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Pathway Optimization for Low-Carbon Plastic Waste-to-Hydrogen Production with Flexible Feed Composition Using a Regression Model

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Conversion of plastic waste into hydrogen is a potential solution to address the issues of growing demand for hydrogen and the massive accumulation of plastic waste simultaneously. However, most studies on plastic-to-hydrogen technology selection were based on predetermined plastic waste composition, limiting their applicability to dynamic real-life operations. To address this, this work introduces a flexible optimisation model capable of accommodating varying compositions of plastic waste. With the aid of regression models, the optimisation model can optimise the plastic-to-hydrogen production pathways, considering economic and environmental performances, without the constraints of specific plastic waste types or mixture compositions. Regression models are developed based on the ultimate analysis data (carbon, hydrogen, nitrogen, oxygen, and sulphur content) to estimate hydrogen yield and purity across various pathways. Thereafter, fuzzy optimisation is employed to identify the trade-off between cost and environmental impact. In addition to the selection of optimal plastic waste-to-hydrogen pathways, the model also considers different purification technologies that can improve the hydrogen purity to various extents. The model demonstrated that pyrolysis-steam reforming combined with PSA is capable of achieving hydrogen purity of 99.999 % with a highest overall satisfaction of 0.7141 (equivalent to total cost of 3.43 M$ and emissions of 528,647 kg CO_2/y) while pyrolysis-catalytic decomposition is more suitable to produce hydrogen with lower purity (55 %).

1. Introduction

According to IEA (2024), around 75 % of global energy usage still relies on fossil fuels, which results in high greenhouse gas emissions, leading to detrimental environmental effects and climate change. Therefore, it is crucial to utilise clean energy sources such as hydrogen energy to address the issues associated with the usage of fossil fuel while fulfilling the escalating energy demand. On the flip side, plastic production currently accounts for approximately 6 % of global oil consumption. This is projected to increase to over 20 % by 2050 (European Parliament, 2017). There is a rapid growth in plastic consumption, which has led to significant environmental consequences and a surge in plastic waste generation. In fact, the Organisation for Economic Co-operation and Development forecasts a rise in global plastic usage from 435 Mt in 2020 to 736 Mt by 2040 (OECD, 2024).
Given the increasing demand for sustainable plastic waste management solutions, the valorisation of plastic waste for hydrogen production through thermochemical pathways has emerged as a viable strategy. Chemical recycling of plastic waste is particularly promising for large-scale applications, facilitating the conversion of plastic waste into valuable products, including hydrogen (Al-Fatesh et al., 2023), which addresses the issue of having a surge of plastic waste and offers an alternative path to produce hydrogen. Among the various chemical recycling pathways, thermochemical recycling has caught the interest of many scholars, given its potential to produce high-value fuels via thermochemical processes such as pyrolysis and gasification (Al-Qadri et al., 2022). For instance, several experimental studies have been conducted to enhance reaction conditions and catalyst efficiency to optimise hydrogen yield and purity. Kim et al. (2025) demonstrated that pyrolysis is highly effective in converting mixed plastic waste into valuable gaseous products, particularly hydrogen. They

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concluded that higher temperatures (800-1000 °C) significantly improve hydrogen production, though the yield varies depending on plastic type. Li and Williams (2024) explored the performance of catalytic steam reforming of plastic waste in hydrogen production. Notably, increasing the reforming temperature from 800 °C to 1000 °C significantly enhanced the hydrogen yield to 83.2 mmol g^{-1} under the presence of tire ash catalyst. Yang et al. (2020) developed a two-stage fluidised catalytic bed reactor system for the continuous co-production of carbon nanotubes and hydrogen from plastic waste gasification. Their findings indicated that optimal hydrogen yield was achieved when the first- and second-stage reactors operated at 600 °C and 800 °C, respectively, with an equivalence ratio of 0.1. However, plastic waste-to-hydrogen technologies have yet to be widely adopted due to limited information in terms of their associated economic and environmental performances.

To date, few studies have focused on the technology selection of plastic waste recycling technologies. Kumar et al. (2025) introduced a P-graph-based method to identify the most cost-effective plastics recycling pathway within the end-of-life supply chain. This approach can generate multiple solutions in terms of total recycling cost, incorporating both capital and operational expenditures. However, the study only considered the mechanical recycling pathway instead of chemical recycling. Majzoub et al. (2024) introduced an extensive mathematical optimisation framework that evaluates various plastic recycling methods, including pyrolysis, gasification, mechanical recycling, and incineration. Both economic feasibility and their contributions to the circular economy (CE) are considered in the model. However, limited plastic waste-to-hydrogen production pathways were considered in their work since hydrogen production is not the sole focus. Hernández et al. (2024) presented a superstructure-based optimisation approach focusing on waste management of low-density polyethylene. While the methodology is robust and inclusive of multiple processing options, it similarly considers limited hydrogen production. In fact, all the aforementioned works relied on fixed input data, omitting the impact of varied plastic compositions on product yields and purities. This restricts the model's flexibility in addressing different cases.

To address this issue, the current study aims to develop an optimisation model that identifies the optimal plastic waste-to-hydrogen production pathway by considering both economic and environmental performances. As inspired by Al-asadi and Miskolczi (2021), this study introduces a novel approach that integrates polynomial regression to estimate hydrogen yield and purity from the ultimate composition of plastic waste (C, H, S, N, and O), which serves as the crucial input for the optimisation model in selecting the most efficient plastic waste-to-hydrogen conversion technology. With this, optimal technology can be selected based on the varied composition of plastic waste compositions, resulting in a less-constrained model that is more flexible to operate.

2. Problem statement

The plastic waste-to-hydrogen conversion pathways considered in this work are shown in Figure 1.

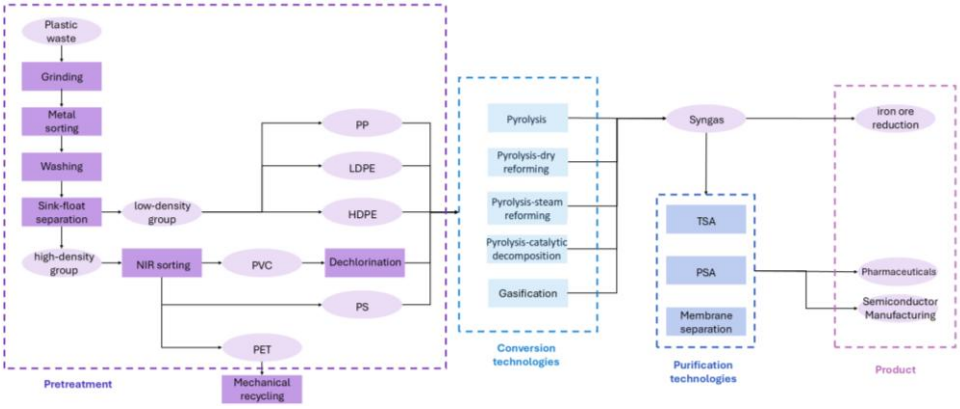

Figure 1: Superstructure of plastic waste to hydrogen conversion technologies. (Abbreviations: NIR sorting (near-infrared sorting), PSA (pressure-swing adsorption) and TSA (temperature-swing adsorption))

The types of plastic wastes considered include High density polyethylene (HDPE), Polyvinyl chloride (PVC), Low density polyethylene (LDPE), Polypropylene (PP), Polyethylene terephthalate (PET) and Polystyrene (PS). This superstructure illustrates four main segments: (i) pre-treatment processes to remove contaminants, and to separate PVC and PET from other types of plastics; (ii) conversion technologies that convert plastic waste into hydrogen; (iii) purification technologies to enhance the purity of hydrogen produced; and (iv) targeted hydrogen products which represent different purity requirement (e.g., high purity hydrogen such as fuel cell-grade; and low purity hydrogen such as those used for fuel blending and metal processing). It is worth noting that PET is excluded from this case study because the pyrolysis of PET results in the production of high-boiling terephthalic acid (TPA) and benzoic acid, which can lead to pipe clogging and corrosion (Li et al., 2022). Consequently, PET

is less suitable for hydrogen production, as the conversion technology primarily relies on thermochemical processes. In fact, the mechanical recycling of PET is already extensively practised at the industrial level. This process is highly cost-effective, simple to operate, and yields high-value products (i.e., recycled PET), which have a growing market demand (Brivio and Tollini, 2022).

3. Model Formulation

The model formulation is presented in the following sections.

3.1 Data collection

The study begins with data collection on the ultimate analysis data of plastic waste, which includes the carbon (C), hydrogen (H), oxygen (O), nitrogen (N), sulphur (S), and chlorine (Cl) content. Production data, including the yield and purity of hydrogen generated through plastic waste-to-hydrogen conversion technologies, is collected. To evaluate the economic performance, cost factors needed for operating and capital expenditures calculation are collected. In terms of environmental aspects, carbon emissions attributed to the operation of the process are collected for the impact evaluation.

3.2 Regression model

With the data collected, the hydrogen yield (Y_p) and the purity of hydrogen yielded from the purification pathway *p* (C_p) are estimated using polynomial regression as shown in Eq(1) and Eq(2), where superscription *Y* and *C* on the right-hand side of the equations also denote hydrogen yield and hydrogen purity, respectively. X represents the independent variable required in the input (i.e., C, H, O, N, S composition), where indexes i and j were used to indicate different components of the input variables, while β represents the associated coefficients. Note that the elemental composition of chlorine (Cl) is not included in the regression model, as it does not contribute to the prediction of hydrogen yield or purity. Instead, it is used separately to assess the need for a dechlorination pretreatment step.

$$Y_p = \beta_0^Y + \sum_{i=1} \beta_i^Y X_i^Y + \sum_{i=1} \sum_{j=i} \beta_{ij}^Y X_i^Y X_j^Y \tag{1}$$

$$C_p = \beta_0^C + \sum_{i=1} \beta_i^C X_i^C + \sum_{i=1} \sum_{j=i} \beta_{ij}^C X_i^C X_j^C \tag{2}$$

3.3 Model constraints

The binary variable B^{purify} is used to determine whether purification is required based on the relationship between total hydrogen purity yielded from the selected pathway *p* (C_p) and targeted purity (C^{target}), as shown in Eq(3). C^{target} refers to the purity level aimed for in the case studies discussed in Section 4. M is an arbitrarily large value used in the Big-M method, ensuring B^{purify} is activated to denote the need of the purification stage ("0" indicates the product needs to go through the purification process; while "1" indicates purification is not required).

$$M \times \left(B^{purify} - 1\right) \leq C^{target} - C_p \leq M \times B^{purify} \tag{3}$$

Eq(4) ensures that one purification method *m* is selected if purification is required. Note that B_m refers to the binary decision variable for purification technology *m*.

$$\sum_{\mathrm{m}} B_m = B^{purify} \tag{4}$$

The yielded hydrogen can then be sent to purification technologies *m* ($\mathrm{Y}_{p,m}$) or directly used as final products without the need of purification ($\mathrm{Y}_p^{by\text{-}pass}$). The resultant flow balance is expressed in Eq(5), while Eq(6) and Eq(7) are used to connect the B^{purify} with the hydrogen flow:

$$Y_p = \sum_m Y_{p,m} + Y_p^{by-pass} \quad \forall p \in P \tag{5}$$

$$Y_p^{by-pass} \leq \left(1 - B^{purify}\right) \times M \quad \forall p \in P \tag{6}$$

$$\sum_{m} Y_{p,m} \leq B^{purify} \times M \quad \forall p \in P \tag{7}$$

As a result, when B^{purify} is equal to "1", $Y_p^{by\text{-}pass}$ will be forced to be "0" as constrained by Eq(6); $Y_{p,m}$ will be constrained to take the value of "0", when purification technology *m* is not selected (B^{purify} = 0).
The yield of hydrogen after purification (Y_m) is obtained using Eq(8), where η_m refers to the purification efficiency of method m. Note that the resultant final yield (Y^{final}) is expressed as Eq(9):

$$Y_m = \sum_{p} Y_{p,m} \times \eta_m \quad \forall m \in M \tag{8}$$

$$Y^{final} = \sum_{m} Y_m + \sum_{p} Y_p^{by-pass} \tag{9}$$

Eq(10) ensures that the final purity of the product (C^{final}) is equal to the purity achievable by the selected purification technology *m* (C_m).

$$C^{final} = \sum_{m} (B_m \times C_m) + \sum_{p} \{C_p \times (1 - B^{purify})\} \quad \forall m \in M \tag{10}$$

3.4 Performance evaluation

Eq(11) computes the total costs ($Cost^{total}$)of the entire system by summing up the pathway total costs ($Cost_p$), purification total costs ($Cost_m$), chlorine pretreatment costs ($Cost^{Cl}$) and other pretreatment costs ($Cost^{Pre}$). The total costs are calculated based on per-unit operating costs and the capital costs.

$$Cost^{total} = \sum_{p} Cost_p + \sum_{m} Cost_m + Cost^{Cl} + Cost^{Pre} \tag{11}$$

Eq(12) demonstrates the total emissions (E^{total}) of the entire system by summing up the pathway total emissions (E_p^{total}), purification total emissions (E_m^{total}), chlorine pretreatment emissions (E^{Cl}) and emissions associated with other pretreatment processes (E^{pre}). The total emissions are computed based on the per-unit operating cost of the pathway.

$$E^{total} = \sum_{p} E_p^{total} + \sum_{m} E_m^{total} + E^{Cl} + E^{pre} \tag{12}$$

Fuzzy optimisation is used because it effectively handles the conflict between the two key objectives, finding a solution that maximises satisfaction for both objectives (Kong et al., 2022). This approach is ideal for optimising conflicting goals at a fuzzy aspiration level, especially when precise values or clear trade-offs are challenging. The expression on the right-hand side of Eq(13) represents the normalised performance (i.e., '0' (worst scenario) and '1' (best scenario)) of the cost and emissions factor (here denoted as Obj^{total}, while *j* refers to different objectives). Obj^{ULV}value is the worst-case values while $Obj^{LLV}$are the best-case values for cost and emissions. λ represents the degree of satisfaction of the least satisfied objective which is maximised in this model. This is to ensure the optimal trade-off between the two aspects ($Cost^{total}$ and E^{total}), without over-prioritising any of them.

$$\max \lambda \leq \frac{Obj^{ULV} - Obj^{total}}{Obj^{ULV} - Obj^{LLV}} \tag{13}$$

4. Case Study Description

The optimisation model was run for two different cases, each targeting a specific hydrogen purity level while considering total costs, emissions, and hydrogen yield. These case studies range from ultra-high purity hydrogen (99.999 %), required for applications such as semiconductor manufacturing and pharmaceuticals (Case 1), to lower-purity hydrogen (55 %), suitable for processes like iron ore reduction (Case 2). The waste considered in the case studies is municipal plastic waste (PW), a common and abundant resource for hydrogen production. The ultimate analysis data of the regression model is available through bit.ly/3FZO9A0. The parameters used in the model are listed in Table 1 (plastic waste composition), Table 2 (cost and emissions

factor of conversion technologies) and Table 3 (cost and emissions factor of purification technologies). As shown in Figure 1, five conversion pathways and three purification pathways are considered in this model.

Table 1: Elemental composition of plastic waste used in this work (Afzal et al., 2023)

C (wt%)	H (wt%)	O (wt%)	N (wt%)	S (wt%)	Cl (wt%)
85.9	14.0	0.1	0.005	0.1	0

Table 2: Cost and emissions factors of each conversion pathway

Technology	CAPEX ($)	OPEX ($/kg PW)	Carbon emissions (kg CO_2/kg H_2)
Pyrolysis	1,020,924	1.25	1.5
Pyrolysis-Catalytic decomposition	1,130,640	2.05	3.05
Pyrolysis-Dry reforming	2,518,224	3.26	4.5
Pyrolysis-Steam reforming	1,657,012	4.89	2.13
Gasification	1,825,178	3.63	2.92

Table 3: Cost, emissions and conversion factors of each purification pathway

Technology	CAPEX ($)	OPEX ($/kg H_2)	Carbon emissions (kg CO_2/kg H_2)	η_m
PSA	643,353	4.45	1.3	0.9
TSA	522,809	6.05	0.66	0.8
Membrane separation	269,775	3.56	0.55	0.8

5. Results and discussions

The result of the case study is demonstrated in Table 4. When ultra-high purity hydrogen (99.999 %) is required, pyrolysis-steam reforming combined with PSA is selected. This is because PSA can achieve extremely high hydrogen purity, making it suitable for industries with strict purity requirements. However, it has a high total cost (3.43 M$/y) and emissions (528,647 kg CO_2/y), primarily due to the energy-intensive nature of the purification process of PSA. Notably, the model reveals that alternative configurations such as pyrolysis-dry reforming, pyrolysis-steam reforming, and gasification are also technically capable of achieving 99.999 % purity when paired with PSA. However, they are not selected due to the resultant lower hydrogen yields and higher costs. For example, pyrolysis-dry reforming with PSA and gasification with PSA exhibit significantly higher capital expenditure, leading to higher total costs and resulting in lower λ of 0.0887 and 0.6810, respectively. These figures indicate that despite being technically feasible, their economic and environmental trade-offs make them less attractive in this context. On the other hand, pyrolysis and pyrolysis-catalytic decomposition are not selected primarily due to lower hydrogen yield (i.e., 24.1 wt% and 57.6 wt%), respectively. Achieving the same output with these technologies would require processing significantly more plastic feedstock, which not only raises operational costs but also amplifies carbon emissions. This finding indicates that in high-purity applications, hydrogen yield could become a decisive factor.

Table 4: Results of the case studies

Case	C^{target} (vol%)	C^{final} (vol%)	$Cost^{total}$ (USD/y)	E^{total} (kg CO_2/y)	λ	Selected technology
1	99.999	99.999	3,427,668	528,647	0.7141	Pyrolysis-steam reforming, PSA
2	55	57.6	1,422,662	434,473	0.9838	Pyrolysis-Catalytic decomposition

In contrast, Case 2 considers a scenario where only 55 % hydrogen purity is required. In this case, pyrolysis-catalytic decomposition is selected. This pathway yields hydrogen at a purity level of 57.6 %, which is sufficient to meet the target. Among the pathways capable of achieving at least 55 % purity, pyrolysis-catalytic decomposition stands out due to its low operating cost and emissions, as shown in Table 2. It offers a lower annual cost of 1.42 M$/y and relatively modest emissions of 434,473 kg CO_2/y as compared to that of Case 1. Pyrolysis alone is not selected in this scenario due to its lower hydrogen yield, typically below 50 wt%.

6. Conclusion

Overall, the results highlight the importance of selecting an appropriate conversion and purification technology based on purity requirements, cost constraints, and yield considerations. The choice of technology ultimately depends on the intended application and the acceptable balance between cost, efficiency, and environmental impact. The case study illustrates how the model flexibly identifies the most appropriate configuration under a purity-driven constraint. Moreover, the model can be extended beyond purity-driven constraints to incorporate additional factors such as maximising hydrogen yield, minimising cost, or achieving specific emissions targets. Future extensions of this work could aim to expand the model to cover a greater spectrum of technologies, enabling more comprehensive assessments across a wider range of potential solutions.

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