CHEMICAL ENGINEERING TRANSACTIONS
VOL. 120, 2025
A publication of AIDIC
The Italian Association of Chemical Engineering
Online at www.cetjournal.it
Guest Editors: Bing Shen How, Viknesh Andiappan, Denny K.S. Ng, Hon Loong Lam, Petar S. Varbanov

ISBN 979-12-81206-21-2; **ISSN** 2283-9216
DOI: 10.3303/CET25120052

Development of P-Graph Models for the Synthesis of Plastic Waste-To-Fuel Supply Chain

Kyla Bianca S. Tuaño*, Hazelyn Lauren R. Kho, Kathleen B. Aviso, Raymond R. Tan

Department of Chemical Engineering, De La Salle University, 2401 Taft Avenue, 0922 Manila, Philippines
kyla_bianca_tuano@dlsu.edu.ph

The conversion of plastic waste into fuel presents a sustainable solution to plastic pollution and fuel shortages. Several plastic waste-to-fuel technologies exist, and the quality and yield of the resulting fuels depend on factors like feedstock composition and treatment processes. Large-scale commercialization is hindered by environmental concerns, particularly carbon emissions. To address this, a systematic optimization approach is necessary to ensure environmental and operational viability. This study applies Process Graph (P-Graph) models to optimize the plastic waste-to-fuel supply chain, identifying network configurations that meet fuel demand while minimizing carbon emissions. An illustrative case study was analysed to delineate the capabilities of the P-graph framework in the fuel distribution system. The case study considers the carbon emissions of networks where the optimal solution yielded a carbon footprint of 0.1229 t CO_2/GJ. Carbon footprint values of the 32 feasible structures were found to range up to 0.1266 t CO_2/GJ. These findings demonstrate the P-Graph framework's potential in supporting low-emission, flexible system designs.

1. Introduction

Plastics have one of the strongest production growths globally, increasing from 2 Mt in 1950 to over 368 Mt in 2019. The increasing consumption has also led to an increase in waste generation, contributing to environmental pollution and greenhouse gas (GHG) emissions. Plastics contribute to particulate emissions, environmental pollution, and adverse human effects (Pilapitiya and Ratnayake, 2024). International organizations like the Nordic Council of Ministers and the United Nations have initiated agreements to mitigate the impacts of plastic pollution (Lau et al., 2020).

There are several established methods to address plastic pollution, including mechanical and chemical recycling, as well as energy recovery (Li et al., 2022). Fuel recovery has gained significant attention. In 2020, the global plastic-to-fuel market was valued at $ 233.5 M and is projected to reach $ 8,800 M by 2028, with a CAGR of 15.8 % (The Insight Partners, 2022). Compared to mechanical and chemical recycling, thermochemical conversion is advantageous for its ability to break down mixed or contaminated plastics into valuable fuels and chemical feedstocks without the need for extensive sorting or cleaning (Wong et al., 2023). Li et al. (2022) identified such thermochemical conversion technologies as heat treatment (HT), including traditional pyrolysis and catalytic cracking. Heat treatment is a general method for plastic waste processing at high temperatures. Thermal energy is supplied to meet the required activation energy for polymer cracking, resulting in combustible gas and liquid oil.

To ensure long-term sustainability, plastic waste-to-fuel technologies must be aligned with broader decarbonization goals. Deep decarbonization of industry requires a transition from fossil-based systems to renewable and low-carbon alternatives. This includes integrating carbon capture and storage (CCS) and adopting cleaner process heat sources. Thermochemical recycling must consider its high Scope 1 emissions. Tan et al. (2025) highlights that optimization models are essential in developing viable decarbonization roadmaps. It can identify emission trade-offs, integrate renewable energy inputs, and apply technologies like CCS or hydrogen-based processing to minimize the carbon footprint of fuel recovery processes.

Paper Received: 15 May 2025; Revised: 18 August 2025; Accepted: 14 October 2025
Please cite this article as: Tuaño K.B.S., Kho H.L.R., Aviso K.B., Tan R.R., 2025, Development of P-Graph Models for the Synthesis of Plastic Waste-To-Fuel Supply Chain, Chemical Engineering Transactions, 120, 307-312 DOI:10.3303/CET25120052

Various studies demonstrate the efficacy of P-graph models in presenting an inexpensive, easy-to-use, flexible, and visual decision-mapping of complex linear systems. For instance, Fan et al. (2020) developed an integrated waste management model using P-graph to optimize municipal solid waste treatment systems. Kumar et al. (2025) recently utilized a P-graph framework to design cost-effective supply chains for end-of-life plastic recycling. Their model accounted for both capital and operational expenditures across various recycling pathways. This approach identified optimal and near-optimal structures that maximized profit and reduced GHG emissions, highlighting the potential of P-graph to support environmentally and economically sustainable decision-making. While these studies demonstrate the applicability of P-graph in waste management, they primarily focus on cost minimization or general municipal waste systems. To date, there remains a lack of research of applying P-graph specifically to plastic waste-to-fuel supply chains with carbon footprint minimization as the main objective. In this study, the P-graph framework is used to synthesize the plastic waste-to-fuel supply chain. This paper intends to develop a decision-support tool for plastic waste management. The rest of this paper is organized as follows: Section 2 gives the formal problem statement. Section 3 discusses the P-graph implementation of the model. In Section 4, an illustrative case study involving various heat treatment units is solved. Section 5 states the conclusions and prospects for future research.

2. Problem statement

The synthesis problem is stated as follows:

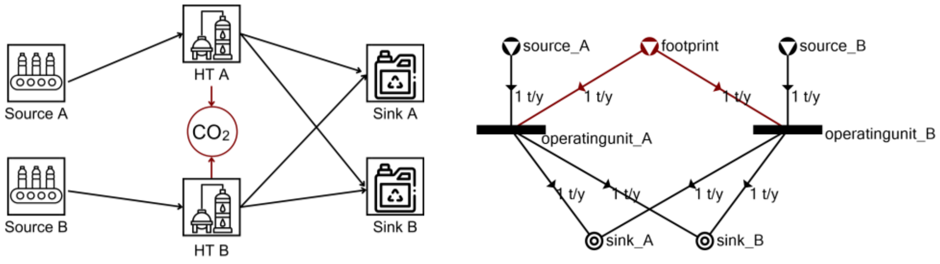
- Given a supply chain system with m number of plastic waste sources;
- Given certain fuel demands with n number of sinks;
- Given operating units, each has a unique carbon footprint and product yield;

The problem is to determine the optimal (and near-optimal) allocation of plastic waste sources to fuel sinks, which minimizes the overall carbon footprint.

3. P-graph model development

P-graph is an approach to process network synthesis (PNS) based on graph theory principles. It is a bipartite graph that uses M-type nodes for material and energy streams and O-type nodes for processes and operations. Three main algorithms based on PNS axioms comprise the P-graph framework (Friedler et al., 1992b). Maximal structure generation (MSG) assembles the O-type nodes into a superstructure of alternative configurations (i.e., maximal structure) using information implicit in their links to the M-type nodes (Friedler et al., 1993). This rigorous procedure prevents human error. Solution structure generation (SSG) identifies all structurally feasible network configurations; each solution structure is a subset of the maximal structure, and identification is algorithmically efficient due to a drastic reduction of the search space in typical PNS problems (Friedler et al., 1992a). The third algorithm, accelerated branch-and-bound (ABB), determines optimal and near-optimal solutions using additional information such as flowrates and cost functions under linearity assumptions (Friedler et al., 1996). ABB is algorithmically faster than the standard branch-and-bound procedure for the equivalent mixed-integer linear programming (MILP) model. Although the original PNS problem was defined in the context of chemical process plant design, P-graph has also been applied to a wide range of analogous “PNS-like” problems (Friedler et al., 2019). Many novel applications map new problems to the classical PNS problem. The book by Friedler et al. (2022) gives a comprehensive introduction to P-graph theory and applications, along with implementation in Python code. The software P-Graph Studio is also available with more complete features, including a graphical user interface (P-Graph, 2024).

Figure 1a illustrates the general source-sink network of a plastic waste-to-fuel supply chain containing two sources and two sinks. Figure 1b represents the P-graph translation of the network. For model demonstration, carbon emissions of plastic-to-fuel technologies are represented by a source node.



a) b)

Figure 1: Plastic waste-to-fuel supply chain represented by (a) general source-sink network and (b) P-graph

In this study, the network components of the supply chain of plastic-to-fuel include plastic waste raw materials, plastic-derived fuel products, and thermochemical waste conversion operating units. Feasible source-sink networks are developed through the following generalized steps: (1) establishing user-defined assumptions, model inputs, and outputs, (2) P-graph modelling, and (3) evaluating optimal and near-optimal solutions. The development of the P-graph model will consider the constraints associated with material balances and carbon emissions. A comparison of the relative advantages of such solutions was made based on their topological features beyond objective function values.

4. Case study

This case study deals with the allocation of plastic waste subjected to demand constraints and environmental impact considerations. The objective function is to minimize the carbon footprint from plastic-to-fuel conversion technologies. Table 1 summarizes the flow rates of each heat treatment (HT) operating unit, including such emissions. All waste plastic sources were assumed to be unlimited to supply compatible plastic waste-to-fuel technologies classified into various types of plastic, including high-density polyethylene (HDPE), polypropylene (PP), and polystyrene (PS). The efficiency of the operating units in converting plastic waste into fuel products is denoted as the conversion rates, in t/y (Li et al., 2022). Data from the existing literature were adopted for specific mixture ratios and their weight per weight conversion values. Traditional heat treatment of equal amounts of PE and PP was reported to yield 55.6 % gasoline (Santos et al., 2019). Lin and Yang (2005) provided a yield value of 91.2 % gases on the catalytic pyrolysis of PP, PE, and PS. Paucar-Sánchez et al. (2023) found 56.7 % gasoline for a simple heat treatment technology.

Table 1: Operating unit streams (Li et al., 2022)

Operating Unit	Technology	Input/s	Rate (t/y)	Output/s	Conversion Rate (t/y)	Emissions (t CO_2/y)
HT1	Catalytic cracking ($BaTiO_3$)	HDPE	1	Liquid oil	0.686	2.04
HT2	Catalytic cracking (HZSM-5)	HDPE	1	Gases	0.726	2.16
HT3	Hydrothermal liquefaction	HDPE	1	Diesel	0.450	1.34
HT4	Simple heat treatment	PE:PP:PS	0.13:0.69:0.19	Gasoline	0.567	1.80
HT5	Catalytic cracking (HZSM-5)	PE:PP:PS	0.62:0.30:0.07	Gases	0.912	2.89
HT6	Pyrolysis of plastic with biomass	PP	1	Diesel	0.556	1.66
HT7	Catalytic cracking (HZSM-5)	PP	1	Liquid oil	0.920	2.74
HT8	Traditional heat treatment at 550 °C	PP	1	Liquid Oil	0.744	2.22
HT9	Traditional heat treatment at 450 °C	PE:PP	0.5:0.5	Gasoline	0.556	1.68
HT10	Traditional heat treatment at 500 °C	PS	1	Liquid oil	0.825	2.87

The supply chain network is also subjected to emissions from the combustion of plastic raw materials. The case study follows the experimental data on CO_2 emissions, in t CO_2 per t fuel (Joshi and Seay, 2019). The CO_2 emission values are based on the combustion of a raw material, where E, in t CO_2/y, was derived from Eq(1).

$$E = y \cdot \dot{F} \tag{1}$$

where y is equivalent to the ratio of CO_2 to fuel (wt/wt) from the experimental data, and $\dot{F}$ is the conversion rate to fuel produced per year. For the sinks, the constraints were based on the transport energy consumption data from the Philippine Energy Situationer Report in 2022 (Philippine DOE, 2022). In Table 2, the percentage requirement for each fuel was quantified from the report with an assumed total demand of 294,000 GJ/y.

Table 2: Sink data (from Philippine DOE, 2022).

Fuel Demand	Requirement
Gases	3.3 %
Diesel	48.2 %
Liquid Oil	2.6 %
Gasoline	42.1 %

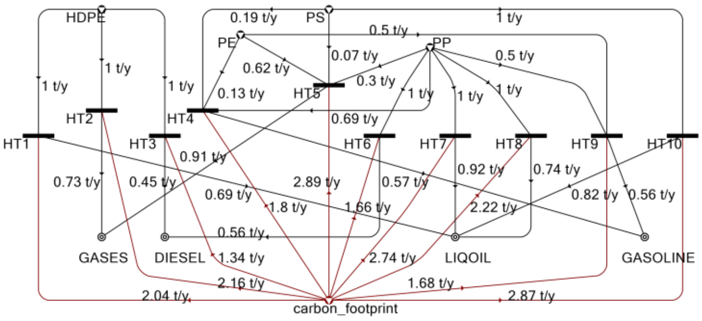


Figure 2: P-Graph superstructure for the case study

The superstructure in Figure 2 is used to represent the source-sink relationships. The carbon footprint is represented by the red raw material node with a cost of 1 $/t to define the objective function of carbon minimization in terms of the cost-minimization nature of the model. From the maximal structure, there were 32 feasible solutions generated using the ABB algorithm with a maximum solutions limit of 100.

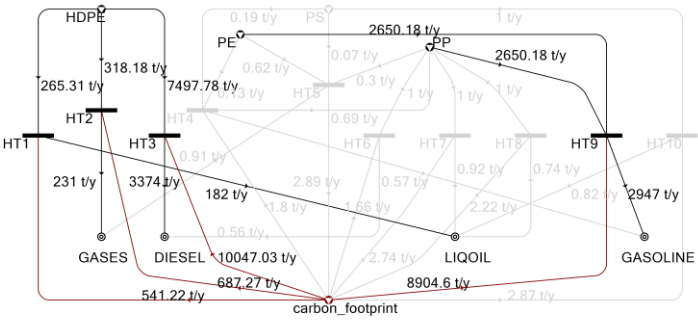


Figure 3: Optimal solution

Figure 3 depicts the optimal solution with the lowest carbon footprint value of 20,180.10 t CO_2/y. All three types of heat treatment technologies for HDPE were included in the structure, signifying the efficiency of using HDPE in plastic-to-fuel supply chains. This is consistent with the results with HDPE having the highest yield, followed by PP, PS, LDPE, and PS (Javed et al., 2023). The carbon footprint values were normalized using net calorific values (NCV) derived from conversion factors in the 1996 IPCC guidelines (IPCC, 2000). The NCV used were 43.33 GJ/t for diesel oil and gases, 44.8 GJ/t for gasoline, and 42.6 GJ/t for crude oil. These values were combined with the carbon emissions, in t CO_2/y, to calculate the carbon footprint in t CO_2/GJ.

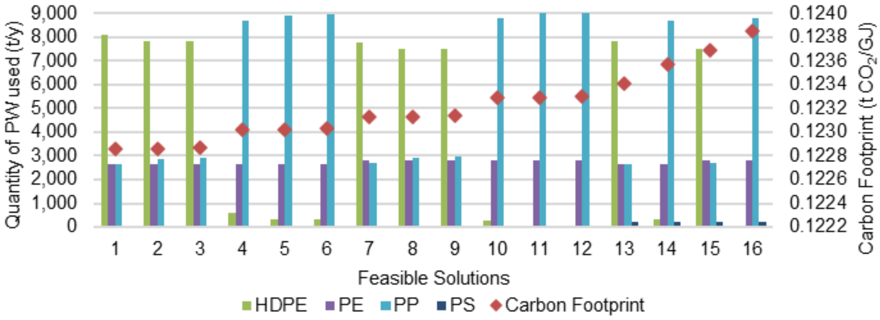


Figure 4: Results for optimal and near-optimal solutions

The performance of the model was further evaluated within 1 % of the lowest carbon emission value. From 32 feasible structures, this premise leads to 15 near-optimal structures. Figure 4 shows the summary of the amount of plastic waste used, in t/y, and the carbon footprint values, in t CO_2/GJ, for each of the optimal and near-optimal solutions. The case study yielded carbon footprint values ranging from 0.1229 to 0.1266 t CO_2/GJ, which are relatively less than the carbon footprint of conventional processes. Based on the data from EPA (2024), the carbon footprint of crude oil consumption can be derived as 0.7034 t CO_2/GJ.

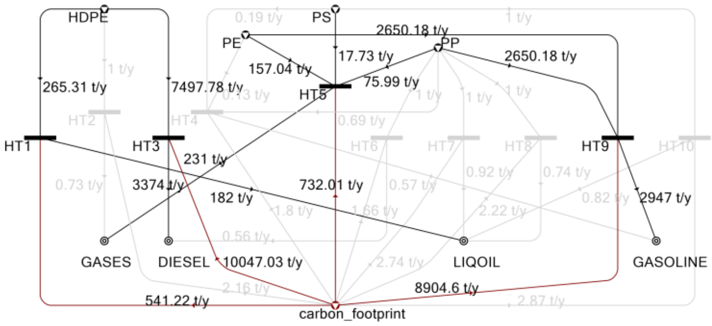
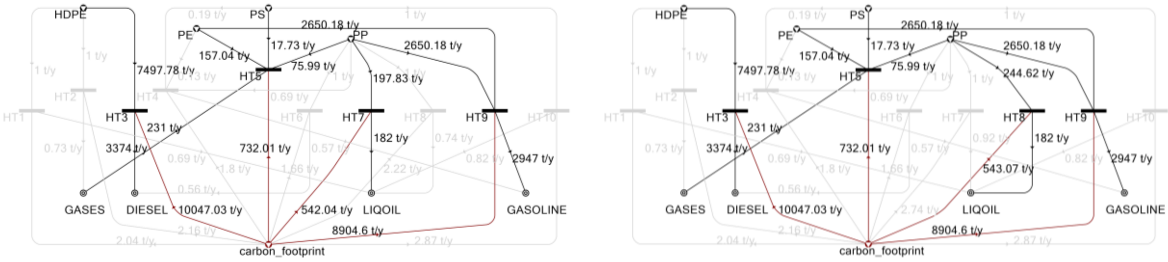


Figure 5: Near-optimal structure 1

Since operational considerations are not always readily consolidated into a mathematical model, it is important to identify multiple configurations for further decision-making. Near-optimal solutions were used to relate the tradeoffs between carbon footprint and raw material utilization. For instance, although the optimal solution yields the lowest footprint value, three technologies depend on the availability of HDPE. Figure 5 shows an alternative supply chain network that uses all four types of plastic waste. The selected solution has a carbon footprint value of 0.1231 t CO_2/y, yielding a 0.16 % difference from the optimal solution. It can be observed that there are two technologies allocated for mixtures compared to the optimal solution, which has one unit for mixed plastic waste.



a) b)

Figure 6: Alternative solutions (a) Near-optimal solution 2 and (b) Near-optimal solution 3

Near-optimal solutions 2 and 3 were considered to exhibit notable differences in technology while having the same carbon footprint as near-optimal solution 1. HT3, HT5, and HT9 are consistent in all three solutions, signifying their reliability in the supply chain. Figure 6a shows near-optimal solution 2, which provides HZSM-5 as an alternative catalyst to $BaTiO_3$ for catalytic conversion to liquid oil. HZSM-5 zeolite accounts for one of the most commonly used catalysts for cracking polyolefins (Abnisa, 2023). Figure 6b represents near-optimal solution 3 as an alternative with simple heat treatment instead of catalytic conversion. Decision-makers may evaluate the implications in operational costs and feasibility for choosing the final configuration.

5. Conclusions

This work developed a P-graph methodology for optimizing plastic waste-to-fuel supply chains. The approach applied the P-graph framework to match plastic waste sources to downstream fuel demands while considering the total carbon footprint of the network. The optimal network yielded the lowest value at 0.1229 t CO_2/GJ among solutions reaching up to 0.1266 t CO_2/GJ. Plastic waste-to-fuel is denoted as a promising alternative to fossil fuel, as these values were less than the carbon footprint of conventional fuel production at 0.7034 t CO_2/GJ. The proposed model is a decision-support tool for evaluating raw material allocation, technology selection, and carbon footprint. Future work may extend the model to better reflect the heterogeneous nature of plastic waste mixtures instead of having fixed mixture ratios. Multi-objective optimization can be explored to quantify the operational costs with emissions. Life cycle assessment (LCA) and sensitivity analysis can help ensure the robustness of the plastic waste-to-fuel models with varying conversion yields and emission factors.

References

Abnisa F., 2023, Enhanced Liquid Fuel Production from Pyrolysis of Plastic Waste Mixtures Using a Natural Mineral Catalyst. Energies, 16, 16031224.

EPA, 2024, U.S. Greenhouse Gas Emissions and Sinks. Environmental Protection Agency, <epa.gov/system/files/documents/2024-04/us-ghg-inventory-2024-main-text_04-18-2024.pdf>, accessed 06.02.2025.

Fan Y.V., Klemeš J.J., Walmsley T.G., Bertók B., 2020, Implementing Circular Economy in municipal solid waste treatment system using P-graph. Science of the Total Environment, 701, 134652.

Friedler F., Aviso K.B., Bertok B., Foo D.C.Y., Tan R.R., 2019, Prospects and challenges for chemical process synthesis with P-graph. Current Opinion in Chemical Engineering, 26, 58–64.

Friedler F., Orosz Á., Pimentel Losada J. (Eds.), 2022, P-graphs for Process Systems Engineering: Mathematical Models and Algorithms. Springer, Cham, Switzerland.

Friedler F., Tarjan K., Huang Y.W., Fan L.T., 1993, Graph-theoretic approach to process synthesis: polynomial algorithm for maximal structure generation. Computers & Chemical Engineering, 17, 929–942.

Friedler F., Tarján K., Huang Y., Fan L.T., 1992a, Combinatorial algorithms for process synthesis. Computers & Chemical Engineering, 16, S313–S320.

Friedler F., Tarján K., Huang Y., Fan L.T., 1992b, Graph-theoretic approach to process synthesis: axioms and theorems. Chemical Engineering Science, 47, 1973–1988.

Friedler F., Varga J. B., Feher E., Fan L.T., 1996, Combinatorially accelerated branch-and-bound method for solving the MIP model of process network synthesis. Chapter In: CA Floudas, PN Pardalos (Eds.), State of the Art in Global Optimization: Computational Methods and Applications. Vol. 7, Springer, Dordrecht, Netherlands, 609–626.

IPCC, 2000, CO_2 emissions from stationary combustion of fossil fuels, Intergovernmental Panel on Climate Change, <ipcc-nggip.iges.or.jp/public/gp/bgp/2_1_CO2_Stationary_Combustion.pdf>, accessed 29.02.25.

Javed N., Muhammad S., Iram S., Ramay M.W., Jaffri S.B., Damak M., Fekete G., Varga Z., Székács A., Aleksza L., 2022, Analysis of Fuel Alternative Products Obtained by the Pyrolysis of Diverse Types of Plastic Materials Isolated from a Dumpsite Origin in Pakistan. Polymers, 15, 15010024.

Joshi C.A., Seay J.R., 2019, Total generation and combustion emissions of plastic derived fuels: A trash to tank approach. Environmental Progress & Sustainable Energy, 39, 13151.

Kumar B., Pimentel J., Cano-Londoño N.A., Ruiz-Mercado G.J., Deak C.T., Cabezas H., 2025, Designing cost-effective supply chains for plastics at the end-of-life. Journal of Cleaner Production, 501, 145227.

Lau W.W.Y., Shiran Y., Bailey R.M., Cook E., Stuchtey M.R., Koskella J., Velis C.A., Godfrey L., Boucher J., Murphy M.B., Thompson R.C., Jankowska E., Castillo A.C., Pilditch T.D., Dixon B., Koerselman L., Kosior E., Favoino E., Gutberlet J., Baulch S., 2020, Evaluating scenarios toward zero plastic pollution. Science, 369, 1455–1461.

Li N., Liu H., Cheng Z., Yan B., Chen G., Wang S., 2022, Conversion of plastic waste into fuels: A critical review. Journal of Hazardous Materials, 424, 127460.

Lin Y.H., Yang M.H., 2005, Catalytic reactions of post-consumer polymer waste over fluidised cracking catalysts for producing hydrocarbons. Journal of Molecular Catalysis A: Chemical, 231, 113-122.

Paucar-Sánchez M.F., Martín-Lara M.A., Calero M., Blázquez G., Solís R.R., Muñoz-Batista M.J., 2023, Towards fuels production by a catalytic pyrolysis of a real mixture of post-consumer plastic waste. Fuel, 352, 129145.

P-Graph, 2024, P-Graph Studio, <p-graph.org/downloads.html>, accessed 23.12.2024.

Philippine DOE, 2022, 2022 energy supply and demand Situationer. Department of Energy Philippines, <doe.gov.ph/energy-statistics/2022-energy-supply-and-demand-situationer>, accessed 21.01.2025.

Pilapitiya P.G.C.N.T., Ratnayake A.S., 2024, The world of plastic waste: A review. Cleaner Materials, 11, 2772-3976.

Santos B.P.S., Almeida D.D., Marques M.F.V., Henriques C.A., 2019, Degradation of Polypropylene and Polyethylene Wastes Over HZSM-5 and USY Zeolites. Catalysis Letters, 149, 798-812.

Tan R.R., Migo-Sumagang M.V., Aviso K.B., 2025, Recent trends in optimization models for industrial decarbonization. Current Opinion in Chemical Engineering, 48, 101118.

The Insight Partners, 2022, Plastic to Fuel Market Size Worth $ 8.8 Billion by 2028 at 15.8% CAGR. Cision PR Newswire, <prnewswire.com/news-releases/plastic-to-fuel-market-size-worth-8-8-billion-by-2028-at-15-8-cagr--the-insight-partners-301614509.html>, accessed 20.03.2024

Wong S.L., Ngadi N., Abdullah T.A.T., Inuwa I.M., 2023, Thermochemical recycling of plastic waste: A promising solution for mixed and contaminated feedstocks. Waste Management, 165, 50–63.