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# Environmental Impacts of Plastic Materials Flow Minimisation Using Data-Driven Pinch Method

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Plastics recycling, as a subclass of material recovery and recycling, features extensive and intensive properties. The intensive properties can be used to define a recyclability criterion and to classify the plastic materials for a symbiotic system (industrial, municipal and commercial) into recyclability categories, where the materials with higher recyclability can be either recycled/reused within the same category or cascaded and made available to categories with lower recyclability. The potential surplus waste materials of lowest-grade recyclability would be destined for waste treatment and disposal, while the potential deficit of materials in the highest-grade recyclability category would have to be fulfilled by supplying fresh plastic material produced from primary raw materials. The current contribution takes this problem formulation as a basis to optimise the plastics recycling of industrial symbiotic systems. It defines a Plastic Material Cascade Diagram and an associated set of Supply-Demand Composite Curves, identifying the recycling bottleneck – a Pinch Point limiting the rate of recycling and determining the most efficient material recycling network design. A case study is formulated to illustrate the usefulness of the new concept in reducing the consumption of raw materials and final waste.

## 1. Introduction

There has been a surge in plastic packaging use as a result of the COVID-19 induced measures, adding to the already substantial volume of plastics produced annually (Klemeš et al., 2020). Ritchie and Roser (2018) reported that the annual production of plastic waste had reached 400 Mt in 2015. Jambeck et al. (2015) forecasted that the amount of ocean plastic waste would increase to 150 Mt by 2025. This results in a significant, simultaneous increase of the released plastic waste, the use of primary resources to produce the material, and the environmental footprints. The highest priority measure to minimise these impacts is the planning of plastics reuse and recycling in an optimal way. Chin et al. (2021) have proposed a data-driven framework for identifying the recyclability and compatibility between sets of plastic waste material sources and demand sinks. The plastic waste issues considerably increased when fighting COVID-19 and vaccinations (Klemeš et al., 2021). Recycling plastic waste requires a definition of the quality of the stream. Huysman et al. (2017) have analysed the compatibility between different polymers on the interfacial tension between them. They defined the substitution ratio of recycled plastic, correlated to the compatibility and derived a quality indicator. Eriksen et al. (2018) have explored various scenarios of plastic recycling and qualitatively defined the plastic waste categorisation based on EU standards. They assessed the polymeric composition and other general residues of the polymers. Brouwer et al. (2019) studied the post-consumer plastic packaging waste in a Dutch recycling plant between 2014 and 2017. They reported that most of the recycled plastics are still suited only for open-loop applications due to impure plastic waste. Brouwer et al. (2020) proposed a categorisation of plastic package waste based on the degradation properties, chemical contamination and physical strength. The categorisation is qualitative , ambiguous and preventing proper threshold for plastic waste categorisation.

Material Pinch Analysis has been proven to be an efficient tool in synthesising resources conservation networks. Water Pinch Analysis was initiated by Wang and Smith (1994) based on the Pinch Analysis concept for heat recovery systems (Linnhoff et al., 1994). El-Halwagi et al. (2003) introduced a graph-based method called

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Material Recovery Pinch Diagram to obtain a minimum supply of external resources by investigating the single quality resource conservation problems. This approach provides more accurate targets that account for source mixing, and the network design can be determined directly. The water cascade analysis was then developed by Manan et al. (2004) and widely applied to minimise freshwater targets. The Pinch Analysis tool is insightful with the graphical approach represented by the Composite Curves that can help to clearly identify the source imbalances and the targets through visual inspection. The recent development of utilising Pinch-based tools is shown by Jia et al. (2020), who proposed a Water Scarcity Pinch Analysis (WSPA) to quantify water scarcity in terms of water quality and quantity. They represent the multiple properties of the water streams as a single quality indicator based on certain pre-set rules on the water categorisation. The indicator is then used to construct the Composite Curves to identify the maximum water flows that can potentially be recycled. Based on the above literature review, the following research gaps can be identified:

(i) There is a need for more studies that combine quantitative and data-driven waste categorisation with Process Integration tools to facilitate more accurate recycling planning. Multiple properties of plastic waste, including chemicals, metals, additives and degradation properties, are not yet considered simultaneously.

(ii) A concept and a procedure are still necessary for obtaining the most resource-efficient plastic material network designs resulting in minimum waste treatment and pollution.

Inspired by the WSPA concept, this work addresses the mentioned gaps by proposing a Plastic Pinch framework, using quality categorisation based on the properties to evaluate the recyclability of the plastic waste. The well-known tree-based classification models are applied, i.e. Decision Tree analysis and Random Forest algorithm (VanderPlas, 2016), to derive a set of interpretable if-then rules for quality patterns determination of the various plastic waste streams. This paper focuses on formulating a criterion for materials recyclability for a given batch of plastic material based on its condition. The criterion formulation is based on the evaluation of the rate of polymer degradation and the rate of leakage of fragments to the environment. The Plastic Pinch procedure then identifies the bottleneck of the recycling rate and facilitates the recycling network design.

## 2. Data-driven Plastic Pinch Analysis Method

Plastic Pinch Analysis (PPA) is designed to evaluate the reusability of plastic waste, given sets of plastic material sources and demands. The evaluation builds upon the recyclability definition (Chin et al., 2021) for plastic waste and obtains targets for the minimum demand of new plastic and to minimise plastic waste sent for final treatment (incineration, landfilling). The procedure of the PPA following the stages:

Step 1: Plastic quality categorisation – identification of the categories using the collected plastic waste data;

Step 2: Identification of the available plastic material sources (samples) and the sinks;

Step 3: Classification of the sources and the sinks (mapping) by the recovery categories (classes) from Step 1, and identification of the plastic material sinks by the same categorisation procedure;

Step 4: Construction of the Composite Curves and identification of the targets: Plastic Pinch Point, minimum fresh plastics, minimum final waste plastics.

Several assumptions are made in this work to simplify the considerations and establish the method:

1. The demands and supplies for plastic materials are put forward by the symbiosis network actors. This can be implemented with contracts between the actors – suppliers, users, the exchange hub. The current work assumes that these transactions are agreed upon and evaluates the technical recyclability.
2. The fresh plastic material is assumed to be always available. The system is considered at a steady state.
3. A class with a smaller number contains higher-quality plastic (waste) material.
4. The materials in each class are forward-compatible. The content of each category/class (except the lowest-quality category) is acceptable for intake by all quality categories/classes of lower quality.
5. Different plastic polymers are incompatible when they are mixed.

*Table 1: Plastic quality categories and recommended uses*

| Categories (Classes) | Intended fate |
|---|---|
| Class 1: Virgin | Fresh plastic as manufactured from virgin resources – petroleum-based or renewables-based |
| Class 2: Industrial | The material can be used for the industrial demands in the SN |
| Class 3: Household | The material can be used for household items in the SN |
| Class 4: Waste | The material cannot be reused/recycled (too contaminated or the polymer is too degraded) and has to be sent for final treatment. |

### 2.1. Step 1: Plastic Quality Categorisation

Similar to the WSPA (Jia et al., 2020), the PPA method adopts quality classes instead of specific detailed plastic chemical/physical parameters. The assessed plastic is divided into several classes based on the suitability for reuse between the sources and the sinks. The exact system of classes can be determined by the engineers and stakeholders in the given system – either an industrial site or a Symbiosis Network (SN). An example of a possible selection of classes is shown in Table 1, and it is assumed that the categories comply with the requirement for cascading formulated just before Step 1. The defined scheme allows the possibility of material cascading in an SN for regional plastics flows optimisation.

### 2.2. Step 2: Identification of sources and sinks

The actors in the SN are surveyed for the plastic materials they would like to share with others, and for the plastic material demands, they have to be satisfied by the SN. The data should include: actor data, source identifier, polymer composition, amount – either finite (t) or flowrates (t/d), heterogeneity – mainly the composition of metals, inclusions and contaminants, degradation state of the polymers. In this case, the Melt Flow Index (MFI) is used as an indicator for the degradation state indicator, but other properties can also be used (Turku et al., 2018). For simplicity, in the current work, the identities of the SN actors are omitted, and heterogeneity is characterised by the concentration of metals. The data collection template is shown in Table 2.

*Table 2. Data collection template*

| **Streams** | **Polymer** | **Flow (t)** | **Properties** |
|---|---|---|---|
| Sources e.g. | Polymer type, e.g. | Flow rate values, e.g. | Properties, e.g. |
| SR1 | PE | 150 | (i) Polymer compositions, |
| … | | … | (ii) Contaminant compositions, |
| SR(n) | | 50 | (iii) Degradation/mechanical properties |
| Sinks | Polymer type, e.g. | Flow rate values, e.g. | Properties, e.g. |
| SK1 | PE | 150 | (iv) Polymer compositions, |
| … | | … | (v) Contaminant compositions, |
| SK(m) | | 50 | (vi) Degradation/mechanical properties |

### 2.3. Step 3: Classification of the Sources and Sinks

The classification of the sources or sinks is based on the collected plastic waste properties data in any recycling system. A logical data analysis with a Machine Learning approach helps in deriving a more informative quality definition of the plastic streams. This study applies the well-known tree-based classification models, i.e. Decision Tree algorithm and Random Forest algorithm, to derive a set of if-then rules for quality patterns determination of the various plastic waste streams, where the qualities can be pre-defined by the stakeholders in the system. By using these if-then rules allow the classification of the sources or sinks into the proper categories.

A traditional decision tree algorithm can be solved by the well-known algorithm, known as the ID3 algorithm, and the improved version called the C4.5 algorithm. These algorithms mainly use the indicators called the Shannon entropy - Eq(1) and information gain- Eq(2) to identify the split points (or thresholds) of the dataset. Another well-known index is the Gini index- Eq(3), which is the basis of the CART algorithm. The Gini index is mainly used for binary classification problems with categorical variables but is also applicable to a continuous dataset with binary splits. Random Forest algorithm is built upon the concept of bagging method, where multiple decision trees are ensemble and return the average results from different runs. The open-source Python package; scikit-learn (VanderPlas, 2016) is used to perform the data-driven classification of the plastic waste

$$Entropy(C) = \sum_{i} -p_i \log_2 p_i \tag{1}$$

$$Gain(C, X) = Entropy(C) - Entropy(C, X) \tag{2}$$

$$Gini = 1 - \sum_{i} (p_i)^2 \tag{3}$$

where 'C' represents a class, '$p_i$' represents the probability of attribute/variable 'i' in class 'C', 'X' is the split point. Gain (C, X) represents the entropy difference after a split on the data using attribute/variable 'X'.

## 2.4. Step 4: Targeting with Plastic Pinch Analysis

Based on the quantity and quality of the plastic sources and sinks, the Composite Curves for supply and demand can be constructed (Figure 1) – the Plastic Source Composite Curve and the Plastic Sink Composite Curve. In Figure 1, the Y-axis denotes the plastic waste quality classes from 1 to 4 (from the highest to lowest quality). The classes are assigned to each source or sink in the previous step. The X-axis denotes the plastic amount. The supplies or the sinks are plotted in stacked curves representing the amount of plastic waste/demands in each quality class quality category. The Source Composite Curve is then shifted horizontally to the right until it is at the right of the Sink Composite Curve. The segment where they touch represents the 'Pinch' quality of the plastic wastes recycling system. The minimum required input raw plastic is represented by the non-overlapping sink segment in the bottom-left of the diagram, and the minimum plastic waste for disposal is represented by the non-overlapping source segment.

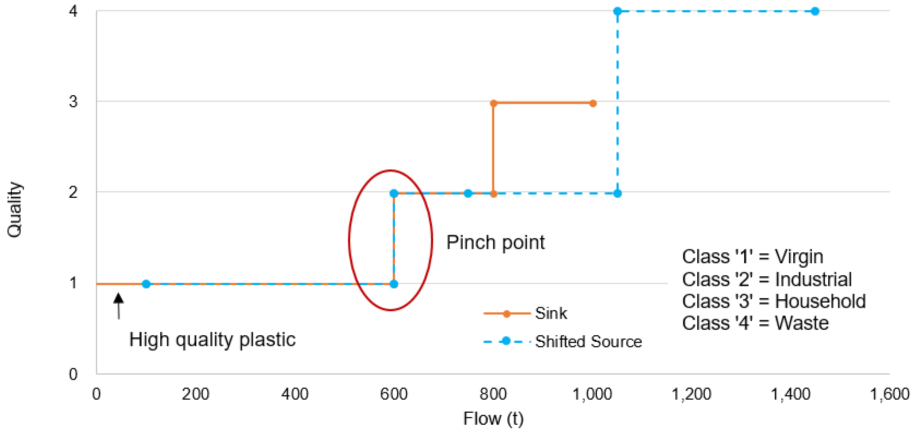

*Figure 1: An example of The Source and Sink Composite Curves*

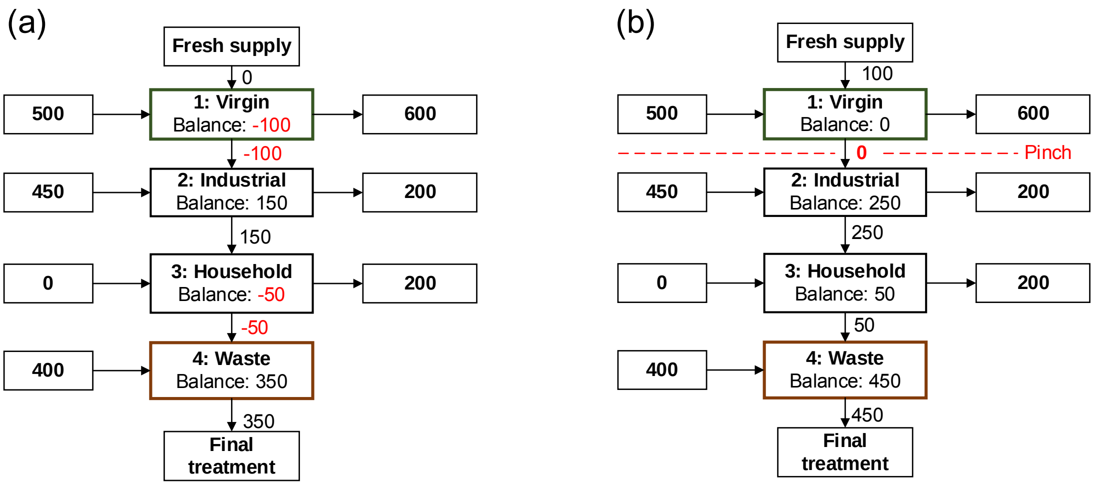

*Figure 2: Plastic Material Cascade Diagram – (a) Infeasible and (b) Feasible*

This kind of recycling planning enables a cascading use of the plastic waste sources - high-quality sources can be used by the demands requiring higher quality first, and then by any lower quality demands - Figure 2. If the Composite Curves are overlapped with a crossover in the case of Figure 1 or a negative flow balance as in Figure 2a, there is insufficient higher quality plastics to meet the demands of the network. In the cascade diagram (Figure 2b), the Pinch Point is identified by the zero flow. This also indicates additional input of plastic materials in class '1' can be added to the system to meet the demands.

## 3. Case Study

An illustrative case study is used to demonstrate the Data-Driven Plastic Pinch framework. The first step identified plastic quality categories. Virgin plastic belongs to Class ‘1’, industrial plastic belongs to Class ‘2’, household plastic belongs to Class ‘3’, and waste belongs to Class ‘4’. It is to be noted that the plastic waste data sample can be collected from any system in a symbiosis network and form a database of plastic waste properties. The data of the plastic waste properties are not shown in this work and can be referred to Chin et al. (2021). The classification of the plastic wastes can then be performed based on the database and applied to any plastic wastes recycling network. The second step involves the identification of the sources and sinks of the system. Table 3 shows the sources and sinks data for the case study, PE denoting polyethylene. The last column of the data represents the quality class of the plastic sources or sinks that are identified with Step 3.

*Table 3. Case study of the sources and sinks*

| **Sources** | Polymer | Flow (t) | Al Metal Concentration (ppm) | Degradation properties | Quality (Class) |
|---|---|---|---|---|---|
| | | | | Melt flow index (g/10 min) | |
| SR1 | PE | 150 | 100 | 0.5 | Industrial (2) |
| SR2 | PE | 300 | 50 | 1.5 | Industrial (2) |
| SR3 | PE | 400 | 500 | 0.1 | Waste (4) |
| SR4 | PE | 500 | 32 | 9.5 | Virgin (1) |
| **Sinks** | Polymer | | Al Metal Concentration (ppm) | Melt flow index (g/10 min) | |
| SK1 | PE | 300 | 100 | 7.7 | Virgin (1) |
| SK2 | PE | 200 | 37 | 5.6 | Industrial (2) |
| SK3 | PE | 200 | 200 | 7.1 | Waste (4) |
| SK4 | PE | 300 | 20 | 8.5 | Virgin (1) |

The third step involves the identification of the classification rules based on the database. The Decision Tree algorithm and Random Forest algorithm are applied to the database, and the results show that the Random Forest algorithm yields better prediction accuracy. The confusion matrix and the classification rules can be found in (Chin et al., 2021). The identified if-then rules can then be applied to the sources and sinks to classify them into the proper classes (see the last column in Table 3).

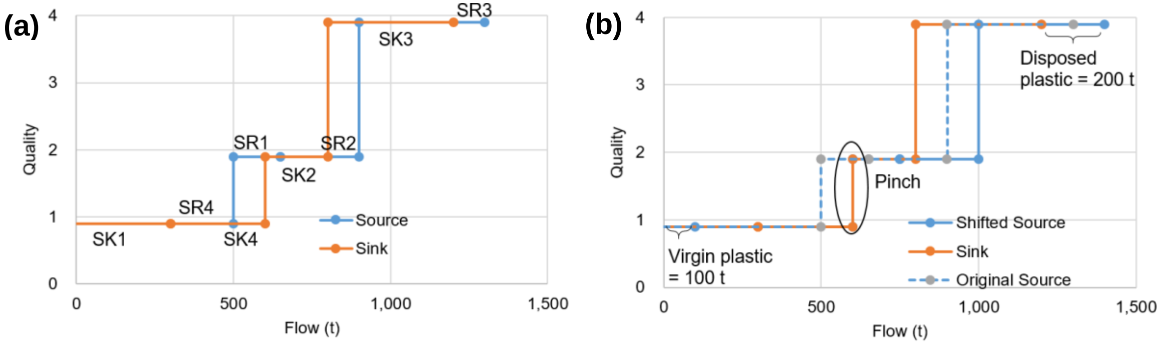

*Figure 3: Composite Curves representation for the case study – (a) Infeasible cascade and (b) Feasible cascade*

After identifying the quality classes of the sources and sinks, the Composite Curves can then be plotted for the system. Figure 3(a) shows the Source and Sink Composite Curves for the case study. It can be seen that there are insufficient sources for the highest quality sink (Class ‘1’). The Source Composite Curve is then shifted to the right until it overlaps with the Sink Composite Curve- see Figure 3(b). Note that a total minimum of 100 t of virgin plastic is required for the system with the Pinch quality class between Class ‘1’ and ‘2’. The minimum plastic waste that is generated is 200 t that is to be sent to incineration or landfilled.

## 4. Conclusions

This work has proposed a Plastic Pinch framework combining the Machine Learning approach to facilitate a more accurate recycling planning of the plastic wastes in any system. The first step includes defining the quality classes of the plastic wastes depending on the demands, and the second step is to identify the sources and sinks streams. In the third step, the Machine Learning-based classification approaches can be used to distinguish the plastic sources and sinks into the pre-defined quality classes that segregate multiple properties of the plastic waste streams. The classification model can be trained with the sampled plastic waste data from different origins. Once the quality classes are defined, the Pinch Analysis framework can then be applied to determine the minimum raw plastic target or the plastic wastes to be disposed of. The Pinch framework is based on the quality class that has been defined by the previous classification approach. An illustrative case study is used to demonstrate the framework, and it shows that 85 % of plastic sources can be recycled. Future work could include more issues such as heterogeneity of plastic wastes, data variations on supplies or demands and unknown quality classes. Future work should also consider the economic and contractual implications of plastic material recycling – including direct exchanges and institutionalising the exchange hubs. Relaxing the steady-state assumption to account for material supplies uncertainty is also important for obtaining practical implementations of the method.

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