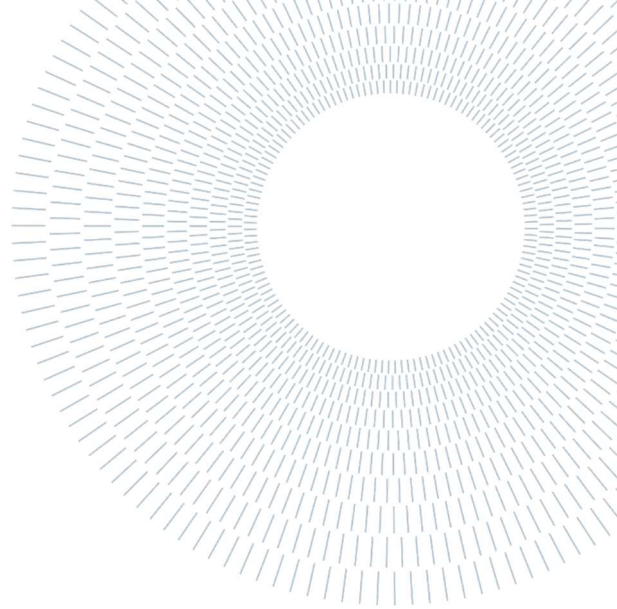




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EXECUTIVE SUMMARY OF THE THESIS

Plastic-to-X Modelling Considering Energy Integration Using a Machine-Learning-Embedded Multi-Objective Graph-Theoretic Optimization Approach: An EU-27 Case Study

TESI MAGISTRALE IN CHEMICAL ENGINEERING – INGEGNERIA CHIMICA

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1. Introduction

The use of plastics has drastically increased over the past 75 years given its affordability, convenience and high performance. Globally, plastic production reached 413.8 Mt in 2023, marking an 11.62% increase from 370.7 Mt in 2018 over the past five years. This increase in plastic production means a corresponding increase in plastic waste generation, which is estimated to reach 12 billion tons of plastic waste disposed in the environment and landfills in 2050. Since plastics do not easily decompose in the environment, their long-term accumulation harms ecosystems. Additionally, disposal methods such as incineration have negative side effects such as the release of CO₂, soot, microplastics, and other airborne pollutants. Not to mention, most of plastic production is fossil-based and relies on energy-intensive processes, resulting in significant CO₂ emissions. Thus, not only is there an urgent need for proper disposal and management of plastic waste, but the decarbonization of plastic production is also vital to mitigate the current

climate change crisis. To achieve this, a transition from the traditional linear economy to a circular economy is essential. In the context of plastic waste management, the circular economy promotes recycling, which can be a combination of closed-loop (plastic-to-plastic) and open-loop (plastic-to-X) recycling strategies. Mechanical recycling is the most established form of plastic-to-plastic recycling, but still faces technical constraints such as polymer incompatibility, thermal degradation, and contamination. These issues call for alternative open-loop recycling methods, especially to achieve full circularity. Chemical recycling methods such as pyrolysis and gasification can convert plastic waste to value added products such as fuels, chemicals, and electricity. However, these technologies still face challenges due to heterogeneous feedstocks and high energy requirements. Moreover, when powered by fossil-based energy, they risk increasing CO₂ emissions, opposing climate goals. Hence, to address this dual challenge of waste management and emissions, integrating renewable energy into plastic recycling systems is critical. Current literature falls short of evaluating plastic recycling pathways at a systems

level including economic, environmental, and energy profile considerations. As a result, this work aims to conduct a comprehensive analysis of four distinct plastic-to-X recycling pathways: plastic-to-plastic via mechanical recycling, plastic to pyrolysis oil, i.e., pyro-oil (fuel) through pyrolysis, plastic to methanol (chemical) via gasification, and plastic to electricity (energy) through incineration. Using a machine learning-embedded multi-objective graph-theoretic (P-graph) optimization approach, the analysis will evaluate each pathway in terms of both economic and environmental performance. The study will also account for four different plastic compositions, i.e., mixed plastics (MP), polyethylene (PE), polypropylene (PP), and polystyrene (PS) to reflect the diversity of real-world plastic waste streams. Furthermore, it will incorporate the energy profiles of the EU-27 countries, along with Norway and Ireland, to assess the impact of varying degrees of renewable energy integration on the overall performance of these pathways. This approach enables a more holistic understanding of how different recycling strategies can be optimized under diverse regional energy contexts, with the goal of simultaneously advancing both circular economic objectives and climate change mitigation.

2. Methodology

The overall research methodology of this work is summarized in Figure 1, which consists of four steps. Step 1 involves investigating various plastic waste recycling pathways by reviewing the literature to identify the available technologies and processes used to convert plastic waste into value-added products. In Step 2, data is collected for each recycling pathway considered, which includes information on CO₂ emissions, associated costs, and energy requirements. Then, Step 3 focuses on model development. First, a surrogate model is constructed to represent each recycling pathway. This is followed by the development of a P-graph model, which serves as the main graph-theoretic multi-objective optimization framework, utilizing the surrogate model (developed with process simulation data) to determine optimal solutions for treating plastic waste. Thus, the work adopts process simulation (Aspen HYSYS), process modelling (Python), and process optimization (P-graph) in an integrated framework (Figure 2).

Finally, in Step 4, the results are processed and analyzed in terms of total CO₂ emissions and net total cost, enabling the evaluation of the most sustainable and cost-effective recycling strategies. In the following subsections, each step of the methodology is discussed in more detail.

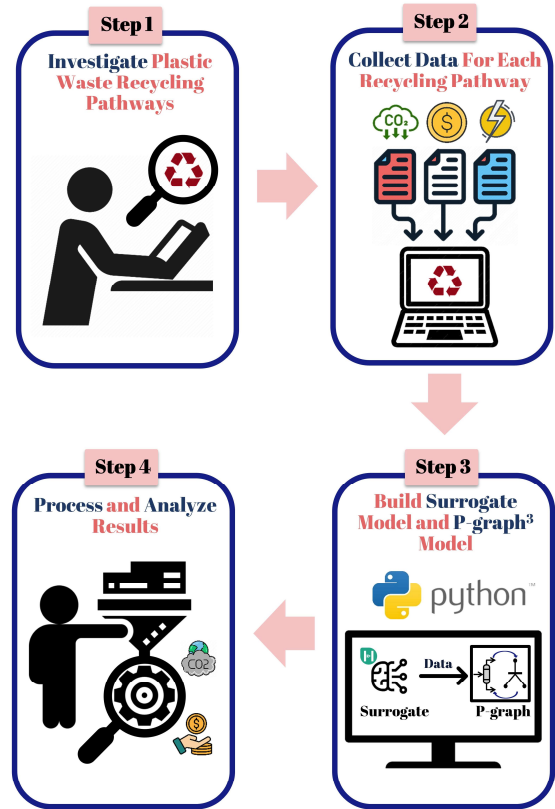


Figure 1: Overall research methodology.

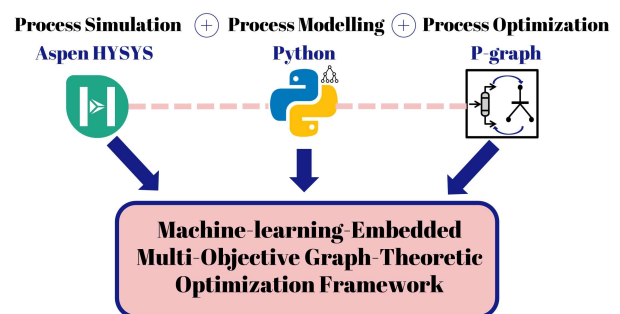


Figure 2: Adopted framework integrating process simulation (Aspen HYSYS), process modelling (Python), and process optimization (P-graph).

2.1. Step 1 Considered Plastic Pathways

In this study, four distinct plastic waste recycling pathways were considered based on their technological maturity, relevance in current

literature, and potential to convert plastic waste into valuable products. These include: (1) plastic-to-plastic recycling through mechanical recycling, (2) plastic-to-fuel, which involves converting plastic waste to pyro-oil oil via pyrolysis, (3) plastic-to-chemical, focusing on the production of methanol through gasification, and (4) plastic-to-energy, where plastic waste is incinerated for energy recovery. These pathways were selected based on insights from literature and represent a broad range of strategies for converting plastic waste into valuable outputs.

2.2. Step 2: Data Collection for Considered Plastic Recycling Pathways

The data collection framework adopted in this study is illustrated in Figure 3. The process begins by selecting the plastic recycling pathway to be analyzed, i.e., this could be plastic-to-plastic, plastic-to-fuel, plastic-to-chemical, or plastic-to-energy. Once the pathway is selected, the next step involves defining the plastic waste composition to be used within that pathway. This may include a MP stream or single streams such as pure PE, PP, or PS. After defining the recycling pathway and plastic composition, the availability of relevant data in the literature is assessed. Specifically, the availability of sufficient data on costs, CO₂ emissions, and energy requirements is for the selected combination is analyzed. If such data is not available, the recycling process must be simulated using a process simulation tool such as Aspen HYSYS to generate the required performance indicators. If the necessary data is available, either from literature or simulations, the next step is to obtain cost, emission, and energy data across varying plastic waste flowrates to support robust modeling. Once this data is collected, a check is performed to determine whether all the desired plastic compositions have been covered. If not, the procedure is repeated for the remaining compositions. When all compositions have been considered, the collected data is then recorded and prepared for surrogate model training, which serves as input for the optimization step, i.e., Step 3.

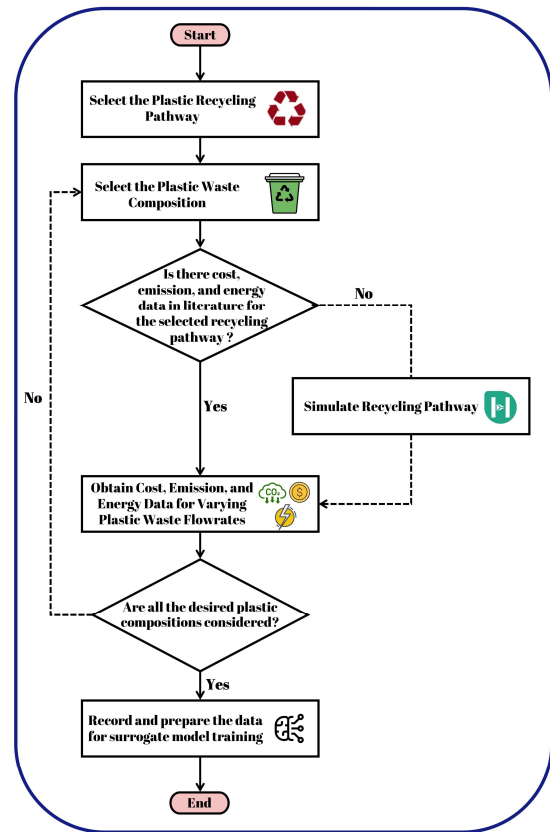


Figure 3: Data collection framework.

2.3. Step 3. Model Development

The model development phase, illustrated in Figure 4, is divided into two sub-steps: Step 3A and Step 3B. In Step 3A, a surrogate model is constructed using the data obtained from the previous step. This model is developed using a decision tree regression algorithm, which is trained on varying plastic waste feed flowrates. The surrogate model is designed to predict three key outputs for each plastic recycling pathway: CO₂ emissions, cost, and electricity requirements. Following this, Step 3B involves the integration of the surrogate models into a P-graph model (a graph-theoretical method introduced by Friedler, et al. [1]) using the P-graph Python library (i.e., Process Graph), which was later introduced by Teng, et al. [2]. Within this machine learning-embedded graph-theoretic optimization framework, each recycling pathway is combined with the electricity generation mix of a selected EU country to reflect region-specific energy impacts. The P-graph model then performs multi-pathway optimization to generate the total CO₂ emissions and net total cost associated with each recycling configuration.

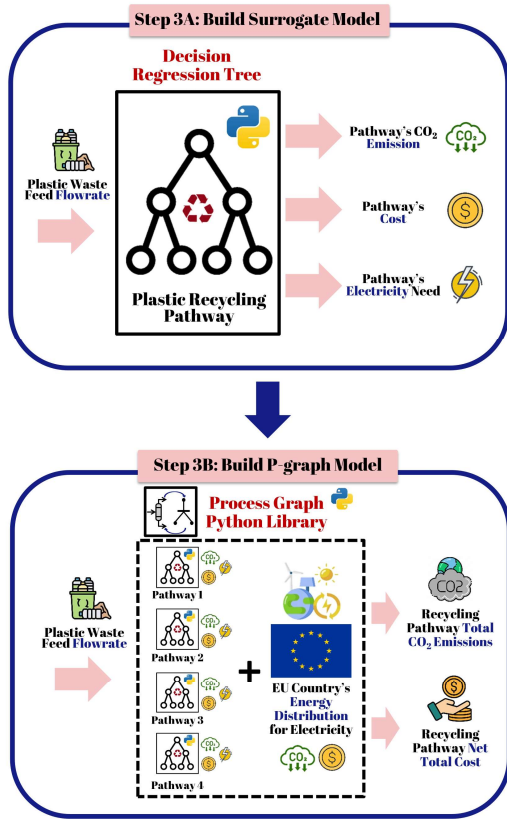


Figure 4: Model development for Step 3: (a) Surrogate model using decision regression tree; (b) P-graph model incorporating energy profiles and recycling pathways.

This work develops a mixed-integer linear programming (MILP)-based mathematical model to determine the optimal plastic recycling pathways considering renewable energy integration. The objective function is solved using the graph-theoretic P-graph framework through a weighted multi-objective optimization approach. The model is designed to evaluate each pathway based on two main criteria: net total cost and total CO₂ emissions, both of which are influenced by the plastic waste composition, selected recycling process, and the electricity mix of the country under consideration. By considering these factors into the model, the aim is to identify cost-effective and environmentally favorable recycling pathways from a large set of possible configurations.

2.4. Step 4. Results Generation and Evaluation

In this step, the fully integrated P-graph model was executed individually for each selected EU country. This was done to reflect the variation in

electricity supply distribution, which influences both the environmental and economic performance of the recycling pathways. For each country-specific run, the model outputs the total CO₂ emissions and total cost associated with the optimal recycling configuration.

3. Case Study Description

The case study conducted in this work focuses on the EU-27 countries, along with Norway and Ireland, resulting in a total of 29 countries. To capture the influence of national electricity profiles on recycling performance, countries are categorized based on their dominant electricity generation source, which is defined as the energy type contributing more than 50 percent to total electricity production. This classification is based on the data by Eurostat [3]. As shown in Figure 5, countries fall into four categories: those primarily reliant on fossil fuels (highlighted in red), those dominated by renewables such as solar, wind, and hydropower (highlighted in green), those with a majority share of nuclear power (highlighted in yellow), and those with a more mixed distribution of energy sources (highlighted in blue). The four plastic compositions are based on plastic bale specifications established by the Deutsche Gesellschaft für Kunststoff-Recycling (DKR). For consistency, a fixed plastic waste flowrate of 10 ton/hr is considered for this case study, allowing for a fair comparison of economic and environmental performance across different compositions and national energy mixes.

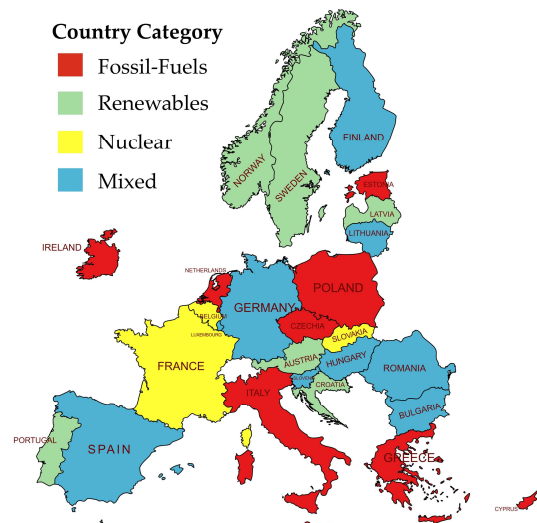


Figure 5: Categorization of EU-27 countries, Norway, and Ireland based on dominant electricity generation source.

4. Results and Discussion

4.1. Plastic-to-X Models

The plastic-to-plastic pathway refers to the mechanical recycling of post-consumer plastic waste into new plastic pellets. This pathway was modeled using process data collected from relevant literature sources. The plastic-to-fuel pathway involves the pyrolysis of plastic waste, which results in three main product fractions, i.e., pyro-oil, pyro-gas (pyrolysis gas), and char. Aspen HYSYS was used to simulate this pathway, and a hydrotreatment unit was incorporated into the simulation to process the crude pyrolysis oil, which is the primary product. The pyro-gas produced during the reaction is also utilized to recover energy through a steam rankine cycle, which generates electricity through a steam turbine. Additionally, part of the thermal energy from the process is recovered as medium-pressure (MP) steam and low-pressure (LP) steam, both of which are assumed to be sold to generate additional revenue. For the plastic-to-chemical pathway, the work adopts the comprehensive simulation model developed by Prifti, et al. [4] which rigorously simulates the plastic-to-methanol process via gasification, reforming, synthesis, and distillation stages. The model has been adapted in this study to accommodate the different plastic waste compositions under investigation. For detailed information regarding the model structure, assumptions, and thermodynamic basis, refer to the original publication. The plastic-to-energy pathway involves the incineration of plastic waste to recover energy in the form of electricity and steam, also modelled using Aspen HYSYS. The thermal energy released is used to drive a Rankine cycle, which generates electricity. Additionally, the system recovers excess thermal energy in the form of MP steam and LP steam, both of which are sold to generate further revenue.

4.2. Surrogate Models

The developed plastic-to-X models described in Section 4.1 serve as the foundation for training the surrogate models evaluated in this section. These models were trained using DT with a number of 360 leaves, beyond which no notable improvement in performance was observed. The model achieves very high predictive accuracy on the test set, with

R^2 and EVS exceeding 0.999 across all plastic streams. This result indicates that more than 99.9 percent of the variance in the predicted variables is captured by the model outputs. To provide further insight into prediction accuracy, the mean absolute error (MAE) was calculated for the CO₂ emissions, total cost, and electricity demand for each pathway and plastic stream. The average MAE for CO₂ emissions remains below 41 kg/year, while that for electricity ranges from approximately 10 to 13 kWh/year. Cost predictions show a similarly low error, remaining under 70 \$/year in all cases. These results further reinforce the reliability of the surrogate models for integration into the P-graph optimization framework.

4.3. Evaluation of Optimal Plastic-to-X Pathways

Table 1 shows the optimal plastic-to-X conversion combinations for different plastic streams in four representative EU countries: Italy (fossil-based), Spain (mixed energy), Austria (renewable-based), and France (nuclear-based). The results show that a clear trend is observed across all countries for the MP stream, where a combination of mechanical recycling and methanol production is consistently selected. This choice can be attributed to the relatively low cost of MP bales compared to purer streams, making mechanical recycling economically attractive. Moreover, methanol production serves as a practical complementary route for the remaining fraction, offering a balanced trade-off between energy demand and material recovery. However, the distribution between the two technologies varies. This difference can be attributed to the energy profile differences, where Italy relies mostly on natural gas, whereas the other countries have a more diversified mix of fossil fuels combined with additional sources like wind, hydro, or biomass. These additional sources reduce the emissions generated of electricity generation, making mechanical recycling, a pathway with higher electricity demand, more attractive compared to methanol production. For PE (DKR-329), the optimal solution is dominated by mechanical recycling, which accounts for 90% of the selected pathway, with the remaining 10% allocated to pyrolysis. This reflects the generally favorable economics of mechanical recycling for high-purity HDPE, while the inclusion of pyrolysis provides

environmental advantages due to its low CO₂ emissions among the available pathways. In contrast, PP (DKR-324) and PS (DKR-331) are predominantly treated through pyrolysis due to the higher pyro-oil yield achieved in these two plastic streams. However, exceptions are observed in countries with cleaner electricity profiles such as Austria and France, where a combination of mechanical recycling and methanol production is favored for the PP stream. This shift can be attributed to the reduced environmental burden provided by low-carbon electricity, which allows the selection of pathways that may not be the most emission-efficient but offer better economic returns. Overall, the results show that both the plastic composition and the national electricity profile influence the selected recycling pathway. Notably, incineration does not appear in any of the optimal configurations, which can be attributed to its relatively high CO₂ emissions, which significantly impact the environmental objective. Aside from these results, P-graph also generated several near-optimal solutions, where the top 1000 near-optimal solutions show the practical advantage of directing plastic waste to multiple treatment options, showing the importance of integrated recycling systems that exploit the strengths of multiple technologies. Overall, the developed P-graph approach is robust in identifying not just a single optimal solution, but a diverse set of high-quality alternatives that are well-suited for the complex and multi-dimensional intricacies of plastic waste management.

Plastic Stream	Optimal Plastic-to-X Combination (%)			
	Italy	Spain	Austria	France
MP	19.2/80.2 (ME/MR)	16/84 (ME/MR)	16/84 (ME/MR)	10/90 (ME/MR)
PE	10/90 (PY/MR)	10/90 (PY/MR)	10/90 (PY/MR)	10/90 (PY/MR)
PP	100 (PY)	100 (PY)	19.2/80.8 (ME/MR)	19.2/80.8 (ME/MR)
PS	100 (PY)	100 (PY)	100 (PY)	100 (PY)

MR = Mechanical Recycling, ME = Methanol Production, PY = Pyrolysis, IN = Incineration

Table 1: Optimal plastic-to-X conversion pathways for different plastic streams across Italy (fossil-based), Spain (mixed-based), Austria (renewables-based), and France (nuclear-based).

5. Conclusions

This work proposes a machine learning-embedded P-graph framework to optimize plastic waste recycling based on cost and environmental impact. Using surrogate models and EU-27 electricity profiles, it evaluates four recycling pathways across representative plastic compositions. Results show that electricity mix and plastic stream type significantly affect optimal choices: mechanical recycling dominates for PE, pyrolysis for PP and PS, and a methanol-mechanical recycling combination for MP streams, while incineration is consistently excluded. Near-optimal solutions reveal the value of multiple pathways, offering greater flexibility. The developed methodology enables a structured, scalable, and energy-integrated evaluation of plastic recycling strategies, supporting data-driven policy and investment decisions towards sustainable plastic management. Future work can expand the pathway set, consider evolving energy scenarios based on climate targets, integrate plant-level data to refine surrogate models, and include a filtering mechanism to eliminate impractical solutions.

6. References

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