System analysis of plastic waste management through chemical recycling

Submitted in partial fulfillment of the requirements for the Doctoral Comprehensive Examination in Chemical Engineering

Farhad Zaker Hosseiny

Department of Chemical Engineering – The Pennsylvania State University

Advisor – Dr. Rui Shi

August 2024

Table of Contents

1.0- Overview

Plastics have become integral to modern life, permeating nearly every aspect of our daily routines. From packaging materials that preserve our food to medical devices that save lives, plastics offer unparalleled versatility, durability, and cost-effectiveness. They play a critical role in various industries, including healthcare, automotive, electronics, and construction, contributing significantly to advancements and efficiencies that define contemporary living. The importance of plastics lies not only in their functional benefits but also in their adaptability, enabling the creation of countless products that enhance our quality of life. Among the various types of plastics, polypropylene is particularly noteworthy for its exceptional chemical resistance, high melting point, and robust mechanical properties.

The short lifespan of plastics, particularly within the packaging sector, results in accumulation of plastic waste shortly after their production. With the ongoing increase in worldwide plastic production, the rate of waste plastic generation exceeds 300 M ton/year globally (PP alone exceeds 60 M ton/year) while approximately 79% of them are landfilled, 12% incinerated, and the rest recycled [1–3]. The traditional methods used to dispose of plastic waste raise significant environmental concerns. Incineration emits carbon dioxides and toxic substances (such as dioxins and furans) which cause air pollution. Additionally, the leachates from landfills contain microplastics and other contaminants that eventually pollute the soil and water. These pollutions pose harmful effects on wildlife and public human health [4–7].

The global plastic waste management market size, valued at ~$37 billion in 2021, is predicted to surpass $47 billion by 2030. While PP acquires the highest market share based on polymer type, on the basis of service type which is categorized into incineration, landfills, collection, and recycling, the recycling segment holds the largest share [8]. At present, mechanical recycling stands as the predominant recycling method, primarily focused on certain types of high-density polyethylene (HDPE) and polyethylene terephthalate (PET) bottles [9,10]. Theoretically, mechanical recycling should be applicable to all types of thermoplastics with minimal quality impacts. However, polyethylene, polystyrene, and polypropylene face challenges in practical implementation. Mechanical recycling often results in downcycling. Thermal-mechanical degradation during the recycling process, along with the presence of contaminants and impurities, adversely impacts the mechanical properties and quality of recycled plastics. This limits the use of recycled materials, making them less suitable for high-quality applications [11–16]. To overcome these challenges associated with mechanical recycling of polyolefins, thermal/chemical routes [17–25] are being studied and developed to enable the production of value-added chemicals from plastic wastes, and among various chemical/thermal recycling methods, pyrolysis is the most widely studied approach [26]. As these methods are currently undergoing development, process optimization is required to achieve favorable economic and minimal environmental impacts. Moreover, due to geo-temporal variations in the composition and quality of plastic wastes, comparative evaluations of cost-effectiveness and environmental impacts are crucial to identify the optimal solution(s) for promoting a circular economy for plastics.

2.0- Goals and Objectives

The ultimate goal of this project is to perform system analysis and optimization on chemical recycling of plastic wastes. By integrating reaction kinetic models, process modeling, Techno-Economic Analysis (TEA), and Life Cycle Assessment (LCA), we will investigate the impact of various design decisions (such as feedstock type, processing technology, and plant capacity), operating conditions (such as temperature, residence time, feedstock composition, etc.), product yield, and location on industrial feasibility, aiming to improve the economic and environmental sustainability of the process. This will help determine the appropriate plastic waste management options for various scenarios where key regional parameters (might) exhibit significant variability and/or limitations that must be addressed. This study will explore the following research questions:

- To what extent does the dynamic nature of the chemical recycling processes impact their sustainability, and how dynamic modeling can be utilized to optimize operating conditions and design parameters to achieve improved sustainability?
- To what extent transportation and logistics impact the sustainability of chemical recycling, and how can they be optimized to achieve improved sustainability?
- How do elements within and beyond the facility's battery limits interact, and what are the associated trade-offs?

We will address these questions by pursuing the following aims:

Aim 1: Developing a baseline LCA/TEA model for waste polypropylene pyrolysis: With this model, we will be achieving two targets. 1) creating a baseline for later comparisons. 2) roughly examining the impact of plant location and feedstock logistics on process sustainability (economic and environmental).

Aim 2: Establishing an advanced sustainable design framework based on reaction kinetic models: In this framework, we will integrate reaction kinetic models, process modeling, and TEA/LCA calculations. This framework will enable us to explore the impact of variation in operating conditions and product yields on system-level sustainability.

Aim 3: Investigating the impact of plant location, feedstock/product logistics, recycling technology, and process configurations on the sustainability of advanced plastic waste management methods: Achieving this aim will enable us to provide a more comprehensive perspective on the limitations, advantages, disadvantages, hotspots, and guidelines, specifically targeting policymakers and researchers in the field of the plastic circular economy.

3.0- Research Background

System analysis of plastic recycling pathways has become a focal point of research due to the ever-growing environmental and economic concerns associated with conventional plastic waste management practices. This review summarizes the key findings from recent studies focusing on the sustainability analysis (economic and environmental) of different plastic waste management methods (with focus being on advanced recycling techniques).

3.1- Economic sustainability analyses background

Sahu [27] and Al-Salem [28] delved into catalytic cracking and hydrocracking, respectively, showing that thermochemical methods can be used to produce high-quality fuels in regions with limited oil and gas resources. They show the process can be profitable, albeit with considerations such as scale and taxation, tipping fees, as well as calorific value of feedstock and efficiencies associated with heat and electricity generation. Later studies further demonstrated the significance of plant size, production rates, operating hours along with plant-size on economic viability [29].

While initial studies were mainly focusing on showing that plastic recycling can be economically feasible, later studies started focusing on comparing different plastic waste management methods. In this regard, some studies show that pyrolysis is the most profitable method among the existing (and developing) recycling methods. However, inconsistent operating conditions, system boundaries, and economic assumptions can also lead to conflicting results and conclusions as well [30,31]. Nevertheless, almost in all studies, advanced methods outperformed conventional methods (landfilling and incineration), with product selectivity and yields identified as key factors for process sustainability.

An evaluation of mechanical, chemical, and combined recycling of mixed plastics waste suggested that combined recycling is superior to individual methods in terms of carbon efficiency, costs, and environmental impacts. However, outcomes were influenced by local or national factors such as waste composition and energy mix, which limited the transferability of the results [32]. Multiproduct pyrolysis-based refinery is another process concept which is being studied in recent years, offering the processing flexibility while showcasing economic competitiveness and environmental benefits. Using advanced heating mediums such as molten salt and optimizing heat integration have been shown to enhance profitability. Integration with solar energy, particularly when using molten salt, has the potential to further improve the economic and environmental sustainability of the process [33,34]. Nevertheless, ensuring a reliable supply of waste, both in sufficient quantity and consistent quality, is crucial for successful implementation of any recycling technology [35,36]. Finally, while economies of scale offer potential for cost reduction, Stallkamp [37] revealed the challenges for business case of automotive plastic waste pyrolysis in Germany, emphasizing the necessity for additional revenue streams and policy interventions. Policy implications included gate fees, subsidies, or CO2 certificate credits to support economic viability.

While the majority of TEA studies have primarily focused on producing lighter components such as ethylene/propylene monomers, aromatics or other value-added chemicals, and transportation fuels, Cappello [38] presented evidence that converting waste polyolefins into lubricants (as a more valuable products) could be a more profitable approach. Their study also suggested that leasing the expensive Pt-loaded catalysts could reduce the minimum selling price of the final product. However, the increased revenue from more valuable products may not always compensate for the higher capital and operational costs [39]. Moreover, it has been demonstrated that the minimum selling price of pyrolysis-derived products (Naphtha and BTX) can compete with petroleum-derived counterparts if either mixed waste plastics cost less than \$0.10/kg or crude oil prices exceed \$60/barrel [40].

3.2- Environmental sustainability analyses background

Both Plastic-to-Plastic (LDPE production) and Plastic-to-Fuel (fuel production) pathways from pyrolyzing non-recyclable plastics is shown to offer environmental benefits compared to conventional routes. The preference between these pathways varies regionally, influenced by factors such as waste management techniques, recycling rates, and water scarcity. Plastic-to-Plastic pathways are generally lower-emitting than current waste practices and conventional plastic production, while Plastic-to-Fuel pathways are less water-intensive and suitable for regions with high plastic incineration rates. Therefore, a holistic approach considering regional characteristics and broader environmental impacts is crucial in determining the optimal use of pyrolysis for non-recyclable plastics [41]. The efficiency of co-product handling, especially fuel gas combustion, plays a crucial role in achieving these environmental benefits. For instance, Life-cycle Greenhouse Gas (GHG) emissions of Ultra-Low Sulfur Diesel (ULSD) derived from non-recycled plastics are 1% to 14% lower than conventional ULSD, depending on co-product handling methods. Additionally, the geographic location of Plastic-to-Fuel facilities influences emissions due to variations in electricity production intensity [42]. Nonetheless, in clear contrast, pyrolysis of mixed waste plastics can also result in excessive GHG emissions [40].

As mentioned above, under certain conditions thermochemical routes can provide environmental benefits in terms of climate change mitigation and resource conservation. However, most other impact categories such as acidification, eutrophication, photochemical and ozone formation, are significantly higher for such recycling methods due to the energy-intensive process units, utility requirements, and purification processes [40,43]. Accordingly, no outright preferred technology emerges for managing or recycling municipal plastic waste; preference depends on the environmental impact category prioritized. Additionally, these necessitate careful consideration of trade-offs and technological advancements. For instance, monomer separation unit can contribute to 49-58% of the total emissions, making it the largest emitter section in a recycling process. Therefore, optimizing pyrolysis conditions to minimize the production of monomers could lead to a reduction in GHG emissions [44]. Furthermore, proper heat integration and adoption of carbon capture technologies, especially in energy-intensive processes such as hydrothermal liquefaction, gasification, and pyrolysis can further reduce the overall GHG emissions [31,44]. Another example in this regard can be the product upgrading via hydrocracking. This process area can contribute to more than 60% of total emissions due to its energy-intensive nature and hydrogen requirements [39].

In addition to influential parameters within process battery limits, such as optimized operating conditions for maximized product yields selectivity and/or minimized energy/utility consumption, efficient waste collection and transportation logistics near urban centers are crucial for sustainability of the process [39]. The product handling system can be as decisive as other parameters, requiring optimization to minimize environmental impacts. Studies have shown that the substitution rate (SR) of conventional steam cracker feedstock with pyrolysis oil can significantly reduce GHG emissions. While both 5% and 20% substitution rates resulted in decreased GHG emissions, the scenario with a 5% SR demonstrated greater reductions. The additional purification steps for pyrolysis oil (such as hydrotreating) in the 20% SR scenario slightly offset the GHG reductions [45].

4.0- Proposed research, methods, and results

As mentioned earlier, the ultimate goal of this research is achievable by accomplishing the three defined aims. These aims are broken down into specified tasks, ensuring that fulfilling them leads to the accomplishment of associated aims.

4.1- Aim 1: Developing a baseline LCA/TEA model for waste polypropylene pyrolysis

4.1.1- Task 1.1: Simulating the process in a process simulator and performing heat & mass balance calculations {completed}

In this task, we assumed a grass-roots, centralized facility designed to process 300 kt of waste polypropylene on an annual basis. The facility operates continuously (24 hours per day) for 330 days a year, totaling 7920 operating hours annually. The facility is envisioned to be situated in the Southern United States, where the volume of polypropylene (PP) waste surpasses this capacity [46,47], ensuring ample feedstock supports uninterrupted plant operations. The feedstock for this process is assumed to be the single-stream waste PP bales, sourced from Material Recovery Facilities (MRFs). Despite the presence of various impurities in these bales, ranging from organic matters to other polymers and metals found in multilayer packaging, which can affect

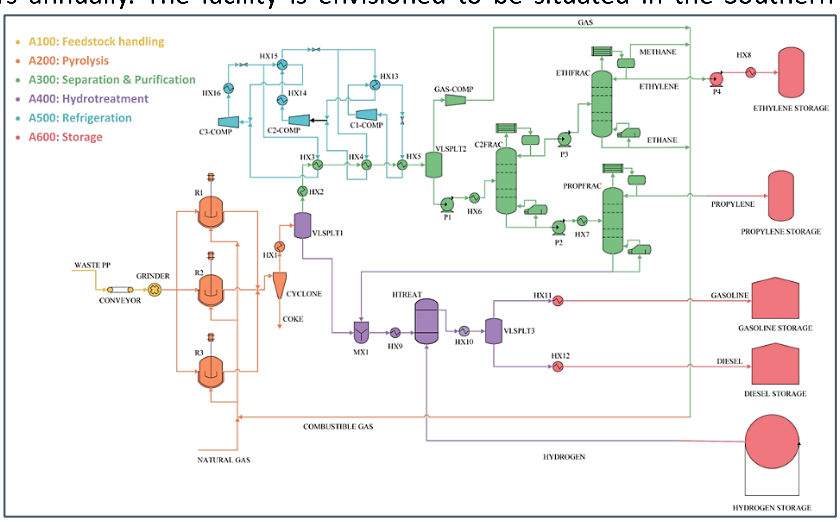


Figure 1: Process flow diagram of polypropylene recycling

product distribution [14], we relied on the product distributions reported in the literature regarding the pyrolysis of PP. This process is comprised of six main areas: feedstock handling, pyrolysis, separation and purification, hydrotreatment, refrigeration, and storage (Figure 1). The products are combustible gas, ethylene and propylene monomers, and gasoline-range and diesel-range blend stocks, with the latter two being the primary products of the process. Pyrolysis is carried out in three parallel batch reactors loaded with fluid catalytic cracking (FCC) catalyst at 450°C and 1 bar, following the operating conditions (in pyrolysis area) and product distribution specified in Achilias' work [48]. Offsite natural gas, along with combustible gas generated on-site, are used to provide the required energy in the reactors for PP pyrolysis. The resulting hydrocarbon vapors are cooled down and separated via flash separators and distillation columns. From the separation and purification area, light and heavy fuel blends are further upgraded through hydrotreating. Finally, the end products are routed to their respective storage tanks. The process schematic is shown by Figure 1. Aspen Plus is used for process simulation and heat and mass balance calculations. Inputs, outputs, and utility consumptions for the process were determined by the software through calculations that consider the facility's processing capacity, product distribution, and energy balance.

4.1.2- Task 1.2: Estimating the capital investments and operational costs, and performing TEA analysis {completed}

Simulation results from Task 1.1 are fed to the Aspen Economic Analyzer (APEA), to calculate the capital investments and fixed operational costs. Variable operational costs such as feedstock purchase and transportation costs, utility costs, and if applicable, costs associated with handling process wastes are estimated manually. Finally, the results were transferred to Microsoft Excel where a comprehensive TEA analysis including various case studies and sensitivity/uncertainty analysis are performed. In this study, the profitability is assessed using three indicators including Net Present Value (NPV), Internal Rate of Return (IRR), and Minimum Selling Price (MSP). NPV is a financial metric used to evaluate the profitability of an investment by calculating the present value of expected cash flows discounted at a specified rate. It compares the current value of cash inflows with the initial investment outlay. A positive NPV indicates that the investment is expected to generate more returns than the initial investment, while a negative NPV suggests the opposite. IRR is another financial metric used to assess the attractiveness of an investment opportunity. It represents the discount rate at which the net present value of cash flows from an investment equals zero. In simpler terms, it's the interest rate at which an investment breaks even. MSP is the product selling price at which the NPV in the specified discount rate is zero.

Considering the average prices in 2022 for feedstocks, catalysts, products, utilities, and other services, economic calculations indicate that over the 30-year lifespan, the plant has the potential to generate revenue with a NPV over $330 million while having an IRR as high as 29.6%. For the refinery described here, minimum fuel selling price is $2.4/GGE (average price of the fuel is ~$3/Gal in the same region in 2022). The analysis reveals that with a total equipment cost (which also includes costs associated with installation) of $189 million, the "Storage" area which include hydrogen and final products storage facilities has the highest contribution to the total equipment cost (Figure 2). Designed for 4-week storage duration, based on design heuristics [49], three spherical hydrogen storage tanks alone cost more than $180 million. Annual operational cost breakdown shows that "Raw material & waste" which includes the purchase costs of feedstocks (waste PP and hydrogen) and catalysts (FCC for pyrolysis and sulfided Co-Mo for hydrotreating) as well as waste (char/wax) handling expenses, and "Transportation" cost which includes the shipping expenses of hydrogen and waste polypropylene to the facility are the major contributors, collectively accounting to approximately 87% (~ $116 million) of the total operational costs (Figure 2). These points highlight the importance of plant location on economic viability for the following reasons: 1) shorter transportation distances can reduce the cost of transporting feedstocks, and 2) the size of storage tanks (especially for hydrogen) can be reduced to 1-2 weeks without compromising uninterrupted plant operations if the plant is located near facilities that regularly supply the process feedstocks. However, in real-world scenarios, facilities that supply waste polypropylene (MRFs and large municipal areas) are often significantly distant from facilities that produce hydrogen (refineries). Therefore, a trade-off is inevitable

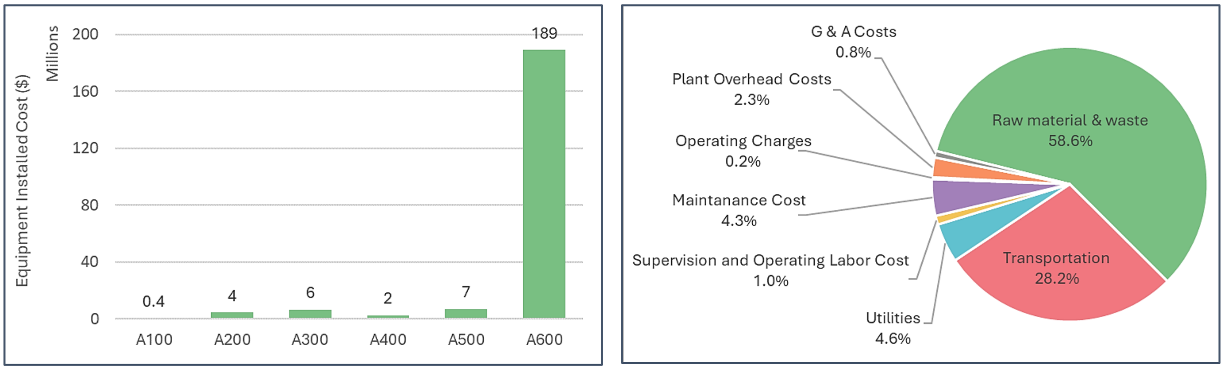


Figure 2: Total equipment cost in in each area (left) and annual operational cost breakdown (right)

when determining the location of the facility with the current process configuration. On-site hydrogen production, particularly for a centralized large-capacity facility, can indeed be an alternative that significantly reduces or eliminates costs associated with hydrogen, including its purchase, transportation, and storage costs.

The impact of varying overall fuel production rate and waste polypropylene price on Minimum Fuel Selling Price (MFSP) is shown in Figure 3. As operating a large-scale centralized recycling plant can substantially boost the demand for waste polypropylene bales in the region, it is considered plausible that the price of waste polypropylene bales could potentially rise to twice the average price of $181 per ton observed in 2022 [50]. The calculations highlight the importance of stability in fuel production, which can be easily disrupted by extended maintenance times or process downtimes (e.g. excessive coke formation on heating surfaces), or by decreasing yields caused by variations in feedstock quality, contamination, and catalyst deactivation. For instance, provided that the plant operates at designed capacity (no decrease in production rate) and the purchase cost of waste polypropylene is less than $345/ton, it is determined that the MFSP would be lower than $3/GGE (as the baseline). However, the same threshold can decrease to approximately $260/ton with just 10% decrease in fuel production rate. This shows that despite economic viability, the profitability of this process highly uncertain. Additionally, although we increased the average price of waste polypropylene by 100% in this analysis, we believe that in the case of increased demand, the final price of waste polypropylene bales could match that of high-density polyethylene (HDPE), which exceeded $400/ton in 2022 [50]. At this price, the MSFP would exceed the market price regardless of the production rate.

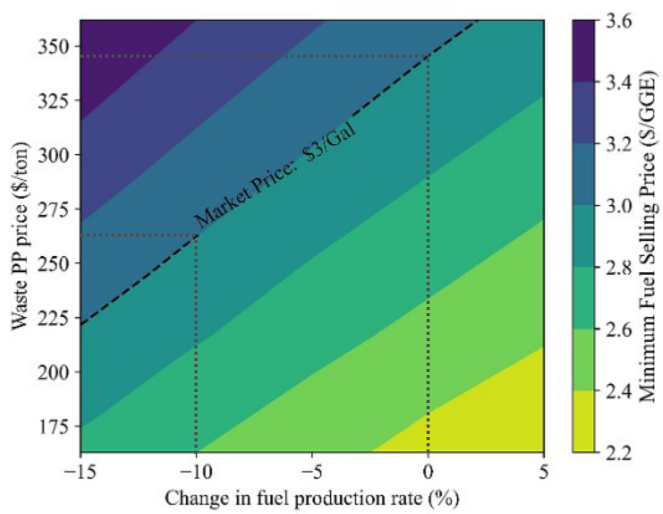


Figure 3: Influence of two major process and economic factors on Minimum Fuel Selling Price

Two additional scenarios were developed with processing capacities of 240 kta and 360 kta to assess their impact on the economic feasibility of the process. Figure 4(a) demonstrates that the total capital investment ranging from $320 million to $460 million changes significantly with capacity. This is mainly due to the significant change in total installed costs of hydrogen tanks ($113MM vs. $135MM vs. $170MM). Since the major components of operational costs (including raw material, transportation, and utility costs) increase linearly with scale, both the annual operational cost and annual income increase linearly with increased capacity, and consequently, the gross earnings, also increase linearly with capacity (gross earnings = income increase - operational cost). Nevertheless, while the 360 kta plant generated the highest NPV over the 30-year plant life due to highest gross earnings, it can be seen that the base case design has the highest IRR (and also the best return on investment) among all scenarios. This lower IRR is because the higher gross earnings in 360 kta case do not fully offset the increase in total capital investment

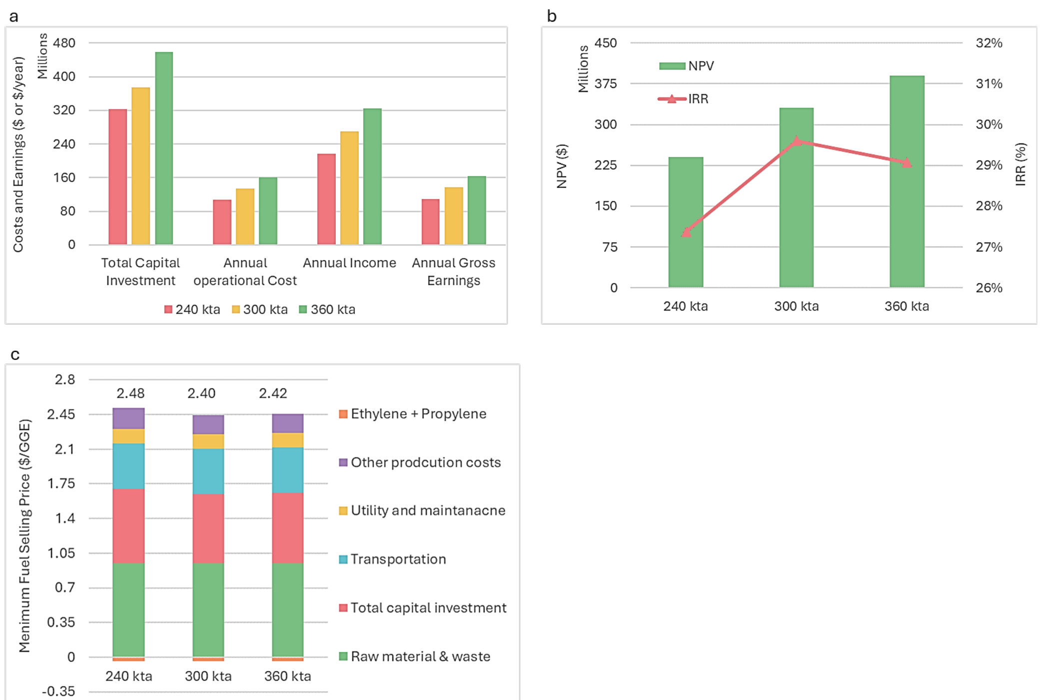


Figure 4: Effect of processing capacity on: a) costs and earnings b) NPV and IRR c) MFSP and its breakdown

(Figure 4(b)). For the same reason, a similar trend is observed in the minimum selling prices, as the MFSPs for three scenarios were $2.48/GGE, $2.4/GGE, and $2.42/GGE, respectively. The MFSP breakdown (Figure 4(c)) indicates that with a contribution over $0.95/GGE, regardless of the capacity, "Raw material & wastes" accounts for the highest portion of MFSP. “Total capital investment” and “Transportation” are the next major contributors. It is also important to note that the sales of by-products (chemical grade ethylene and propylene) have a negligible impact on the minimum selling price of the fuel products.

4.1.3- Task 1.3: Assessing the environmental impacts of process {ongoing}

For this task, the data from Task 1.1 will be fed to OpenLCA software [51] to assess the environmental impacts associated with plastic recycling. The LCA study will adopt a cradle-to-gate system scope, where cradle refers to the output(s) of Material Recovery Facilities (MRF) and the gate refers to the output(s) of the plastic recycling plant being studied. Since this task is still ongoing, this section will describe the proper conduction of LCA based on the ISO standards [52,53].

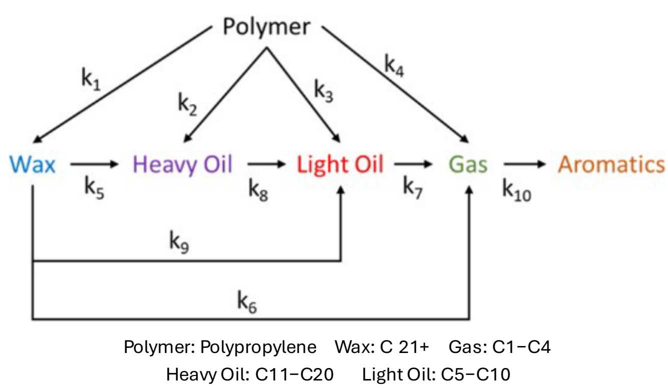
The first step of LCA is goal and scope definition. The ISO standard requires specifying the intended application, the reasons for the study, the audience, and whether results will be released publicly are defined. Also, in this step, the “boundary” is defined detailing what information is relevant in the study and how the study will be conducted. This includes the identification of a functional unit. Clear definition of the function of a process is key for comparability between LCA studies. In case of having byproducts in the system, the method for attributing a share of environmental impact to coproducts should be defined. Allocation should be avoided, if possible, through system expansion or subdivision. In the case that allocation is unavoidable, impact can be attributed to a coproduct based on a biophysical chemical property such as the mass of the coproduct or its heating value. In the second step, inventory analysis entails generating a list of input and output flows across the system boundary. Data collection, validation and connection to unit processes and functional units as well as data aggregation are performed in this step. The quality and uncertainty of the data should be reported, where possible. In the third step, the impact assessment involves taking the flows identified in step 2 and assessing their environmental impact using sustainability indicators, such as global warming (GWP) [54,55]. The final step, interpretation, should be conducted throughout the entire LCA process to ensure consistency across all steps. This involves transforming the data into meaningful results that can be used for decision-making.

4.2- Aim 2: Establishing an advanced sustainable design framework based on reaction kinetic models

4.2.1- Task 2.1: Integrating reaction kinetic models in process simulations {completed}

The primary target in this task is to replace the static yield data with reaction kinetic models in the Aspen Plus simulations. This will enable us to dynamically monitor product yields and utility consumption under various operating conditions, allowing us to optimize the conditions to achieve predefined goals, such as maximizing process profitability and/or minimizing environmental impacts. Additionally, we can pursue other objectives, such as maximizing the yield of desired product(s) or minimizing utility consumption, depending on the situation.

The first step in this process is choosing an appropriate kinetic model among the available options. In this regard, we incorporated the model developed by Kulas et al. [56]. The reaction pathways for this model are shown in Figure 5. The lumped-type kinetic model is comprised of 10 reactions and 6 lumped species. All the reactions are assumed to be first-order and irreversible, and the aromatic fractions are formed from the gas phase Diels-Alder reaction followed by dehydrogenation, and unimolecular cyclization reactions followed by dehydrogenation [57].



$$\frac{dP}{dt} = -k_1P - k_2P - k_3P - k_4P$$

$$\frac{dW}{dt} = k_1P - k_5W - k_6W - k_9W$$

$$\frac{dH_{Oil}}{dt} = k_2P + k_5W - k_8H_{Oil}$$

$$\frac{dL_{Oil}}{dt} = k_3P + k_9W + k_8H_{Oil} - k_7L_{Oil}$$

$$\frac{dGas}{dt} = k_4P + k_6W + k_7L_{Oil} - k_{10} \times Gas$$

$$\frac{dA}{dt} = k_{10} \times Gas$$

$$k_i = A_i e^{-E_{a,i}/RT}$$

Figure 5: Polypropylene decomposition reaction pathways and associated rate equations

Temperature dependencies of rate constants are described by the Arrhenius law. The activation energies (E) and Arrhenius constants (A) were determined by fitting the rate equations to the experimental data in MATLAB using the method of least squares. Hence, by solving the system of Ordinary Differential Equations (ODEs), it is possible to predict the product distribution at different temperature levels and vapor residence times. The system of ODEs is solved numerically using the 4th order Runge-Kutta (RK4) method for its accuracy, robustness, adaptability, and ease of implementation [58]. The preliminary code was developed in MATLAB for test runs, proper timestep selection, and later refinements. This approach allows for iterative testing and optimization before implementing the final solution in Aspen Plus. The timestep was set to 0.01 seconds, which was sufficiently small to ensure that 1) the calculations are accurate, and 2) the timestep size does not affect the final results. The final run before integration process involved replicating the reference data. As shown in Figure 6, the product distribution predicted by our program was consistent with the reference data, demonstrating the applicability of the program.

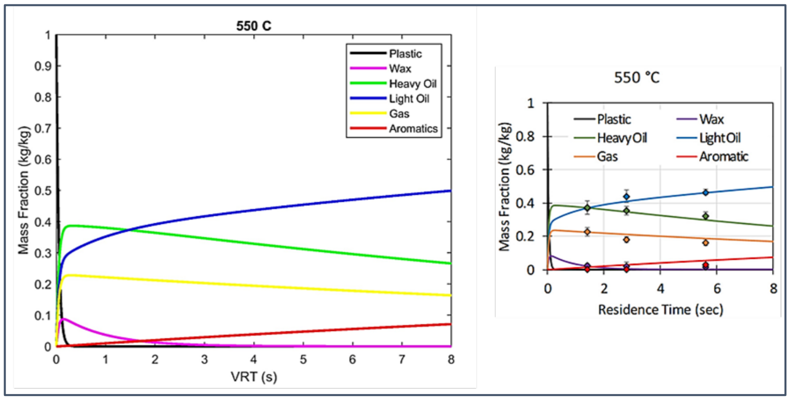


Figure 6: Model predictions (left) and reference data (right) for product distribution

The first step in integration process was to modify the previous process scheme (developed in Task 1.1) because of the differences in product distributions and final products of the kinetic model and previous yield data. In the kinetic model, the final products are combustible gas and pyrolysis oil, with the latter comprising "Light Oil," "Heavy Oil," and "Aromatics" fractions. The modified process scheme is comprised of 4 main areas: feedstock handling, pyrolysis, separation & purification, and storage, as shown schematically in Figure 7. While the feedstock handling, pyrolysis, and storage areas are identical to the previous process scheme, the separation & purification area in the new model only includes flash separators and does not require any distillation columns, resulting in a much less sophisticated design.

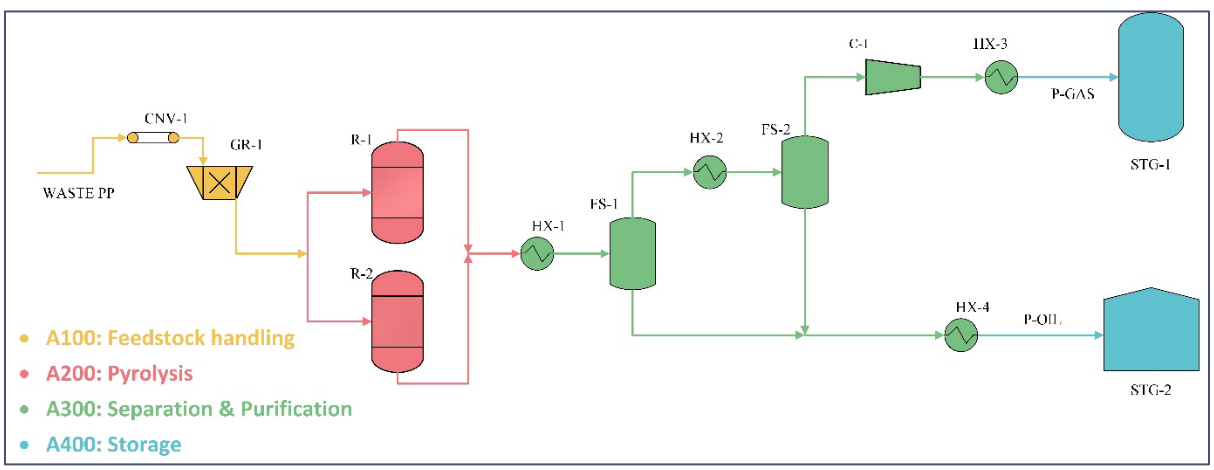


Figure 7: Process flow diagram of modified process

With the modification to the process scheme, the program was then converted to FORTRAN 77 language as Aspen Plus is only compatible with this programming language [59]. Finally, the converted code was used in a flowsheet calculator in Aspen Plus where it takes residence time and reactor temperature as inputs and export the calculated mass fractions to the reactor outlet. This approach allows for dynamically determining the components yields in different operating conditions (temperature and residence time, the two variables in the kinetic model), thus enabling condition optimization for any defined target. For instance, if we prioritize P-Oil (pyrolysis oil) as the primary product of the process, lower temperature levels and higher residence times maximize its yield. However, beyond 4 seconds of residence time, there is no further increase in the yield of P-Oil, as shown in Figure 8.

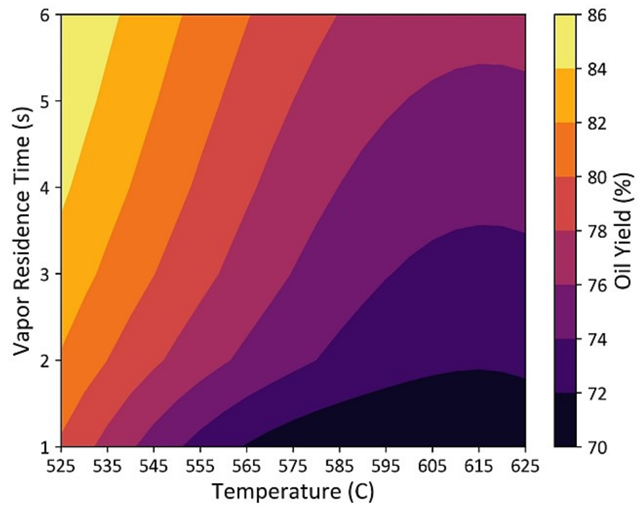


Figure 8: P-Oil yield in different operating conditions

4.2.2- Task 2.2: Integrating the TEA/LCA calculations in simulations {ongoing}

As mentioned previously, the goal of Aim 2 is to establish an advanced sustainable design modeling framework that integrates reaction kinetic models, process modeling, and TEA/LCA calculations, in order to explore the impact of variation in operating conditions and product yields on system-level sustainability.

As the first step, a code for calculating the minimum selling price was developed and applied to a flowsheet calculator in Aspen Plus. Reactors, heat exchangers, and the compressor were sized for the worst-case scenario, which involves the highest temperature level and lowest residence time. This ensures that the equipment can operate properly under various conditions, including the worst-case scenario. Invariable cost terms, including total capital expenditures (CAPEX) and fixed operational costs (F-OPEX), once calculated by APEA, along with feedstock purchase and transportation costs, were manually used as constant parameters. Finally, utility costs and product sales revenue were considered variable inputs in the program, as they change with operating conditions. Having all the components required for cash-flow analysis, the minimum selling price was calculated numerically using iterative Secant method with a fractional perturbation of the independent variable, known as the "modified secant method" [60]. Similar to Task 2.1, the code was initially developed in MATLAB for test runs and refinements before being converted to FORTRAN 77 and applied to the flowsheet calculator.

The analysis reveals that the operating conditions maximizing the P-Oil yield (Figure 8) correspond to the highest revenue, defined as "Revenue = Product sale - utility cost" in Figure 9(a). This is due to two factors: 1) The sale price of P-Oil is higher than that of P-Gas ($634/ton vs $192/ton), and 2) lower heat duties in the reactor and heat exchangers, along with reduced power requirements in the compressor, minimize utility consumption when P-Oil production is maximized. For this part of the analysis, we assumed the sale price of P-Oil to be equal to the average price of crude oil in 2023, and the sale price of P-Gas to be equal to that of natural gas (based on heating value) [61–64]. Since other components in the cash-flow analysis (CAPEX, F-OEPX, and feedstock purchase and transportation costs) remains independent of operating conditions, the minimum selling price of the P-Oil (as the target product) follow the same trend, as demonstrated in Figure 9 (b).

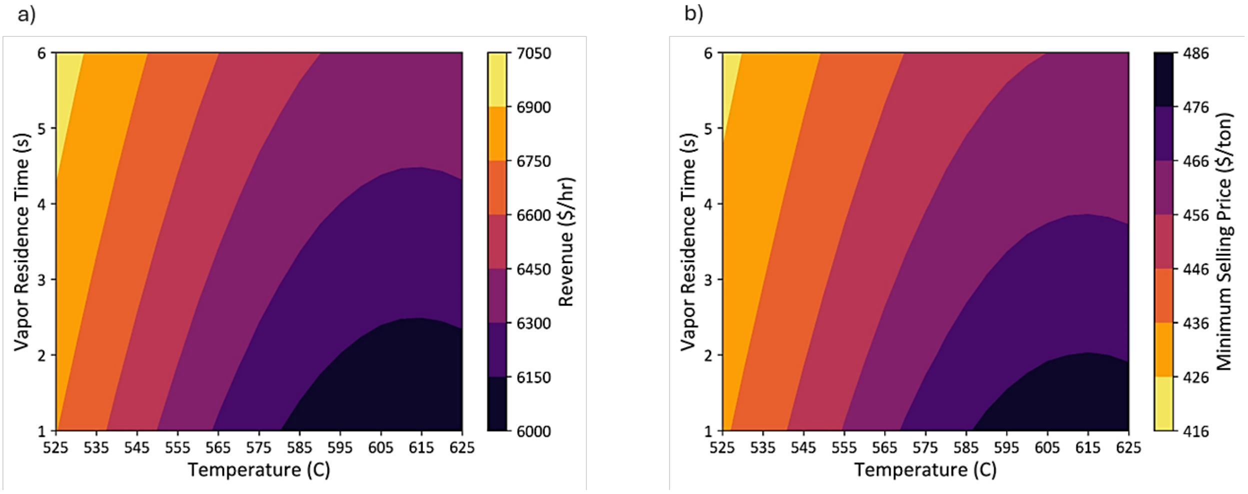


Figure 9: Impact of operating conditions on revenue (a) and minimum selling price (b)

Univariate sensitivity and uncertainty analysis (at optimum operating condition) reveal that feedstock purchase cost, total capital investment, and feedstock transportation cost are the most influential parameters, respectively (Figure 10). Variations in fixed operational cost, tax rate, by-product price, and utility costs have a similar impact on the minimum selling price of P-Oil and are minor compared to the first three parameters. The variation extant in feedstock price was chosen based on price fluctuations in 2023 [50]. For all other parameters, the ranges were selected based on reasonable values found in the literature, our engineering judgments, and uncertainties in values we based our calculations on. Furnace heating efficiency shows the least impact on minimum selling price. This is mainly due to the limitations of the kinetic model as it is unable to capture the influence of heat transfer on product distribution, while studies show the opposite [65]. In this study, furnace efficiency only affects natural gas consumption, which is a component of the utility cost. Consequently, it has an even smaller impact than the overall utility cost.

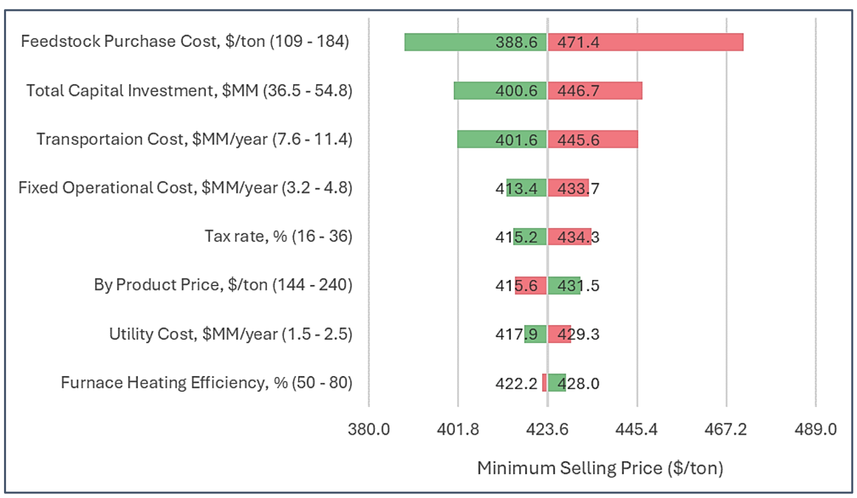


Figure 10: Single variable sensitivity analysis

The concurrent impact of changes in feedstock purchase cost and process downtime on the minimum selling price of P-Oil is shown in Figure 11. Compared to the same analysis in Task 1.2, within the price range and downtimes of this study, the minimum selling price is predominantly influenced by the cost of waste PP bales. However, it is worth mentioning that at each waste PP price level, the difference in MSPs associated with 25 and 85 days of downtime is approximately $55/ton. This price difference is still significant and highlights the importance of process stability. The notable trend differences between the results of this analysis and the corresponding one in Task 1.2 lies in the variation ranges of feedstock prices in the two studies. In previous analysis, as a rough estimation, we assumed that the purchase cost of waste PP bales could rise to twice the average price in 2022. In this analysis, however, the upper limit was set at \$1050/ton, equivalent to the average price of waste HDPE bales. This assumption is based on the idea that if the demand for waste PP increases, its price could rise to match that of waste HDPE. This upper limit is more than seven times the average price of waste PP in 2023 [50]. Assuming 330 operational days for the facility (equivalent to 35 days of downtime), as long as the purchase cost of waste PP bales is less than \$323/ton, the MSP of P-Oil remains below \$634/ton, which is the average price of crude oil in the US in 2023 and serves as the reference market price for P-Oil in this study.

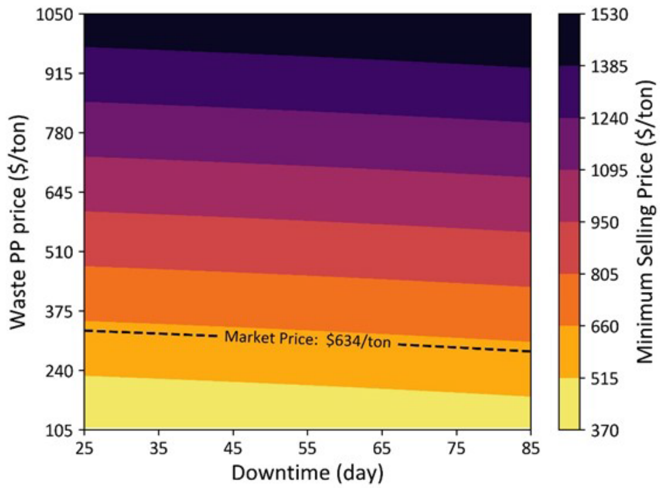


Figure 11: Influence of two major process and economic factors on Minimum Fuel Selling Price

Despite the novelty of using kinetic model (rather than static yields), our approach is still limited by the simplicity and constraints of the integrated kinetic model. Indeed, by adopting more sophisticated kinetic models, we will be able to more rigorously investigate the impact of various operating parameters on process sustainability and conduct more advanced optimizations and sensitivity analyses.

Regarding environmental sustainability, similar to MSP calculator, a separate program will be developed and applied to a flowsheet calculator in Aspen Plus to assess the impact of operating conditions on the environmental impact of the process. Compared to MSP calculations, this program will be less complicated as it will primarily feature straightforward impact assessment calculations. Nonetheless, it is evident that the same limitations will persist due to the simplicity of the integrated kinetic model.

4.3- Aim 3: Investigating the impact of plant location, feedstock/product logistics, recycling technology, and process configurations on sustainability of advanced plastic waste management methods

In contrast to Aims 1 and 2, Aim 3 will shift the focus to the outside of the battery limits of the processing facility to rigorously assess the impact of feedstock and product logistics on system-level sustainability. In the next step, we will use these findings to further optimize the process within the battery limits. This aim will be achieved by completing the two defined tasks as described in the following sections.

4.3.1- Task 3.1: Quantifying logistic impacts on system sustainability {future work}

The primary goal of this task is to uncover the hidden footprint of logistics on system sustainability. Only a limited number of studies have examined this particular aspect. One such study [66] demonstrated that the inherent value of plastic waste changes with location, as shown in Figure 12. The inherent value represents the amount of value plastic waste generates within the value chain. For this analysis, we will employ the Geographic Information System (GIS) developed by United States Environmental Protection Agency (EPA) known as the "Recycling Infrastructure and Market Opportunities Map" [67], illustrated in Figure 13. These data will be used as inputs (and constrains) in The Freight and Fuel Transportation Optimization Tool (FTOT), a tool developed by United States Department of Transportation. This tool serves as a versatile scenario-testing tool aimed at optimizing the transportation of materials in energy and freight contexts. As an open-source software in python environment, FTOT functions include detailed analysis of transportation requirements and constraints, optimizing routing and flows across multimodal transportation networks, estimating costs associated with routing solutions, assessing emissions and vehicle distances, analyzing facility utilization, and other relevant metrics categorized by commodity, transportation mode, and facility. Additionally, FTOT can suggest potential facility locations based on optimized transportation patterns, making it invaluable for scenario comparisons and strategic decision-making in logistics and supply chain management [68]. The results of this task will reveal the impact of location and logistics on system sustainability more rigorously, enabling location optimization. Additionally, these results will allow us to refine our sustainability analysis and conduct more advanced scenario analyses in the subsequent task.

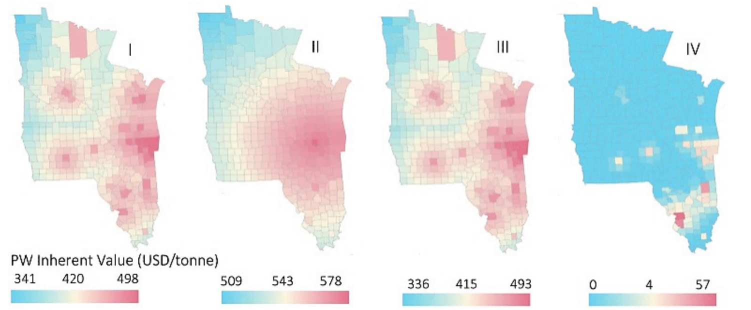


Figure 12: Inherent value of plastic waste in the study region (upper Midwest region of the US) [61]

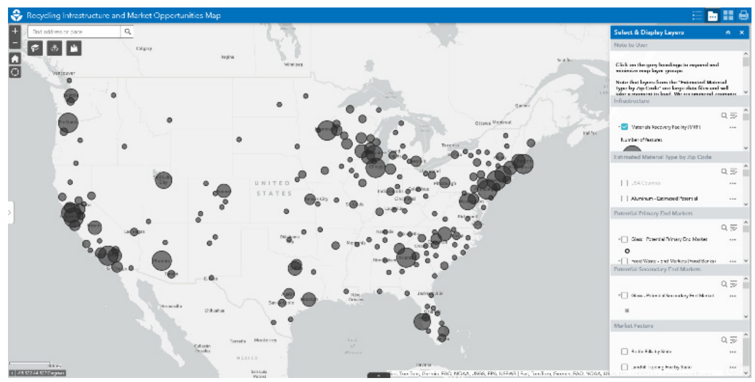


Figure 13: Recycling Infrastructure and Market Opportunities Map

4.3.2- Task 3.2: Performing a system level optimization for plastic waste management {future work}

In previous aims (with their associated tasks), the impact of various factors, ranging from operating conditions and process configuration to logistics and transportation, have been studied independently. In this task, however, the primary goal is to connect those factors to: 1) evaluate how their interactions impact process sustainability and demonstrate the associated trade-offs, and 2) present a more comprehensive perspective on sustainability of advanced plastic waste management methods. Fulfilling this task requires conducting various scenario analyses on:

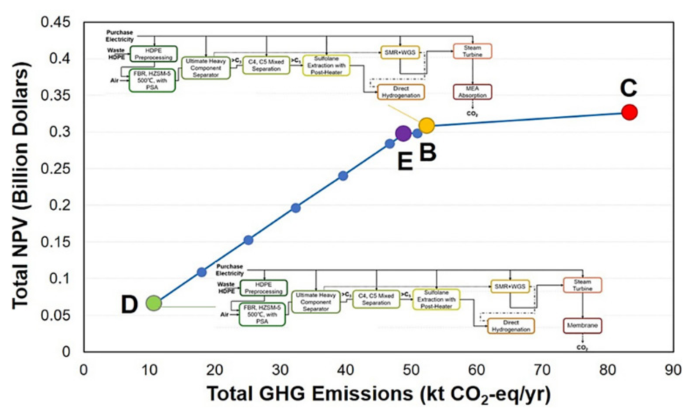


Figure 14: trade-offs between the total NPV and total life cycle GHG emissions in a landscape of design [69]

- **Recycling technologies:** examining Hydrothermal Liquefaction (HTL) and other technologies under optimized operating conditions with different feedstocks.
- **Plant location and configuration:** evaluating centralized versus decentralized setups based on capacity.
- **Facility integration:** comparing standalone grass-root designs with integration into existing facilities.

- **Process scheme:** Analyzing downstream separations and product upgrading in the context of a grass-root design.

For this task, we will primarily rely on the knowledge and frameworks which will have been developed by that date. The results of various scenario analyses and the trade-offs between different economic and environmental sustainability metrics and design decisions can be visualized similarly to some novel works in this field [69], as illustrated by Figure 14.

Completing this task will fulfill Aim 3 of this research, thus achieving the project's ultimate goal of performing system analysis and optimization of chemical recycling for plastic wastes.

5.0- Intellectual Merit

Here we pursue to perform system analysis on converting plastic wastes into valuable products. By integrating Life Cycle Assessment (LCA) and Techno-Economic Analysis (TEA), this study will provide a comprehensive evaluation of the environmental and economic impacts of chemical recycling processes, offering critical insights into their sustainability and feasibility. Almost all studies in this field used static yield data and their system boundary was limited to the recycling facility. In this study, we look to develop an advanced sustainability assessment platform that integrates reaction kinetics with LCA/TEA calculations and process design, while also expanding the system boundary to include logistics and transportation. We investigate a landscape of process designs through advance sustainability assessment model coupled with uncertainty/sensitivity analysis to prioritize research and improve decision-making. The insights gained from this study can help design more efficient and flexible plastic waste management processes, enhance logistics, and enable more advanced optimizations in subsequent research.

6.0- Broader Impact

This project will develop an advanced sustainability assessment platform that provide a comprehensive evaluation of the economic and environmental impacts of thermochemical processes for plastic recycling, offering essential insights into their sustainability and practicality. Expanding the system boundary to include logistics and transportation will further deepen our understanding of the environmental and economic impacts of advanced plastic waste management methods. This approach will help identify limitations, hotspots, and trade-offs, thereby enhancing policy-making and strategic decision-making, and promoting the development of more sustainable practices in plastic waste management. Ultimately, this work will help bridge the gap between laboratory-scale innovations and large-scale applications, supporting the transition to a circular economy.

7.0- References

[1] Global plastic production. Statista n.d. https://www.statista.com/statistics/282732/global-production-of-plastics-since-1950/ (accessed February 6, 2024).

[2] Martín AJ, Mondelli C, Jaydev SD, Pérez-Ramírez J. Catalytic processing of plastic waste on the rise. Chem 2021;7:1487–533. https://doi.org/10.1016/j.chempr.2020.12.006.

[3] Geyer R, Jambeck JR, Law KL. Production, use, and fate of all plastics ever made. Sci Adv 2017;3:e1700782. https://doi.org/10.1126/sciadv.1700782.

[4] Okunola A A, Kehinde I O, Oluwaseun A, Olufiropo E A. Public and Environmental Health Effects of Plastic Wastes Disposal: A Review. J Toxicol Risk Assess 2019;5. https://doi.org/10.23937/2572-4061.1510021.

[5] Worm B, Lotze HK, Jubinville I, Wilcox C, Jambeck J. Plastic as a Persistent Marine Pollutant. Annu Rev Environ Resour 2017;42:1–26. https://doi.org/10.1146/annurev-environ-102016-060700.

[6] Halden RU. Plastics and Health Risks. Annu Rev Public Health 2010;31:179–94. https://doi.org/10.1146/annurev.publhealth.012809.103714.

[7] Galloway TS. Micro-and nano-plastics and human health. Marine Anthropogenic Litter 2015:343–66.

[8] Factors F and. Study on Global Plastic Waste Management Market Size to Hit US$ 46.87 Bn, at a CAGR of 4.5% by 2030. Facts and Factors n.d. https://www.fnfresearch.com/news/global-plastic-waste-management-market (accessed February 6, 2024).

[9] Ormonde E, DeGuzman M, Yoneyama M, Loechner U, Zhu X. Plastics recycling. Chemical Economics Handbook 2019:56.

[10] Kusenberg M, Eschenbacher A, Djokic MR, Zayoud A, Ragaert K, De Meester S, et al. Opportunities and challenges for the application of post-consumer plastic waste pyrolysis oils as steam cracker feedstocks: To decontaminate or not to decontaminate? Waste Management 2022;138:83–115. https://doi.org/10.1016/j.wasman.2021.11.009.

[11] Stern C, Frick A, Weickert G. Relationship between the structure and mechanical properties of polypropylene: Effects of the molecular weight and shear-induced structure. J of Applied Polymer Sci 2007;103:519–33. https://doi.org/10.1002/app.24156.

[12] González-González VA, Neira-Velázquez G, Angulo-Sánchez JL. Polypropylene chain scissions and molecular weight changes in multiple extrusion. Polymer Degradation and Stability 1998;60:33–42. https://doi.org/10.1016/S0141-3910(96)00233-9.

[13] Schyns ZOG, Shaver MP. Mechanical Recycling of Packaging Plastics: A Review. Macromol Rapid Commun 2021;42:2000415. https://doi.org/10.1002/marc.202000415.

[14] Vogt BD, Stokes KK, Kumar SK. Why is Recycling of Postconsumer Plastics so Challenging? ACS Appl Polym Mater 2021;3:4325–46. https://doi.org/10.1021/acsapm.1c00648.

[15] Al-Salem SM, Lettieri P, Baeyens J. Recycling and recovery routes of plastic solid waste (PSW): A review. Waste Management 2009;29:2625–43. https://doi.org/10.1016/j.wasman.2009.06.004.

[16] Westlie AH, Chen EY -X., Holland CM, Stahl SS, Doyle M, Trenor SR, et al. Polyolefin Innovations toward Circularity and Sustainable Alternatives. Macromol Rapid Commun 2022;43:2200492. https://doi.org/10.1002/marc.202200492.

[17] Rorrer JE, Ebrahim AM, Questell-Santiago Y, Zhu J, Troyano-Valls C, Asundi AS, et al. Role of Bifunctional Ru/Acid Catalysts in the Selective Hydrocracking of Polyethylene and Polypropylene Waste to Liquid Hydrocarbons. ACS Catal 2022;12:13969–79. https://doi.org/10.1021/acscatal.2c03596.

[18] Simón D, García MT, de Lucas A, Borreguero AM, Rodríguez JF. Glycolysis of flexible polyurethane wastes using stannous octoate as the catalyst: Study on the influence of reaction parameters. Polymer Degradation and Stability 2013;98:144–9. https://doi.org/10.1016/j.polymdegradstab.2012.10.017.

[19] Ügdüler S, Van Geem KM, Denolf R, Roosen M, Mys N, Ragaert K, et al. Towards closed-loop recycling of multilayer and coloured PET plastic waste by alkaline hydrolysis. Green Chem 2020;22:5376–94. https://doi.org/10.1039/D0GC00894J.

[20] Celik G, Kennedy RM, Hackler RA, Ferrandon M, Tennakoon A, Patnaik S, et al. Upcycling Single-Use Polyethylene into High-Quality Liquid Products. ACS Cent Sci 2019;5:1795–803. https://doi.org/10.1021/acscentsci.9b00722.

[21] Zhang F, Zeng M, Yappert RD, Sun J, Lee Y-H, LaPointe AM, et al. Polyethylene upcycling to long-chain alkylaromatics by tandem hydrogenolysis/aromatization. Science 2020;370:437–41. https://doi.org/10.1126/science.abc5441.

[22] Erkiaga A, Lopez G, Amutio M, Bilbao J, Olazar M. Syngas from steam gasification of polyethylene in a conical spouted bed reactor. Fuel 2013;109:461–9. https://doi.org/10.1016/j.fuel.2013.03.022.

[23] Honus S, Kumagai S, Fedorko G, Molnár V, Yoshioka T. Pyrolysis gases produced from individual and mixed PE, PP, PS, PVC, and PET—Part I: Production and physical properties. Fuel 2018;221:346–60. https://doi.org/10.1016/j.fuel.2018.02.074.

[24] Fekhar B, Gombor L, Miskolczi N. Pyrolysis of chlorine contaminated municipal plastic waste: In-situ upgrading of pyrolysis oils by Ni/ZSM-5, Ni/SAPO-11, red mud and Ca(OH)2 containing catalysts. Journal of the Energy Institute 2019;92:1270–83. https://doi.org/10.1016/j.joei.2018.10.007.

[25] Toledo JM, Aznar MP, Sancho JA. Catalytic Air Gasification of Plastic Waste (Polypropylene) in a Fluidized Bed. Part II: Effects of Some Operating Variables on the Quality of the Raw Gas Produced Using Olivine as the In-Bed Material. Ind Eng Chem Res 2011;50:11815–21. https://doi.org/10.1021/ie200145p.

[26] Tian W, Song P, Zhang H, Duan X, Wei Y, Wang H, et al. Microplastic materials in the environment: Problem and strategical solutions. Progress in Materials Science 2023;132:101035. https://doi.org/10.1016/j.pmatsci.2022.101035.

[27] Sahu JN, Mahalik KK, Nam HK, Ling TY, Woon TS, bin Abdul Rahman MS, et al. Feasibility study for catalytic cracking of waste plastic to produce fuel oil with reference to M alaysia and simulation using ASPEN Plus. Env Prog and Sustain Energy 2014;33:298–307. https://doi.org/10.1002/ep.11748.

[28] Al-Salem SM, Papageorgiou LG, Lettieri P. Techno-economic assessment of thermo-chemical treatment (TCT) units in the Greater London area. Chemical Engineering Journal 2014;248:253–63. https://doi.org/10.1016/j.cej.2014.03.053.

[29] Fivga A, Dimitriou I. Pyrolysis of plastic waste for production of heavy fuel substitute: A techno-economic assessment. Energy 2018;149:865–74. https://doi.org/10.1016/j.energy.2018.02.094.

[30] Bora RR, Wang R, You F. Waste Polypropylene Plastic Recycling toward Climate Change Mitigation and Circular Economy: Energy, Environmental, and Technoeconomic Perspectives. ACS Sustainable Chem Eng 2020;8:16350–63. https://doi.org/10.1021/acssuschemeng.0c06311.

[31] Hernández B, Kots P, Selvam E, Vlachos DG, Ierapetritou MG. Techno-Economic and Life Cycle Analyses of Thermochemical Upcycling Technologies of Low-Density Polyethylene Waste. ACS Sustainable Chem Eng 2023;11:7170–81. https://doi.org/10.1021/acssuschemeng.3c00636.

[32] Volk R, Stallkamp C, Steins JJ, Yogish SP, Müller RC, Stapf D, et al. Techno-economic assessment and comparison of different plastic recycling pathways: A German case study. J of Industrial Ecology 2021;25:1318–37. https://doi.org/10.1111/jiec.13145.

[33] Gracida-Alvarez UR, Winjobi O, Sacramento-Rivero JC, Shonnard DR. System Analyses of High-Value Chemicals and Fuels from a Waste High-Density Polyethylene Refinery. Part 1: Conceptual Design and Techno-Economic Assessment. ACS Sustainable Chem Eng 2019;7:18254–66. https://doi.org/10.1021/acssuschemeng.9b04763.

[34] Jiang G, Wang J, Al-Salem SultanM, Leeke GA. Molten Solar Salt Pyrolysis of Mixed Plastic Waste: Process Simulation and Technoeconomic Evaluation. Energy Fuels 2020;34:7397–409. https://doi.org/10.1021/acs.energyfuels.0c01052.

[35] Riedewald F, Patel Y, Wilson E, Santos S, Sousa-Gallagher M. Economic assessment of a 40,000 t/y mixed plastic waste pyrolysis plant using direct heat treatment with molten metal: A case study of a plant located in Belgium. Waste Management 2021;120:698–707. https://doi.org/10.1016/j.wasman.2020.10.039.

[36] Chhabra V, Parashar A, Shastri Y, Bhattacharya S. Techno-Economic and Life Cycle Assessment of Pyrolysis of Unsegregated Urban Municipal Solid Waste in India. Ind Eng Chem Res 2021;60:1473–82. https://doi.org/10.1021/acs.iecr.0c04746.

[37] Stallkamp C, Hennig M, Volk R, Stapf D, Schultmann F. Pyrolysis of mixed engineering plastics: Economic challenges for automotive plastic waste. Waste Management 2024;176:105–16. https://doi.org/10.1016/j.wasman.2024.01.035.

[38] Cappello V, Sun P, Zang G, Kumar S, Hackler R, Delgado HE, et al. Conversion of plastic waste into high-value lubricants: techno-economic analysis and life cycle assessment. Green Chem 2022;24:6306–18. https://doi.org/10.1039/D2GC01840C.

[39] Olafasakin O, Ma J, Zavala V, Brown RC, Huber GW, Mba-Wright M. Comparative Techno-economic Analysis and Life Cycle Assessment of Producing High-Value Chemicals and Fuels from Waste Plastic via Conventional Pyrolysis and Thermal Oxo-degradation. Energy Fuels 2023;37:15832–42. https://doi.org/10.1021/acs.energyfuels.3c02321.

[40] Yadav G, Singh A, Dutta A, Uekert T, DesVeaux JS, Nicholson SR, et al. Techno-economic analysis and life cycle assessment for catalytic fast pyrolysis of mixed plastic waste. Energy Environ Sci 2023;16:3638–53. https://doi.org/10.1039/D3EE00749A.

[41] Das S, Liang C, Dunn JB. Plastics to fuel or plastics: Life cycle assessment-based evaluation of different options for pyrolysis at end-of-life. Waste Management 2022;153:81–8. https://doi.org/10.1016/j.wasman.2022.08.015.

[42] Benavides PT, Sun P, Han J, Dunn JB, Wang M. Life-cycle analysis of fuels from post-use non-recycled plastics. Fuel 2017;203:11–22. https://doi.org/10.1016/j.fuel.2017.04.070.

[43] Jeswani H, Krüger C, Russ M, Horlacher M, Antony F, Hann S, et al. Life cycle environmental impacts of chemical recycling via pyrolysis of mixed plastic waste in comparison with mechanical recycling and energy recovery. Science of The Total Environment 2021;769:144483. https://doi.org/10.1016/j.scitotenv.2020.144483.

[44] Gracida-Alvarez UR, Winjobi O, Sacramento-Rivero JC, Shonnard DR. System Analyses of High-Value Chemicals and Fuels from a Waste High-Density Polyethylene Refinery. Part 2: Carbon Footprint Analysis and Regional Electricity Effects. ACS Sustainable Chem Eng 2019;7:18267–78. https://doi.org/10.1021/acssuschemeng.9b04764.

[45] Gracida-Alvarez UR, Benavides PT, Lee U, Wang M. Life-cycle analysis of recycling of post-use plastic to plastic via pyrolysis. Journal of Cleaner Production 2023;425:138867. https://doi.org/10.1016/j.jclepro.2023.138867.

[46] Census profile: South Region. Census Reporter 2023. http://censusreporter.org/profiles/02000US3-south-region/ (accessed November 16, 2023).

[47] Polypropylene Recycling Coalition. The Recycling Partnership n.d. https://recyclingpartnership.org/polypropylene-coalition/ (accessed November 17, 2023).

[48] Achilias DS, Roupakias C, Megalokonomos P, Lappas AA, Antonakou EV. Chemical recycling of plastic wastes made from polyethylene (LDPE and HDPE) and polypropylene (PP). Journal of Hazardous Materials 2007;149:536–42. https://doi.org/10.1016/j.jhazmat.2007.06.076.

[49] Turton R, Shaeiwitz J, Bhattacharyya D, Whiting W. Analysis, synthesis, and design of chemical processes. 5th edition. Boston: Prentice Hall; 2018.

[50] Secondary Materials Pricing, RecyclingMarkets.net n.d. https://www.recyclingmarkets.net/secondarymaterials/ (accessed May 17, 2024).

[51] Hildenbrand J, Srocka M, Ciroth A. OpenLCA 2024.

[52] ISO 14040:2006. Environmental management — Life cycle assessment — Principles and framework. International Organization for Standardization. Geneva: 2006.

[53] ISO 14044:2006. Environmental management — Life cycle assessment — Requirements and guidelines. International Organization for Standardization. Geneva: 2006.

[54] Bare J. TRACI 2.0: the tool for the reduction and assessment of chemical and other environmental impacts 2.0. Clean Techn Environ Policy 2011;13:687–96. https://doi.org/10.1007/s10098-010-0338-9.

[55] Huijbregts MAJ, Steinmann ZJN, Elshout PMF, Stam G, Verones F, Vieira M, et al. ReCiPe2016: a harmonised life cycle impact assessment method at midpoint and endpoint level. Int J Life Cycle Assess 2017;22:138–47. https://doi.org/10.1007/s11367-016-1246-y.

[56] Kulas DG, Zolghadr A, Shonnard D. Micropyrolysis of Polyethylene and Polypropylene Prior to Bioconversion: The Effect of Reactor Temperature and Vapor Residence Time on Product Distribution. ACS Sustainable Chem Eng 2021;9:14443–50. https://doi.org/10.1021/acssuschemeng.1c04705.

[57] Gracida-Alvarez UR, Mitchell MK, Sacramento-Rivero JC, Shonnard DR. Effect of Temperature and Vapor Residence Time on the Micropyrolysis Products of Waste High Density Polyethylene. Ind Eng Chem Res 2018;57:1912–23. https://doi.org/10.1021/acs.iecr.7b04362.

[58] Gerald CF, Wheatley PO. Applied numerical analysis. 7. ed., [repr.]. Boston, Mass. Munich: Pearson, Addison Wesley; 2007.

[59] Aspen Plus User Models V8.2. Aspen Technology, Inc. 2013.

[60] Chapra SC. Applied numerical methods with MATLAB for engineers and scientists. 3rd ed. New York: McGraw-Hill; 2012.

[61] U.S. Energy Information Administration (EIA). Short-Term Energy Outlook n.d. https://www.eia.gov/outlooks/steo/realprices/ (accessed May 27, 2024).
[62] U.S. Energy Information Administration (EIA). Crude oil used by U.S. refineries continues to get lighter in most regions n.d. https://www.eia.gov/todayinenergy/detail.php?id=41653 (accessed May 27, 2024).
[63] U.S. Energy Information Administration (EIA). United States Natural Gas Industrial Price (Dollars per Thousand Cubic Feet) n.d. https://www.eia.gov/dnav/ng/hist/n3035us3a.htm (accessed May 27, 2024).
[64] U.S. Energy Information Administration (EIA). British thermal units (Btu) - U.S. Energy Information Administration (EIA) n.d. https://www.eia.gov/energyexplained/units-and-calculators/british-thermal-units.php (accessed May 27, 2024).
[65] Di Blasi C. Kinetic and Heat Transfer Control in the Slow and Flash Pyrolysis of Solids. Ind Eng Chem Res 1996;35:37–46. https://doi.org/10.1021/ie950243d.
[66] Ma J, Tominac PA, Aguirre-Villegas HA, Olafasakin OO, Wright MM, Benson CH, et al. Economic evaluation of infrastructures for thermochemical upcycling of post-consumer plastic waste. Green Chem 2023;25:1032–44. https://doi.org/10.1039/D2GC04005K.
[67] United States Environmental Protection Agency (EPA). Recycling Infrastructure and Market Opportunities Map n.d. https://www.epa.gov/circulareconomy/recycling-infrastructure-and-market-opportunities-map (accessed July 18, 2024).
[68] United States Department of Transportation (DOT). The Freight and Fuel Transportation Optimization Tool | Volpe National Transportation Systems Center n.d. https://www.volpe.dot.gov/our-work/policy-planning-and-environment/volpe-tool-evaluates-freight-and-fuel-transport-options (accessed July 18, 2024).
[69] Zhao X, You F. Waste high-density polyethylene recycling process systems for mitigating plastic pollution through a sustainable design and synthesis paradigm. AIChE Journal 2021;67:e17127. https://doi.org/10.1002/aic.17127.