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FOURIER TRANSFORM INFRARED SPECTROSCOPY (FTIR) OF PYROLYSIS OF POLYPROPYLENE MICROPARTICLES AND ITS CHEMICAL REACTION MECHANISM COMPLETED WITH COMPUTATIONAL BIBLIOMETRIC LITERATURE REVIEW TO SUPPORT SUSTAINABLE DEVELOPMENT GOALS (SDGs)

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Abstract

The purpose of this study was to identify the effect of pyrolysis on the change in the structure of chemical compounds in polypropylene analysed using Fourier Transform Infrared (FTIR). The process was done by pyrolyzing 350 g of 3000-μm polypropylene particles using a batch reactor (Length × Width × Height = 44.5×35.5×25 cm) connected to condensers. The condensers were connected series and completed with sample collectors. Condenser 1 (Length × Height = 44.5 × 35.5×25 cm) was connected to the reactor and condenser 2 (a diameter of 14.8 cm × height of 15.8 cm) was connected to condenser 1. The reaction was done at temperatures between 64-86.6°C for 240 minutes. The condensation process was carried out at a temperature of 24°C. The result obtained in condenser 1 was a 2-phase liquid (35 mL) with a pungent smell. The upper fluid was yellowish, and the lower fluid was brown. Condenser 2 produced a 1-phase liquid (50 mL) with colourless and kerosene-like smells. The FTIR analysis showed that samples from condenser 1 (phase 1; top phase) and condenser 2 contain the same compound and mostly water, whereas condenser 1 (phase 2; bottom phase) showed the presence of C-H out of plane functional groups, C-H alkenes, isotactic polypropylene bonds, alkanes, and alkene C=C strain. Further, it had C=C bonds which were not found in pure polypropylene. This occurs due to structural reorganization in polypropylene which was characterized by the breaking of the C-C bending bonds. This research provides important insight into the role of the condenser in the polypropylene pyrolysis process and its influence on the chemical and physical properties of the resulting liquid. This study can also support current issues in the Sustainable Development Goals (SDGs).

Keywords: Condensers, FTIR, Polypropylene, pyrolysis.

1.Introduction

Polypropylene (PP) is a polymer produced from the polymerization process of propylene gas with the chemical structure $(C_3H_6)_n$. Polypropylene has a high glass transition (Tg) of around 190 – 200°C, a melting point of 160 – 166°C, and has low thermal conductivity of 0.12 w/m. Polypropylene has high chemical resistance but low impact resistance. The high crystallinity of polypropylene can cause high, rigid, and hard strain forces [1, 2].

Polypropylene production in Indonesia reaches 600,000 tons/year and the need for polypropylene in the world increases every year with an average annual increase of 9.7%. Polypropylene plastic is widely used in making drink bottles, food boxes, and food storage [3]. Based on data from the Badan Pusat Statistik (BPS) regarding Indonesian Environmental Statistics in 2018, plastic waste in Indonesia reached 65.2 million tons per year (https://www.worldbank.org/en/country/indonesia/publication/plastic-waste-discharges-from-rivers-and-coastlines-in-indonesia; retrieved on May 2025). One type of plastic that contributes to waste is polypropylene plastic. This type of plastic is a plastic that is difficult to degrade and is usually disposed of directly into the environment without prior processing [4, 5].

At present, the processing of polypropylene-type plastic as one way of handling waste can be done through various methods. Currently, various methods can be used to proceed with plastic waste. Some people proposed the use of alternative plastic, such as bioplastic [6-8]. Other researchers give ideas for reusing, and recycling plastic [9], or even give regulations [10]. Some methods for solving plastic issues are mechanical shredding methods for transforming plastic into small pieces to make it easy for further processes [11, 12]. Others are the pyrolysis methods for decomposing plastic into simple fractions with high heating [13, 14], and processing methods using chemical reactions to modify the structure of plastic and change it into a valuable product [15].

Research on how to solve polypropylene issues has been well-documented and attracted attention from researchers (see Fig. 1 from bibliometric analysis in Scopus database), showing an increasing number of publications time by time. Bibliometric analysis is one of the excellent methods to understand current research trends, as reported elsewhere [16-24]. Table 1 shows some previous studies on pyrolysis of polypropylene plastics. Some of these methods are carbonation [25], co-carbonization [26], hot pressing [27], pyrolysis (polypropylene and polystyrene) [28], and pyrolysis (using an optical infrared separator) [29].

From the current studies shown in Table 1, there has been no research analysing FTIR from the results of pyrolysis of polypropylene plastic. Therefore, we selected the pyrolysis method to process polypropylene plastic because the method can be done easily and possibly carried out on a small scale. Pyrolysis was chosen because it can produce renewable fuels and other valuable products that can be useful for everyday life [30-36].

As a continuation of our previous studies [37-39], the purpose of this study was to identify the effect of pyrolysis on the change in the structure of chemical compounds in polypropylene analysed using Fourier Transform Infrared (FTIR). This research provides important insight into the role of the condenser in the polypropylene pyrolysis process and its influence on the chemical and physical properties of the resulting liquid.

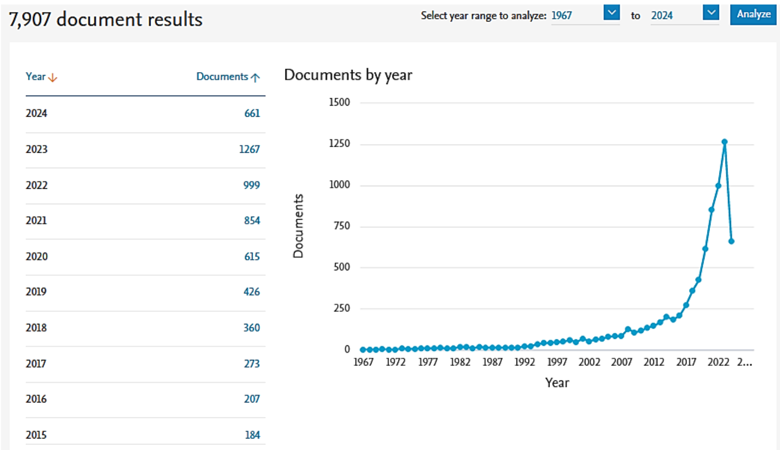


Fig. 1. Scopus database for research trend for "polypropylene waste" taken on May 2024. Detailed information for the bibliometric analysis is explained elsewhere [23].

Table 1. Previous studies on pyrolysis of polypropylene plastics.

No.	Title	Author/Ref.	Note
1	Penerapan teknologi pengolahan sampah plastik menjadi briket arang plastik (study case: Bank sampah Asy-Syifa Berkah)	Amyranti et al. [25]	Polypropylene is used as plastic charcoal briquettes combined with PET (polyethylene) type plastic through the material carbonation method.
2	Valorization of waste biaxially-oriented polypropylene plastic films by its co-carbonization with almond leaves	Adeneyi et al. [26]	Biaxially oriented co-carbonization (BOOP) polypropylene waste for hybrid biochar production
3	Pemanfaatan limbah plastik polyprophylene (PP) dan sekam padi menjadi papan partikel	Meldayanoor and Rusuminto [27]	Polypropylene plastic combined with rice husks is used as particle board using the "Hot Pressing" method.
4	Pengolahan plastik polystyrene dan polypropylene menjadi liquid fuel menggunakan katalis gamma alumina (γ-Al_2O_3) dan zeolit teraktivasi dalam single stage separator	Aswan et al. [28]	Pyrolysis with Polystyrene and Polypropylene plastic types with variations of 20% Zeolite catalyst and 10% Gamma Alumina catalyst.
5	Recycling of polypropylene recovered from a composting plant: Mechanical behavior of compounds with virgin plastic	Badini et al. [29]	Recycling of polypropylene is carried out by recovery involving a sorting step carried out using an optical infrared separator and a washing treatment. Then, pelletize the recovered polypropylene, mix it with commercial polypropylene raw materials, and make the item by injection moulding.

This study can also support current issues in the Sustainable Development Goals (SDGs), while SDGs have become one of the popular issues recently [40-44]. In addition, different from other studies, we have novelties in this study in optimizing the size of the condensers used. Different condenser sizes can create different results. It can increase the surface area of condensation and improve the separation efficiency and the formation of pyrolysis resulting liquid. The larger condenser can provide a wider contact area between the pyrolysis vapor and the condenser surface. Thus, it can increase the cooling rate [45]. Then the quality and quantity of liquid products produced can be more optimal and the separation of product fractions can be more effective based on their boiling point. This approach in addition to improving process efficiency, can also reduce the energy required for cooling and is environmentally friendly.

2. Method

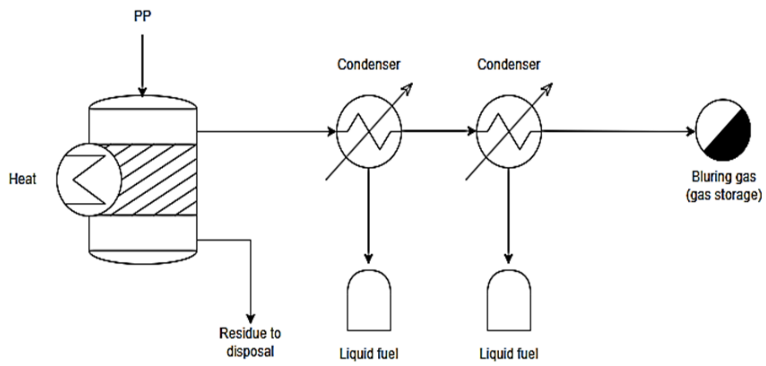
The tools used in this experiment include a rectangular can measuring 44.5×35.5×25 cm, a cylindrical can with a diameter of 14.8 cm and a height of 15.8 cm, an aluminum pipe with a diameter of 8 mm (length = 25 cm), an aluminum pipe with a diameter of 19 mm (length = 50 cm), glue, LPG gas (as the combustion source), a silicone hose with a diameter of 13 mm (length = 25 cm), a water container, a thermocouple, a gas stove, and a regulator. The materials used are pure polypropylene particles (350 g), plasticine, and water.

The process flow diagram of polypropylene pyrolysis is shown in Fig. 2(a). The pyrolysis process used Liquid Petroleum Gas (LPG) as the heat source. The system was a closed batch reactor (Length × Width × height = 44.5×35.5×25 cm), where the reactor was connected to an aluminum pipe that serves as the gas flow medium. The gas flowing through the aluminum pipe condensed in two different condenser variations. The gas condensed in the condenser when its temperature was lower than the temperature of the gas in the reactor. The combustion residue from pyrolysis (exhaust gas) was collected in the gas storage (blurring gas). Then, Fig. 2(b) shows the flow chart of the pyrolysis procedure. Polypropylene pyrolysis was conducted by heating 350 g of polypropylene particles in the reactor at a temperature of ±86.6°C for 240 minutes. Every 30 minutes, the reactor temperature was periodically checked using a thermocouple (see Table 2). The vapor/gas produced from the heating process was directed into two different condensers connected by an aluminum pipe. The cooling process occurs in condenser 1 and condenser 2, resulting in liquids with different characteristics.

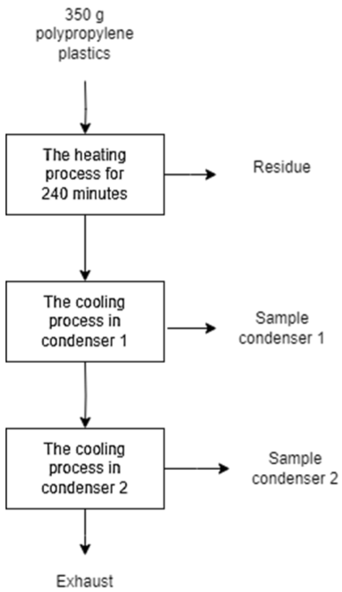
Table 2. Time and pyrolysis temperature.

No.	Time (min)	T (°C)
1.	30	64
2.	60	68.4
3.	90	65
4.	120	86.6
5.	150	86.6
6.	180	86.6
7.	210	86.8
8.	240	86.6

The sample characterization was performed using a Shimadzu 8400 Fourier Transform Infrared (FTIR) instrument. This analysis was conducted to determine the functional group structure present in the condenser sample. Potassium bromide (KBr) was added to the sample, which was then homogenized using a mortar and pestle and moulded into pellets. The sample was subsequently analysed using the FTIR instrument.



(a) The process flow diagram of polypropylene pyrolysis.



(b) flow chart of the pyrolysis procedure.

Fig. 2. (a) Process flow diagram pyrolysis and (b) Flow chart pyrolysis.

3. Results and Discussion

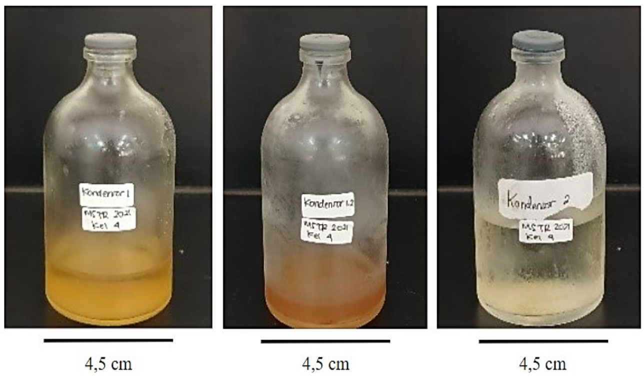
When the pyrolysis process takes place, the long chain of hydrocarbons is cut into shorter ones. Furthermore, a cooling process is carried out on the gas resulting from produced gasses. Thus, it will condense and form a liquid. This liquid will be accommodated in condenser 1 and condenser 2. Detailed information regarding the physical properties of samples is shown in Table 3. Then, the appearance of the samples is shown in Fig. 3.

The reactor temperature at the initial 30 minutes was around 64°C assuming that the plastic ore was still in the process of melting. In this study, there was a decrease in temperature to 65°C within 90 minutes. This decrease in temperature can occur due to heat loss to the environment. This can occur through conduction where heat from within will be transferred to the reactor wall and will be transferred to the surrounding environment.

After the temperature decreased, there was a significant temperature increase, and as the heating temperature increased, the substances contained in the plastic pellets decomposed completely. This is based on the Arrhenius equation, which states that the higher temperature allows the greater thermal decomposition constant. Thus, increasing the rate of pyrolysis causes the hydrocarbon vapor to condense into hydrocarbon liquid more quickly. At 120 – 240 minutes, the temperature became constant at 86.6°C. This temperature is quite different from the melting point of polypropylene, indicating that the pyrolysis occurring in the reactor was not completely decomposed.

Table 3. Physical properties of pyrolyzed polypropylene plastic pyrolysis.

PP (g)	Combustion Temp (°C)	Burning Time (min)	Combustion Results	Vol (mL)	Physical properties of the sample
350	86.6	240	Condenser Sample 1 (phase 1)	25	The liquid is yellowish, smells slightly pungent
			Condenser Sample 1 (phase 2)	10	Colloids are brownish, smell slightly pungent
			Condenser Sample 2	50	Colourless liquid, smells distinctively like diesel



(a) (b) (c)

Fig. 3. (a) Pyrolysis Product from Condenser 1 (phase 1; top phase); (b) Pyrolysis Product from Condenser 1 (phase 2; bottom phase); and (c) Pyrolysis Product from Condenser 2.

Based on Table 3, there are three samples obtained from 2 different condensers. In condenser 1, a yellowish liquid of 35 mL was produced. The resulting liquid in condenser 1 had 2 phases that did not dissolve each other. Therefore, the resulting liquid was separated and given two different labels. The upper fluid (phase 1; top phase) was yellowish and the lower fluid (phase 2; bottom phase) was brownish and slightly colloidal. The colloid produced in condenser 1 bottom phase (phase 2) was formed due to a reaction between fuel and existing rust that exists in condenser 1. Also due to the formation of micelle between water and oil phase. The volumes of each phase were phase 1 (25 mL) and phase 2 (10 mL), which were produced from 350 g of polypropylene.

In contrast to the sample produced in condenser 1, the sample produced in condenser 2 was a colourless liquid and the volume produced was much larger (50 mL) with a distinctive smell like kerosene. This is because the condensation process takes longer. Based on experimental results, heating 350 g of PP plastic at a temperature of 86.6°C for 240 minutes produces a liquid with a total volume of 85 mL.

After obtaining liquids labelled with condenser 1 (phase 1), condenser 1 (phase 2), and condenser 2 samples, analysis was carried out using the FTIR instrument. The sample produced in condenser 1 must be separated because it had 2 different phases. The results of characterization using FTIR are combined into the scheme shown in Fig. 4. Table 4 presents FTIR data for further analysis. To ensure the analysis, FTIR data was compared to literature [37, 46-48].

The spectrum had a wavenumber scale of 4000 – 500 cm^{-1} and transmittance of 20 – 100%. The peaks that appeared in the spectrum can provide information about the type of chemical bonds and functional groups present in the sample. There are different forms of spectrum. In pure polypropylene, there are sharp peaks at various wavenumbers, indicating the presence of typical peaks for polypropylene, namely isotactic bonds at wavenumbers 800-980 cm^{-1} and the presence of C-C bond bending at 1170 cm^{-1}. In the spectrum of condenser sample 1 (phase 1; top phase) and condenser sample 2, there are peaks with widened and elongated shapes. This peak is characteristic of the presence of hydrogen bonding (H_2O), which is shown at wavenumbers 3463.27 cm^{-1} for Condenser Sample 1 (phase 1; top phase) and 3309.96 cm^{-1} for Condenser Sample 2. Meanwhile, in condenser 1 (phase 2; bottom phase), it has quite sharp peaks and can be interpreted well. Among these are the most prominent peaks not found in condenser samples 1 and 2.

Based on Table 4, FTIR for pure polypropylene showed the presence of nine peaks with different wavenumbers. The wavenumbers at 2950, 2916, 2868, and 2836 cm^{-1} describe the presence of C-H stretching groups, whereas peaks 1456 and 1378 cm^{-1} are specific spectra of polypropylene containing CH_2 deformation and CH_3 symmetrical formation form, respectively. Peaks at 998, 974, and 842 cm^{-1} show isotactic polypropylene bonds. Lastly, the spectrum at the peak of 1167 cm^{-1} shows C-C bending which is the polypropylene backbone itself.

In the condenser sample 1 (phase 1; top phase) (see Table 4), five peaks with different wavenumbers were obtained. The peak at a wavenumber of 671.25 cm^{-1} describes the presence of an alkene functional group (C-H). The peak at a wavenumber of 1643.41cm^{-1} indicates an alkene functional group C=C stretching. The peak at a wavelength of 2067.76 cm^{-1} indicates the presence of an alkane functional group (C-H). The peak at a wavenumber of 2939.61 cm^{-1} indicates the presence of C-H sp^3. The peak at a wavenumber of 3463.27 cm^{-1} indicates the presence of water (H_2O) because it has a long and widened shape.

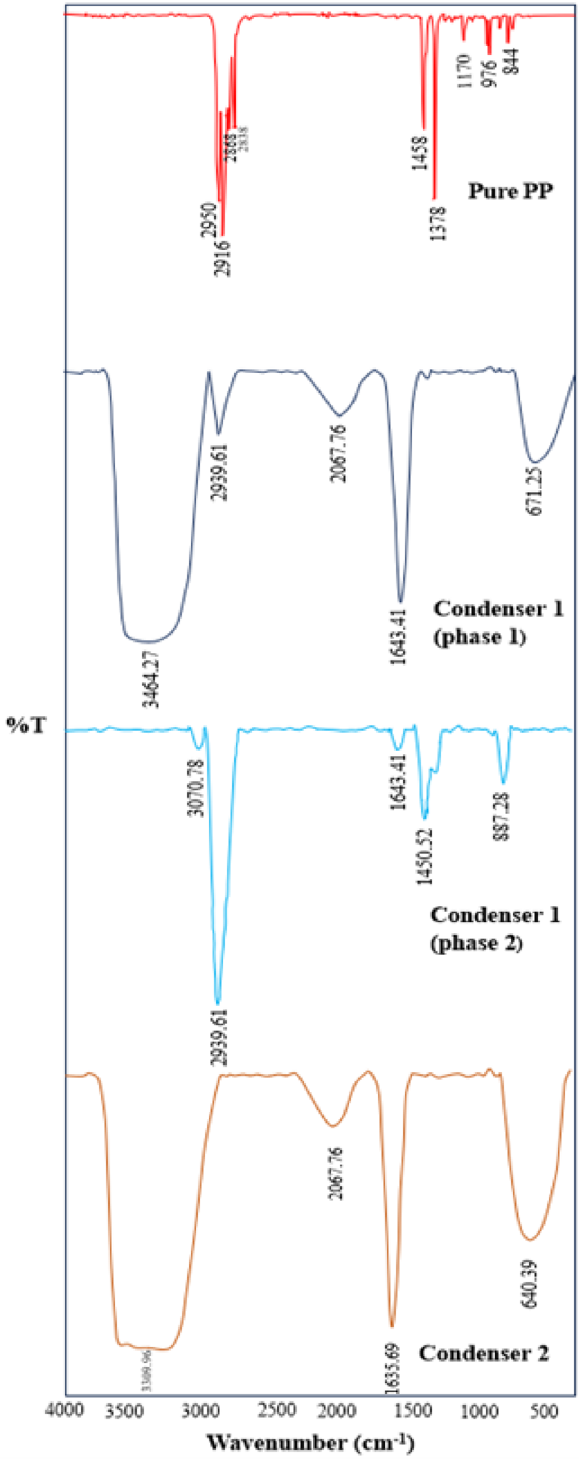


Fig. 4. FTIR Spectrum (a) pure polypropylene; (b) condensers 1 (phase 1); (c) condensers 1 (phase 2); and (d) condensers 2

Table 4. Comparison of FTIR data.

No.	PP (cm^{-1})	Condenser Sample 1 (phase 1) (cm^{-1})	Condenser Sample 1 (phase 2) (cm^{-1})	Condenser Sample 2 (cm^{-1})	Function Group
1	-	-	-	640.39	C-H out of plane bend
2	-	671.25	-	-	Alkene (C-H)
3	844	-	887.28	-	Isotactic polypropylene bonds
4	976	-	-	-	Isotactic polypropylene bonds
5	1170	-	-	-	C-C bending
6	1378	-	-	-	CH_3 symmetrical shape formation
7	-	-	1450.52	-	Alkana (scissors/bending)
8	1458	-	-	-	CH_2 deformation
9	-	-	-	1635.69	Alkene C=C stretching
10	-	1643.41	1643.41	-	Alkene C=C stretching
11	-	2067.76	-	2067.76	Alkana (C-H)
12	2836	-	-	-	C-H stretching
13	2868	-	-	-	C-H stretching
14	2916	-	-	-	C-H stretching
15		2939.61	2939.61	-	C-H stretching
16	2950	-	-	-	C-H stretching
17	-	-	3070.78	-	Alkane C-H stretching
18	-	-	-	3309.96	Hydrogen Bonding (H_2O)
19	-	3463.27	-	-	Hydrogen Bonding (H_2O)

For the sample in condenser 2 (see Table 4), four peaks with different wavenumbers were obtained. At the first peak at a wavenumber of 640.39 cm^{-1}, it describes the presence of a C-H bend functional group. For the second peak at a wavenumber of 1635.69 cm^{-1}, there is an alkene functional group C=C stretching. For the third peak at a wavelength of 2067.76 cm^{-1}, it indicates the presence of an alkane functional group (C-H). Finally, the fourth peak at a wavenumber of 3309.96 cm^{-1}, indicates the presence of hydrogen bonds, whereas the FTIR spectrum interprets the presence of water (H_2O) because it has a long and widened shape.

As explained earlier, in condenser FTIR data 1 (phase 2; bottom phase), there is a new bond formation that was not identified in pure polypropylene FTIR data. In these data (see Table 4), it obtained five peaks, namely the first peak with a wavenumber of 887.28 cm^{-1} (the presence of a C-H functional group out of plane bend or indicating the presence of isotactic polypropylene bonds), the second peak with a wavenumber of 1450.52 cm^{-1} (an alkane functional group (scissors/bending), the third peak with a wavenumber of 1643.41 cm^{-1} (an alkene group C=C stretching), the fourth peak with a wavenumber of 2939.61 cm^{-1} (a C-H sp^3 functional group), and the fifth peak with a wavenumber of 3070.78 cm^{-1} (an alkane C-H stretching functional group).

The FTIR spectrum of condenser 1 (phase 1; top phase) and condenser 2 samples shows more water content, the functional group content in these samples cannot be identified properly. However, condenser 1 (phase 2; bottom phase) does not show the presence of water, so it can be used as a comparison with the pure polypropylene FTIR spectrum.

The peak comparison (see Table 4) between the FTIR spectra of pure polypropylene and the FTIR of polypropylene pyrolysis results in condenser sample 1 (phase 2; bottom phase) shows a difference. This has the possibility of thermal decomposition at high temperatures in the presence of oxygen, that is, there is a break of chemical bonds in the polymer chain. This process produces various types of small molecules, including molecules that have C=C double bonds.

Based on the comparative analysis of functional groups, the chemical structure of pyrolyzed polypropylene undergoes thermal decomposition at high temperatures resulting in a C=C double bond. Based on the reaction (Fig. 5), the formation of C=C double bonds go through several stages: (i) Breaking the polymer chain bonds of C-H and C-C bonds; (ii) Formation of free radicals; and (iii) Formation of double bond C=C.

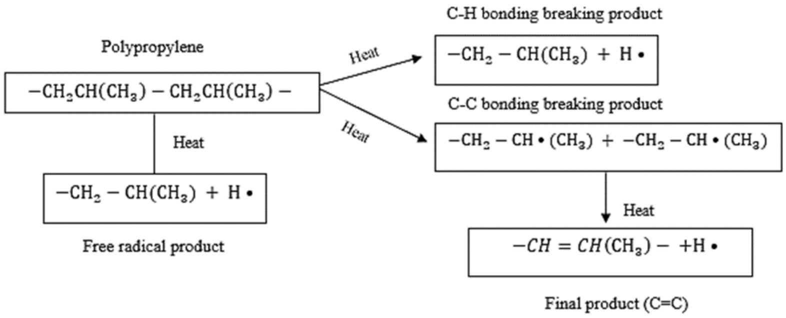


Fig. 5. Polypropylene pyrolysis reaction scheme.

There are several reactions:

(i) Polymer Chain Termination (C-H bond)

(a) C-H Bond Termination

$$-CH_2CH(CH_3)-CH_2CH(CH_3)- \quad \text{heat} \rightarrow \; -CH_2-CH(CH_3) + H\bullet$$

(b) C-C Bond TC-C Bond Termination

$$-CH_2CH(CH_3)-CH_2CH(CH_3)- \quad \text{heat} \rightarrow \; -CH_2-CH\bullet(CH_3) + -CH_2-CH\bullet(CH_3)$$

In the presence of high temperatures, the bonds in the polypropylene chain including C-H bonds and C-C bending begin to break. This causes the formation of free radical H at the points of breaking these bonds.

(ii) Free Radical Formation

$$-CH_2CH(CH_3)- \quad \text{heat} \rightarrow \; -CH_2-CH(CH_3)\bullet +H\bullet$$

The breaking of C-H and C-C bonds forms alpha radicals and polymer radicals. Where these free radicals can react with each other to form new structures. Some radicals can recombine to form single bonds, while some other radicals can undergo reorganization (loss of hydrogen atoms) leading to the formation of C=C double bonds.

(iii) Formation of Double Bond C=C

$$-CH_2 - CH(CH_3) \bullet + - CH_2 - CH(CH_3) \bullet \text{ heat} \rightarrow -CH = CH(CH_3) - \ +H \bullet$$

Free radicals formed tend to be very reactive and can interact with other free radicals around them. Free radicals that undergo reorganization (loss of hydrogen atoms) combine to form a C=C double bond. Thus, although pure polypropylene does not have a C=C double bond in the FTIR spectrum, the pyrolysis process of polypropylene plastic involves breaking and reorganizing the bond under high thermal conditions to form a new structure containing the C=C double bond.

Finally, this study adds new information regarding the pyrolysis of polypropylene. Since this polypropylene has been well-used in daily use products, this study will be beneficial for further processes, especially relating to the burning/pyrolysis of plastic waste. Indeed, this will bring benefits for solving current issues in the SDGs, while SDGs have been well-reported in current research trends [49-53].

4. Conclusion

This study identified the effect of pyrolysis on the change in the structure of chemical compounds in polypropylene analysed using FTIR. The process was done by pyrolyzing 350 g of 3000-μm polypropylene particles using a batch reactor (Length × Width × Height = 44.5×35.5×25 cm) connected to condensers. The reaction was done at temperatures between 64-86.6°C for 240 minutes. The condensation process was carried out at a temperature of 24°C. The results from FTIR analysis were then compared to create a proposal mechanism in the reaction during the pyrolysis. This research provides important insight into the role of the condenser in the polypropylene pyrolysis process and its influence on the chemical and physical properties of the resulting liquid. This study can also support current issues in the SDGs.

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