time on polystyrene catalytic cracking process

3.3.2 Effect of Temperature on Liquid Yield

In the fly ash cracking of polystyrene, the operating temperature significantly influences the pyrolysis product yields. In order to study the optimum reaction temperature, the polystyrene was catalytically degraded in the temperature between 400℃ - 500℃ for maximizing liquid product yield under optimum reaction conditions. The resultant plot is portrayed in Fig.9. The maximum amount of liquid yield (88.4%) was obtained at 425℃ and at 450℃ it reduced to 78.4%. Beyond the 425℃, the liquid yield reduced to 79.5% and 72.8% for the 475℃ and 500℃ respectively. Adil (2013) conducted HDPE catalytic cracking with Co-Mo catalyst in the temperature ranging between 410-450℃ and the maximum liquid product (78%) was yielded at 440℃. However, Panda and Singh (2013) reported the liquid yield has increased with the temperature above 400 ℃ and decreased with the temperature beyond 500℃.

3.3.3 Effect of Time on Liquid Yield

The effect of reaction time on polystyrene catalytic cracking process is shown in Fig.10. In the fly ash cracking of polystyrene, the maximum liquid yield was obtained at 60 min as 88.4%. Beyond the 60 min of reaction time was preferable for pyro gas production. At 75 min of reaction time, the product yields were found as 24.6% of pyro gas, 74.2% of liquid yield and 1.2% of char residue and the reaction time of 90 min the product yields were found as 35.5% of pyro gas, 63.5% of liquid yield and 1.0% of char residue respectively. Sonawane *et al.* (2015) reported the maximum conversion of liquid yield (86.4%) was observed at 65 min of reaction time from polypropylene catalytic cracking process.

3.4 Characterization of liquid fuel

The liquid fuel quality was checked using physico-chemical property, GCMS and FTIR analysis. The characterization of liquid fuel was discussed in this section.

3.4.1 Physico-Chemical Properties of liquid fuel

The liquid fuel density was 0.825 g/cc, which is almost equal to the commercial diesel density (0.807) value. The kinematic viscosity of liquid fuel was found as 1.4 cSt, which having a similar kinematic viscosity of gasoline fuel (1.17 cSt) and lower than the diesel fuel (1.9-4.1 cSt) values (Sharuddin *et al.* 2016). Pour point was used to examine the suitability of fuel for low-temperature installations (Johnson *et al.* 2015). The pour point was -3 ℃, which may be acceptable for a most geographic region (Kumar & Singh 2013). The cloud point temperature was found as +9 ℃, which had a lower cloud point than the conventional diesel (-12℃). This reveals that the produced liquid fuel was easy to handle in all the regions. Flashpoint used to analyse the fire hazards of fuel and the flashpoint temperature was determined as 36℃. This is a lower flashpoint value than the commercial diesel (52℃) and close value with commercial gasoline (42 ℃) value (Sharuddin *et al.* 2016). Gross calorific value (GCV) was found as 44.68 MJ/kg, which is higher than the commercial diesel (43.0) and commercial gasoline (42.5).

3.4.2 FTIR analysis of liquid fuel

Fig.11 shows the FTIR spectra of liquid fuel obtained from the fly ash cracking of polystyrene under optimum reaction conditions. The presence of alkene is detected at 3077 cm^{-1} in a strong appearance with respect to =C-H stretching vibrations. C-H stretching vibrations in strong appearance at 2976 cm^{-1} shows that the presence of alkane groups. The presence of aldehyde is detected at 2728 cm^{-1} in a strong appearance with respect to C-H stretching vibrations. The presence of aromatic compounds is detected at 1577 cm^{-1} and 1460 cm^{-1} in weak appearance with C=C stretching vibrations. The presence of alkyl halide is detected at 1357 cm^{-1}, and 1277 cm^{-1} in a strong peak with C-F stretching vibration. =C-H Bend stretching is detected at 821 cm^{-1} indicates that the presence of alkene. The presence of alkyl halide is detected at wavenumbers of 584 cm^{-1} with C-I stretching vibrations. Also, it was inferred from the FTIR analysis, the fuel consists of aliphatic and olefinic compounds with a major constituent of aromatic compounds. Lee *et al.* (2002) reported the FTIR analysis of liquid fuel obtained from polystyrene catalytic cracking consists more than 99% of aromatic groups with a minor quantity of paraffin's. This is due to the high stability of the aromatic compounds which inhibit the further secondary cracking.

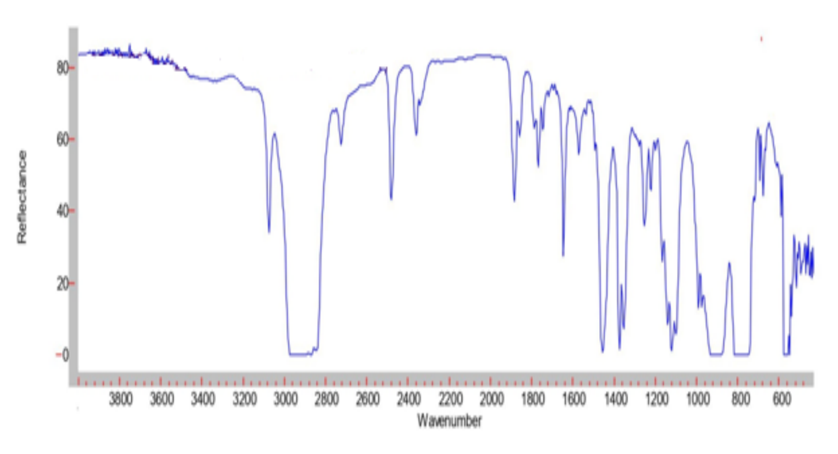


Fig.11 FTIR spectra of the liquid fuel obtained by the fly ash cracking of polystyrene

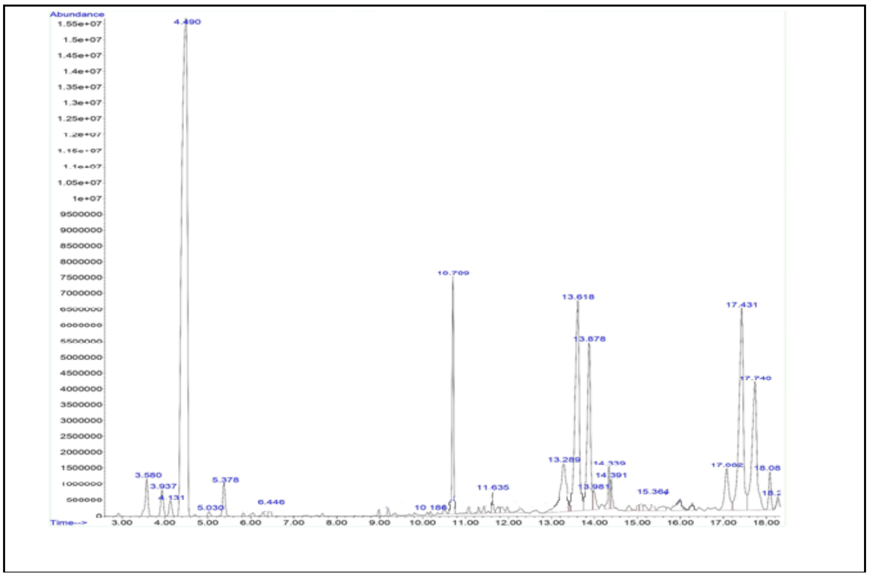


Fig.12 GC/MS analysis of the liquid fuel obtained by the fly ash cracking of polystyrene

3.4.3 GC/MS analysis of liquid fuel

The GC/MS analysis of the liquid fuel is shown in Fig.12. The assay report according to the retention time 3.580, the compound is Pentane, 2-methyl-, retention time 4.487 compound is n-Hexane, the retention time 10.707 compound is 2,4-Dimethyl-1-heptene, retention time 13.416 compound is 3-Tetradecene (E)-, retention time 13.877 compound is Tetradecane, the retention time 17.427 compound is 1-Pentadecene, the retention time 17.743 compound is Octane, 4-methyl-, the retention time 18.276 compound is Dodecyl isobutyl carbonate and few more hydrocarbons with smaller peak. The appeared hydrocarbon chain compounds mostly contain mixed fractions of gasoline, kerosene and diesel range products carbon number of C_3-C_{24}. These findings are in good association with the reported literature (Nisar et al., 2020). Nisar *et al.,* (2020) reported the catalytically cracked liquid oil from the polystyrene contains petroleum products with C_3-C_{24} carbon numbers.

3.5 Simulation output of the polystyrene catalytic cracking model

Prior to the assembling of model blocks for the catalytic cracking process, the operating condition of each block was introduced. At a flow rate of 100 kg/h, the operating temperature at 425 ℃ and inert atmospheric conditions, the polystyrene was inlet into the reactor through the material stream. The vapor fractions were produced as a top product, while the char residue was produced as a bottom product in the reacting system. The desirable vapor fractions are then fed into the condensing system to acquire high-grade products such as petroleum fuel.

3.5.1Material and energy balance of the pyrolysis reactor

The simulation environment of polystyrene catalytic cracking process is shown in Fig.13. The reactor block's operating conditions are tabulated in Table 4. The material stream polystyrene in a reactor block as a solid-state and its vapor fraction is zero. The polystyrene was converted into char residue and vapor fraction at various temperature ranges. Likewise, the mass flow rate of the vapor fraction is more than the char residue flow rate. Moreover, the material stream polystyrene's heat flow was equally distributed to the heat flow of vapor fraction and char residue. Furthermore, the catalytic cracking was an endothermic reaction and its heat of reaction at 25℃ was found as 1.89×10^5 kJ/k mol.

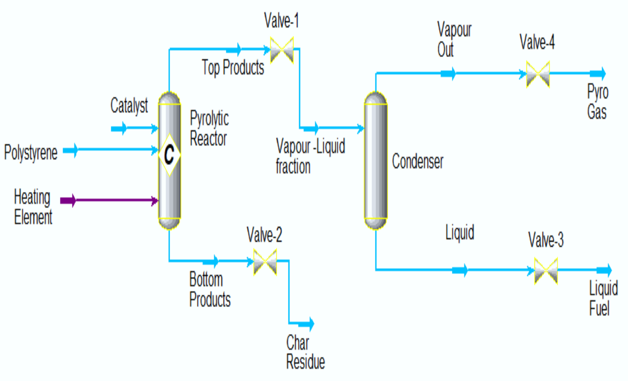


Fig.13 Simulation environment of the catalytic cracking of polystyrene

Table 4
Operating conditions of the reactor for catalytic cracking of Polystyrene

Operating variable	Polystyrene Fed	Vapor liquid fraction	Char residue
Vapor fraction	0	1	0
Reaction temperature [°C]	425	410	30
Relative pressure [atm]	1	1	1
Feed flow rate [kg/h]	100	98.74	1.26
Heat flow [kJ/h]	375.50	336.40	39.10

Table 5
Component flow rate around the reactor of Polystyrene catalytic cracking

Components	Polystyrene Fed (kg/h)	Vapor liquid fraction (kg/h)	Char residue (kg/h)
C_8H_8	100	0	0
H_2	0	3.848	0
CH_4	0	0.614	0
C_2H_6	0	0.770	0
C_2H_4	0	0.688	0
C_3H_6	0	0.0032	0
C_3H_8	0	0.062	0
C_4H_{10}	0	0.032	0
C_8H_{16}	0	35.85	0
$C_{16}H_{32}$	0	46.33	0
$C_{28}H_{56}$	0	10.54	0
C	0	0	1.26

Table 6
Operating conditions of the condenser for catalytic cracking of polystyrene

Operating variable	Vapor liquid fraction	Pyro gas	Liquid fuel
Vapor fraction	1	1	0
Reaction temperature [°C]	410	35	38
Relative pressure [atm]	1	1	1
Feed flow rate [kg/h]	98.74	5.14	93.6
Heat flow [kJ/h]	336.4	22.1	314.30

Table 5 represents the flow rate of reactant and product stream of catalytic cracking in a reactor block. According to the results, it was inferred that the mass of reactant is equally balanced with the mass of products leaving. Then, the results are a good association with the conservation law of mass.

3.5.2 Material and energy balance of the condenser

The operating conditions and energy flow around the condenser during condensation of vapor fraction into desired products are tabulated in Table 6. From Table 6, the vapor mixtures from the reactor were then fed into the condenser in which the vapor fraction is 1 whereas the vapor fraction of liquid fuel is 0 and 1 of pyro gas. Moreover, it was observed from the results, the temperature of the liquid fuel and the pyro gas is not as much as that of the vapor fraction temperature.

Table 7 expresses that component flow rate around the condenser during the condensation. At the end of the simulation, the product yield distribution was found to be 93.6% of liquid fuel, 5.14% of pyro gas and 1.26% of char residue individually. It was inferred that the simulated model for the catalytic cracking is substantial to fit the experimental data in terms of liquid fuel conversion. These investigations are in reasonable agreement with earlier researches (Adeniyi *et al.,* 2018 and Garieb Alla & Ali, 2014). Adeniyi *et al.* (2018) simulated the LDPE thermal cracking process and the maximum conversion of liquid product (92.88%) was obtained at 450℃ and inert atmospheric conditions. Garieb Alla & Ali (2014) simulated the thermal cracking of various waste plastics and results were found as 95.2% of liquid yield and 4.6% of non-condensed gases.

4. Conclusions

The polystyrene catalytic cracking experiment has been conducted in a pilot-scale pyrolytic reactor and the optimum operating conditions were found as 425℃, 45 min of reaction time, and 1:4 of catalyst to polystyrene feed ratio, for maximum liquid yield of 88.4%. Furthermore, the steady-state simulation of polystyrene catalytic cracking process was modelled through Aspen Hysys simulator and the simulated model produced 93.6% of liquid yield. Comparisons between the experimental and simulated results show that the error is 5.2%. These variations are provided reasonable agreement between the experimental and simulated results. The developed simulation mode can be a manual for scale-up studies and will give an aspiration to the researcher's for understanding the actual product ranges.

Table 7
Component flow rate around the condenser for catalytic cracking of polystyrene

Components	Vapor liquid fraction (kg/h)	Pyro gas (kg/h)	Liquid fuel (kg/h)
C_8H_8	0	0	0
H_2	3.848	2.99	0
CH_4	0.614	0.608	0
C_2H_6	0.770	0.764	0
C_2H_4	0.688	0.682	0
C_3H_6	0.0032	0.0032	0
C_3H_8	0.062	0.061	0
C_4H_{10}	0.032	0.032	0
C_8H_{16}	35.85	0	36.22
$C_{16}H_{32}$	46.33	0	46.72
$C_{28}H_{56}$	10.54	0	10.66
C	0	0	0

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