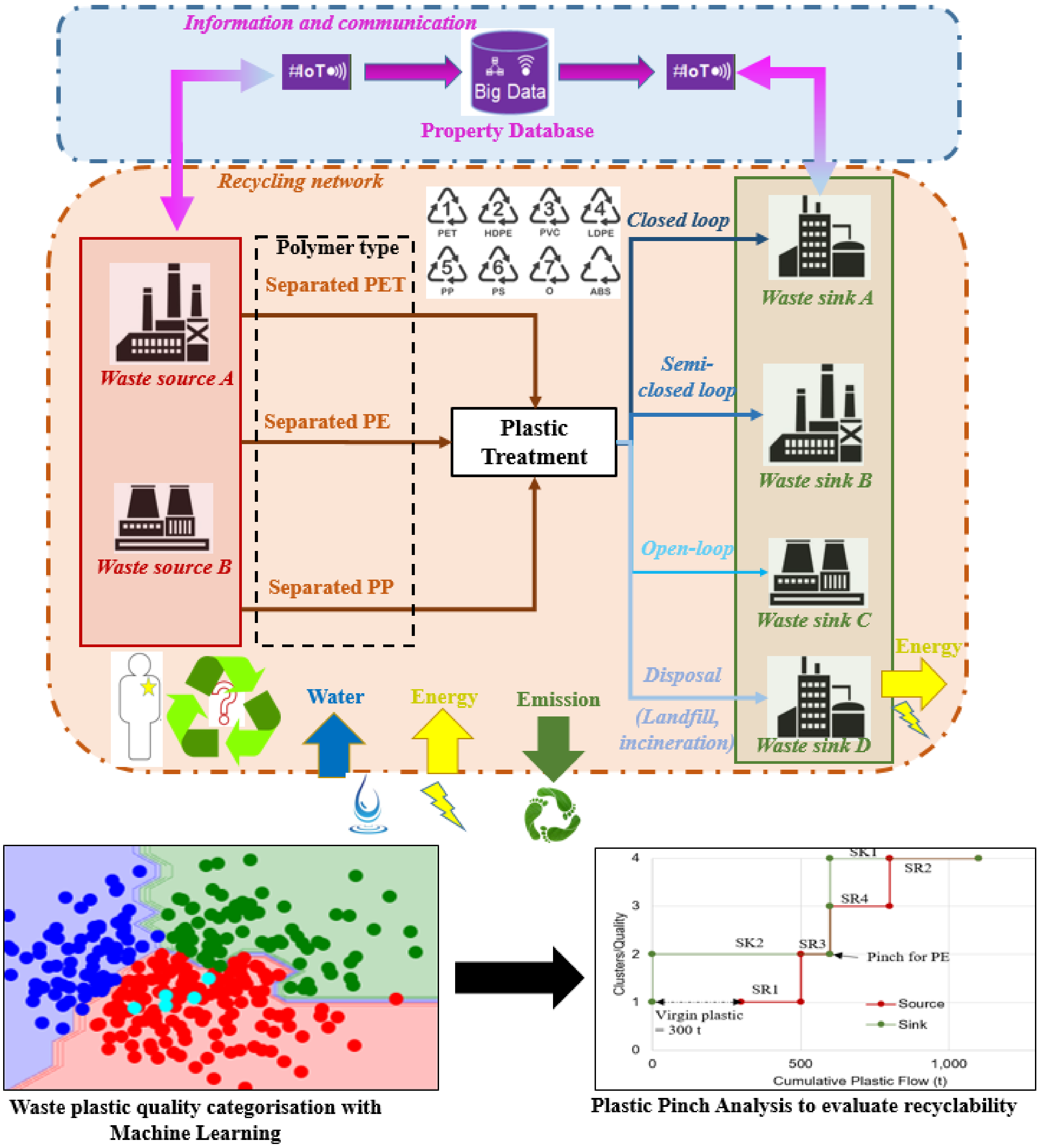
Plastic circular economy framework using hybrid machine learning and pinch analysis

Graphical abstract



Highlights

- Quality-oriented recycling of plastic waste is proposed.
- Data-driven plastic pinch analysis to evaluate plastic waste recycling potential.
- Machine learning approaches to define quality grades of plastic polymers.
- The study showed maximum recyclability is 38% for PET, 100% for PE and 92% for PP.
- The environmental impacts of recycling and treatment technologies are compared.

Plastic circular economy framework using hybrid machine learning and pinch analysis

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Abstract

The worldwide plastic waste accumulation has posed probably irreversible harm to the environment, and the main dilemma for this global issue is: How to define the waste quality grading system to maximise plastic recyclability? This work reports a machine learning approach to evaluating the recyclability of plastic waste by categorising the quality trends of the contained polymers with auxiliary materials. The result reveals the hierarchical resource quality grades predictors that restrict the mapping of the waste sources to the demands. The Pinch Analysis framework is then applied using the quality clusters to maximise plastic recyclability. The method identifies a Pinch Point – the ideal waste quality level that limits the plastic recycling rate in the system. The novel concept is applied to a problem with different polymer types and properties. The results show the maximum recycling rate for the case study to be 38 % for PET, 100 % for PE and 92 % for PP based on the optimal number of clusters identified. Trends of environmental impacts with different plastic recyclability and footprints of recycled plastic are also compared.

1. Introduction

Plastic waste pollution has been a consistent threat to societies regardless of the global advancement of technology (Huysman et al., 2017). Ritchie and Roser (2018) reported that the annual production of plastic waste had reached 400 Mt in 2015. It is expected that about 0.2 Gt of plastic will be ended up in landfills by 2025 if the trend persists, and the expected amount of ocean plastic waste would increase to about 150 Mt by 2025 (Jambeck et al., 2015). The plastic surge is more significant during the pandemic of COVID-19 as it induces measures on higher usage of plastic packaging, causing further damage to the environment (Klemeš et al., 2020). The plastic waste issues considerably increased when fighting COVID-19 and vaccinations (Klemeš et al., 2021). The highest priority mitigation measure is to minimise virgin plastic consumption by maximising the recycling rate of plastic waste. It is highlighted by Lazarevic et al. (2010) that the optimal virgin material substitution ratio should be identified by recycling high-quality plastic waste to ensure greater environmental benefits. This underlines a better understanding of the plastic material characteristics and its recyclability is needed to maximise the environmental benefits.

The main hurdle for plastic waste recycling is the complex fraction of the plastic waste streams, which also consists of a complex blend of several polymers (Ragaert et al., 2017). It was identified that the waste streams with more than 20 wt % for the contamination fractions are sent to incineration, wasting the potential of the secondary materials (Huysveld et al., 2019). Gradus et al. (2017) analysed the cost-effectiveness of plastic waste incineration and treatment options in the Netherlands. Despite the cost of collection and treatment of plastic recycling being high, the post-separation of waste can reduce the cost of recycling, rather than source separation. They also mentioned that the post-separation of plastics provides a higher quality of plastic waste, enabling a higher recycling rate of plastic. Faraca et al. (2019) analysed the environmental life-cycle cost perspective for hard plastic waste recycling options, and they concluded that quality-oriented mechanical recycling options are preferable from both environmental and economic perspectives. More straightforward mechanical recycling can be more beneficial than incineration due to considerable emissions from incinerating a large amount of plastic waste. Their studies have proven that resource quality is the driving force toward cost-effective and environmentally-friendly recycling to achieve a sustainable Circular Economy.

Ragaert et al. (2020) extensively analysed the composition and mechanical properties of the mixed plastic waste case study for recyclability study. PVC is one of the hurdles for recycling plastic and they proposed that the waste stream can be treated with PVC removals as well as non-ferrous metals. Akbar and Liew (2020) assessed the recycling potential of carbon-fibre reinforced plastic waste in the construction industry. Several pathways for mechanical and chemical recycling of plastic waste are reviewed by Ragert et al. (2020) and, more recently, Vollmet et al. (2020), who reviewed options for the chemical recycling of polymers to enhance recycling rates. They provide several options for closing the loops for polymers, which are preferable to incineration or landfilling. Coates and Getzler (2020) proposed and analysed the option for the chemical recycling method by transforming polymers back to monomers and then purifying them for repolymerisation. Successful research reported by Tournier et al. (2020) is using enzymes to reduce plastic waste (PET) into fully functional plastic bottles. Mikula et al. (2021) also reviewed the production of 3D printing filaments from secondary plastic resources and showed that this approach is promising in closing the loop of plastic recycling. Several options include converting plastic to value-added products like solvents or fuel additives via an integrated biomass process (Beydoun and Klankermayer, 2020) and carbon nanotube products (Alireza and Gordon, 2012). Various works have proven that minimising and recycling plastic waste is a major way forward for treating plastic waste (Klemeš, et al., 2020). However, prior to recycling plastic waste, the various complex properties should be taken into consideration when planning the recycling pathways.

Regarding the plastic waste recycling planning studies, Huysman et al. (2017) have developed a Circular Economy performance indicator for plastic waste, mainly based on the Cumulative Exergy Extraction from the Natural Environment (CEENE) method, which analyses the impact of the recycling process. The approach is coupled with compatibility estimation between different polymers. The substitution ratio of recycled plastic is based on the quality indicator and is correlated with interfacial tension between polymers. Incompatible polymers blend has poor mechanical properties such as high brittleness (Ragaert et al., 2017). Min et al. (2020) has analysed the critical factors for ocean plastic degradation based on limited data from various publications. Eriksen et al. (2019) have defined the plastic waste categorisation based on EU standards qualitatively and according to different applications (e.g. food grade, pharmaceutical uses, and other usages). They assessed the polymeric composition and other general residues of the polymers. Faraca and Astrup (2019) also evaluated the plastic waste from the recycling centres in Denmark and distinguished them into applicability, impurity, lifetime, and polymeric compositions. The quality grades of plastic are mainly identified through the specific application of recycled waste. Brouwer et al. (2020) later provided a general categorisation guideline depending on the physical strength, degradation, and chemical composition of the plastic waste. However, the categorisation only provides a qualitative guideline for the practitioners, and it can be difficult to identify a proper quality grade to maximise the recycling of plastic waste. This calls for a tactical approach to systematic quantifying the quality classes of plastic waste with complex properties.

Material Pinch Analysis has been proven to be an efficient tool in the problem of resources conservation network synthesis. 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 Material Recovery Pinch Diagram to obtain a minimum supply of external resources by investigating the single quality resource conservation problems. A detailed review of the Pinch Analysis application can be found in Klemeš et al. (2018). This approach provides more accurate fresh resources requirements that account for source mixing, and the network design can be determined directly. While those developments on Mass Integration have been very helpful for the recycling and reuse of materials in the industry, where the streams are more homogeneous, the reuse of mass flows in the general economy features less homogeneous flows, with varying composition and quality levels. This problem is made more difficult by the variation of the regulations for material recycling across countries. Typical problems of this type are presented by regional water scarcity evaluation- see Jia et al. (2020) and minimisation and by the recycling of material resources at various scales – site, city, region.

Many publications have laid a foundation in plastic waste recycling planning, but a critical gap that exists is the lacking of a proper defined plastic waste recyclability within a regional system. Plastic waste trading is still restricted by the current recycling capacity due to the lack of a plastic chemical information system. To the best of the authors' knowledge, the correlation between complex plastic quality and plastic recyclability has not yet been investigated.

To fill the knowledge gaps, two key steps have been taken by collaborations of the current authors and developed a prototype of an AI-driven plastic waste categorisation method (Chin et al., 2021) for identifying the recyclability of plastic waste flows and batches. The other step has been the Plastic Pinch Analysis concept (Varbanov et al., 2021), which defines the basics of plastic cascade recycling. These works are inspired by the family of Process Integration methods (Klemeš et al. 2018) and draw an analogy from the Water Scarcity Pinch concept (Jia et al., 2020). To obtain a fully usable data-driven Plastic Pinch Analysis method, these two prototype components need further development to achieve:

(i) A general data-driven workflow integrating the available waste streams data, covering the suppliers of secondary raw materials (sources) and the potential users (sinks), with the plastic conservation network synthesis problem

(ii) A clear system of concepts for quantifying the qualities of mixed-polymer and mixed-composition samples

(iii) The construction of a cascade model where each material cascade enables the exchange and reuse of a separate internally compatible set of materials. Materials in the same category can be recycled to the demands with similar categories or cascaded to lower quality categories. This helps evaluate the plastic recyclability within a region/system.

The concept developed in this work stems from the general life cycle of plastic materials, as well as the established separation and recycling practices. The ultimate aim is to formulate a site-level integration with Big Data analytics to form a chemical information system for plastic waste recycling- see Fig. 1. The qualities of the plastic waste can be modelled using the Machine Learning framework, using the existing available centralised database. The data samples can be collected from an existing plastic recycling system presented in Fig. 1, and the general database can be formulated from the samples. In this case, the qualities of the plastic waste from different plants can be identified using the database as the benchmark, and in turn, it helps to predict the waste quality for any system. The plastic waste exchange between industrial and domestic users has become more accurate and informative by allowing information exchange between suppliers and demands. The flow network starts the consideration from the extraction of primary resources and includes the stages for raw material preparation, forming products, distribution/use of the products, waste separation and processing, recycling and landfilling.

In addition to that general flow pattern, it is also known that there are different applications for plastic materials (Grigore et al., 2017), such as food and drink, household items, gardening items, building, and interior items. Those applications define a set of material classes, which impose different quality and cleanliness requirements on the material sources. Taking a batch or a sample of waste plastics (termed a Source) and determining its future fate presents a recycling planning problem. That can be modelled as a mapping of the source to a set of alternative sinks, as illustrated in Fig. 2, whether be closed-loop, semi-closed loop or open-loop recycling applications (Huysman et al., 2017). In that Fig., a set of sinks, which pose sufficiently close quality requirements, form a class of materials. Following that logic, the potential applications determine the classes of materials, and the potential source of secondary raw material has to be classified within one or several of those classes. The main questions to be answered are the recyclability of the plastic waste within that system. The environmental impact of the recycling system should be studied as well, by analysing the emissions as well as potential water and energy consumption.

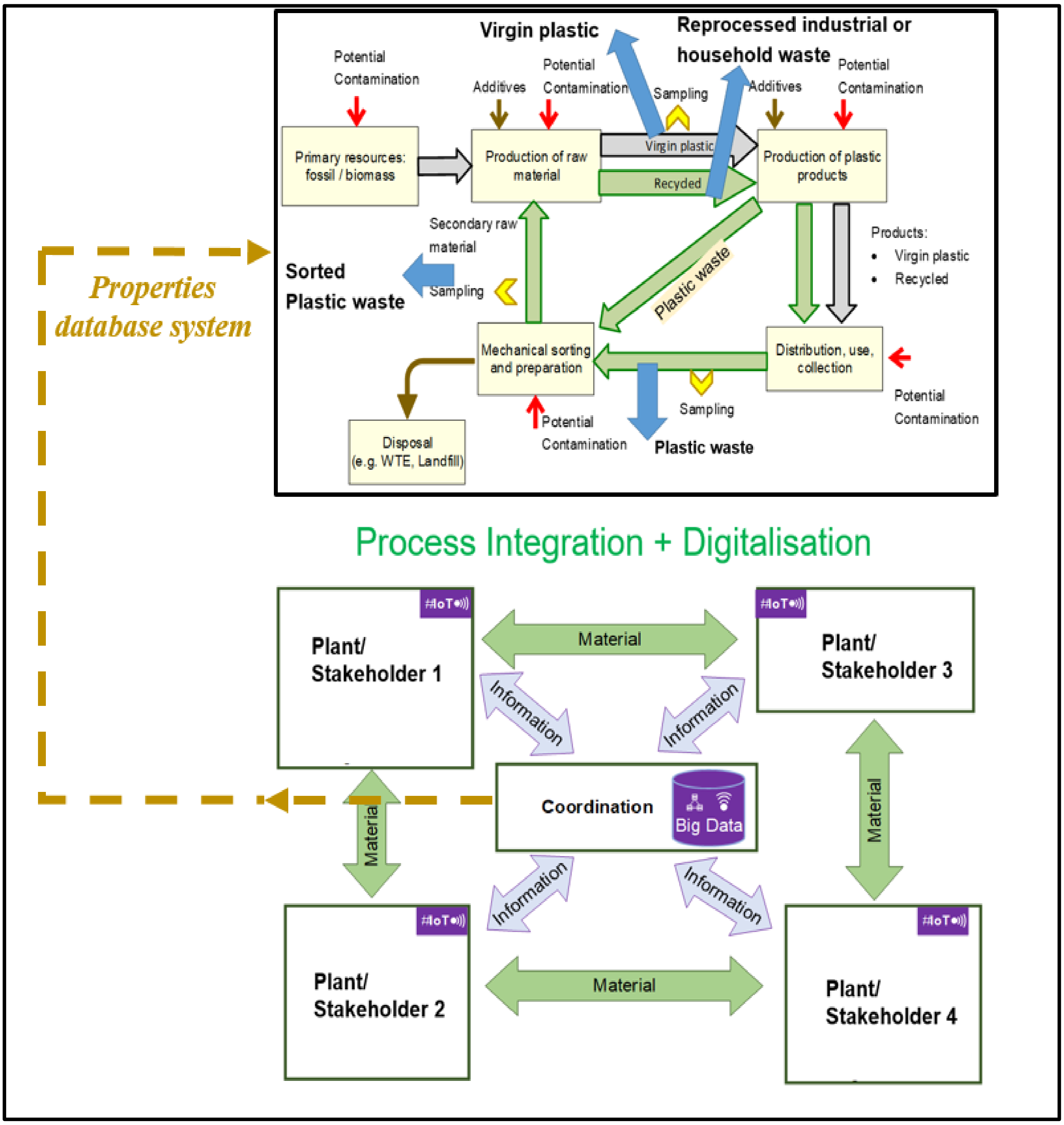


Fig. 1. Material exchange between stakeholders aided by using big data analytics with a database based on a plastic value chain with a recycling system (Adapted and modified from Eriksen et al. (2017)).

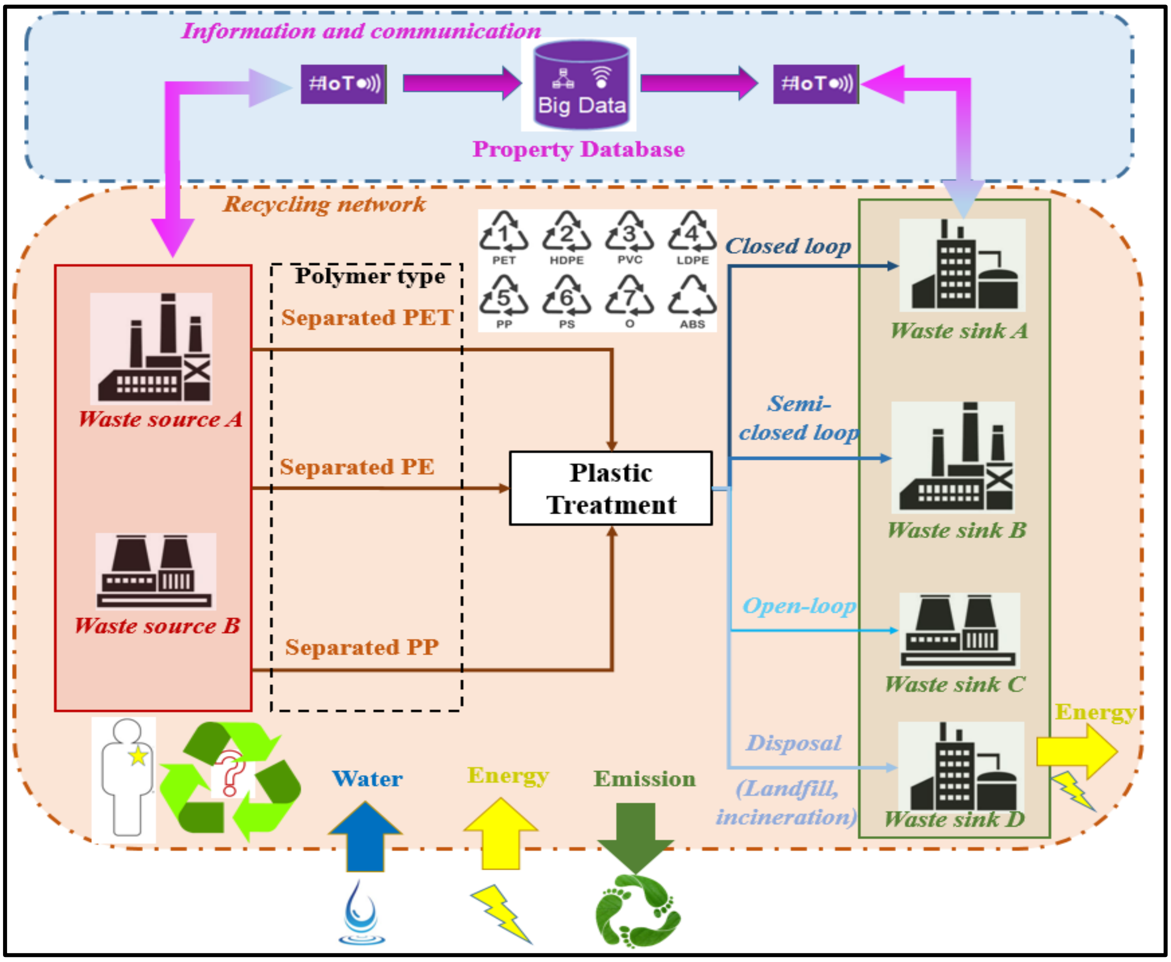


Fig. 2. Mapping of plastic sources for different applications with a data-driven approach.

2. Material and methods

2.1 Database formation

To characterise the effect of complex properties of plastic waste the optimal recycling planning, the datasets utilised in this study consist of various bulk properties of plastic waste streams, including three polymers types: PE, PET and PP to mimic the regional property database. Each polymer types consist of data samples with mechanical properties, degradation properties, metal contaminations and impurities. For metal contaminations, there are 13 types of metals in the dataset for each polymer type, namely As, Cd, Co, Cr, Cu, Fe, Hg, Li, Mn, Ni, Pb, Sb, Ti and Zn. The data samples for metal contaminations are retrieved from the experimental study of Eriksen et al. (2017) that are sourced from an existing plastic recycling system. Their data are limited due to few samples available: 16 for PE, 26 for PET and 10 for PP, including all the plastic waste from different origins: virgin plastic, recycled industrial and household waste, and unwanted waste. The rest of the datasets are interpolated from the existing data.

The degradation of plastic waste happens for various factors, including exposure to high temperatures or exposure to ultraviolet radiation. They could break the polymers intermolecular chain links, which in turn affects the plastic waste usability. The degradation can be quantified by measuring the viscosity of the polymers. In this work, the intrinsic viscosity (IV) property is used for the polymers PET, while the melt flow index is used for polymer PE and PP as it measures the ease of flow for thermoplastic polymer. Lower values of MFI/higher values of IV for a similar polymer indicate higher polymer strengths, which means less degradation of the plastic waste. The values provided in the dataset are estimated based on IV from Bredikhin et al. (2017) and MFI from Eriksen et al. (2019), but they can differ depending on the specific processes. The dataset in this work is just a benchmark dataset for demonstrating the proposed framework.

The dataset also includes mechanical properties, which in this case mainly focus on the tensile strength of the plastic waste. Due to limited data availability, the tensile strengths for each polymer type in the datasets are estimated from the experimental data of Eriksen et al. (2019). In reality, this is correlated with the polymer's strength index, which is MFI or IV. The impurities included in the datasets consist of papers, cardboard, food residues and other unknown substances. The datasets are estimated based on the standard ranges provided in Brouswer et al. (2019) that indicate the range of the impurities amount acceptable for recycled plastics based on specific applications. The polymeric composition of non-target polymers is also estimated based on the specification with a similar reference. Specification of the non-target polymers compositions for the target polymers is assumed to be known in the demand sites through information exchange.

2.2 Plastic pinch analysis

This work focuses on providing a user-friendly tool for targeting the minimum virgin plastic flow according to the quality grade of plastic waste. Pinch Analysis is an efficient framework without the need for complex mathematical formulation in targeting the maximum recycling rate of the waste stream, constrained by the quality of the waste. The approach is user-friendly and can be illustrated with graphical visualisation, allowing the insights of the problem and solutions to be visualised. The users can tweak the graphical solutions themselves as well to determine the alternative solutions. The pinch analysis concept is mainly based on the two variables: quality and the quantity of the material sources/supplies and sinks/demands. For plastic waste recycling, the main hurdle is the definition of the quality grade due to the complex properties of plastic waste, which hinders accurate plastic waste recycling planning. Since the quality class of plastic waste is determined using the Machine Learning tools, this eases the problem formulation, and the outcomes of the learning tools help in defining the quality constraints for the problem of the plastic waste conservation network. The theoretical explanation of the machine learning framework applied is explained in Table S1 and S2.

The illustration of how the quality class can be integrated with the Pinch Analysis tool is shown through database formulation, as shown in Fig. 1. The composite curves for supply and demand can be constructed, as illustrated in Fig. 3(a). The plastic source composite curve is made up of the available plastic waste sources in the case study that can be recycled, while the plastic sink composite curve is for the demands requirements. Both composite curves are constructed by stacking each segment of sources/sinks in descending order of quality grade, where each segment represents a source/sink stream. Y-axis denotes the plastic waste quality classes from the highest to lowest quality- which is defined by the machine learning algorithms). The horizontal axis is the plastic amount (can be flow or flowrate). 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 waste recycling system. The pinch segment shows the quality bottleneck of the plastic waste in the system. The minimum required input raw plastic is denoted by the shifted amount of the source composite curve, while the minimum plastic waste to be disposed of is denoted as the extra source segment that is not overlapped with sink composite curve.

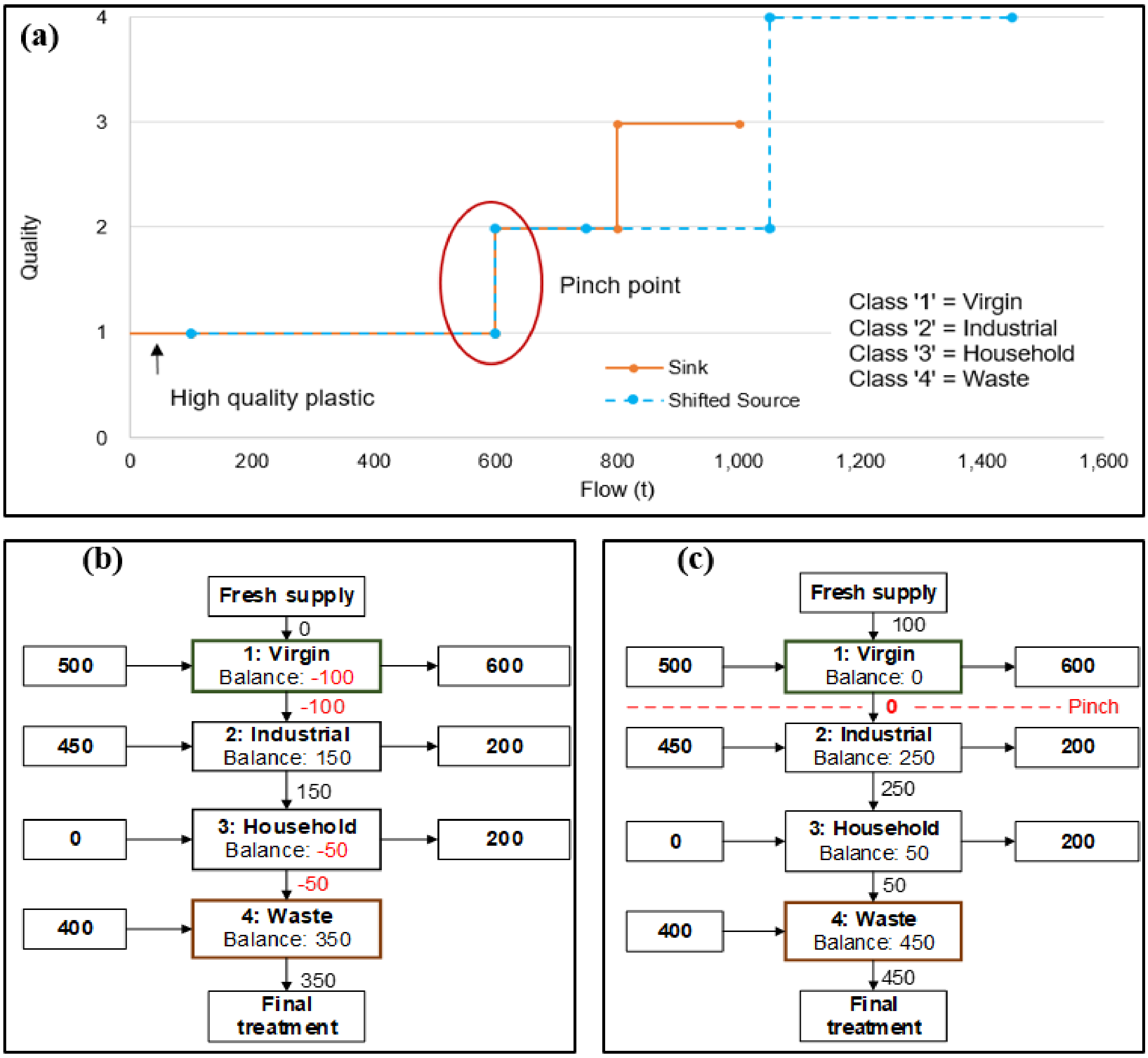


Fig. 3. (a) An example of source and sink composite curve and plastic material cascade diagram (b) Infeasible and (c) Feasible.

The pinch analysis is analogous to the cascading use of plastic waste sources. The highest quality plastic sources should be used for demands that have higher quality requirements of the plastic. If the highest quality source is used up, the next highest quality source should have resorted. The recursive use of the resources in this way ensures the recycling potential of the sources is maximised, and the reliance on the raw materials can be minimised (El-Halwagi et al., 2003). Fig. 3 shows the cascading diagrams where they show the pathways of the plastic waste sources. Fig. 3(b) shows that it is an insufficient good quality plastic waste to fulfil the demands. In this case, a fresh supply is required, as denoted in Fig. 3(c).

3. Results

3.1 Quality grading with machine learning

The data-driven framework for quantifying the quality levels of the plastic waste streams and integrating them with the optimisation of the plastic waste recycling rate is proposed in Fig. 4. Although the current dataset requires more data on the properties of all polymer types, the current work demonstrates the application of machine learning in quantifying the quality clusters of existing waste streams. The use of data-driven approaches could shed light on the information on the available plastic waste and allow better-informed categorisation of the plastic waste based on its complex properties, which also allows easier planning of waste recycling. The pinch analysis method followed up by machine learning allows users to gain crucial intuitions on the resource quality bottlenecks of the current production or recycling system. Tree-based models are employed for data classification due to their high results interpretability. Prior to classification, data pre-screening might be required, and in reality, there are mislabeled data or imbalanced datasets. This work utilises a custom sampling method to filter out the noises of the data with undersampling and estimate data for imbalanced data scenarios using the oversampling method. This work utilises K-Nearest Neighbour (KNN) algorithm to analyse mislabeled data and filter the mislabeled ones. The code is available on github.

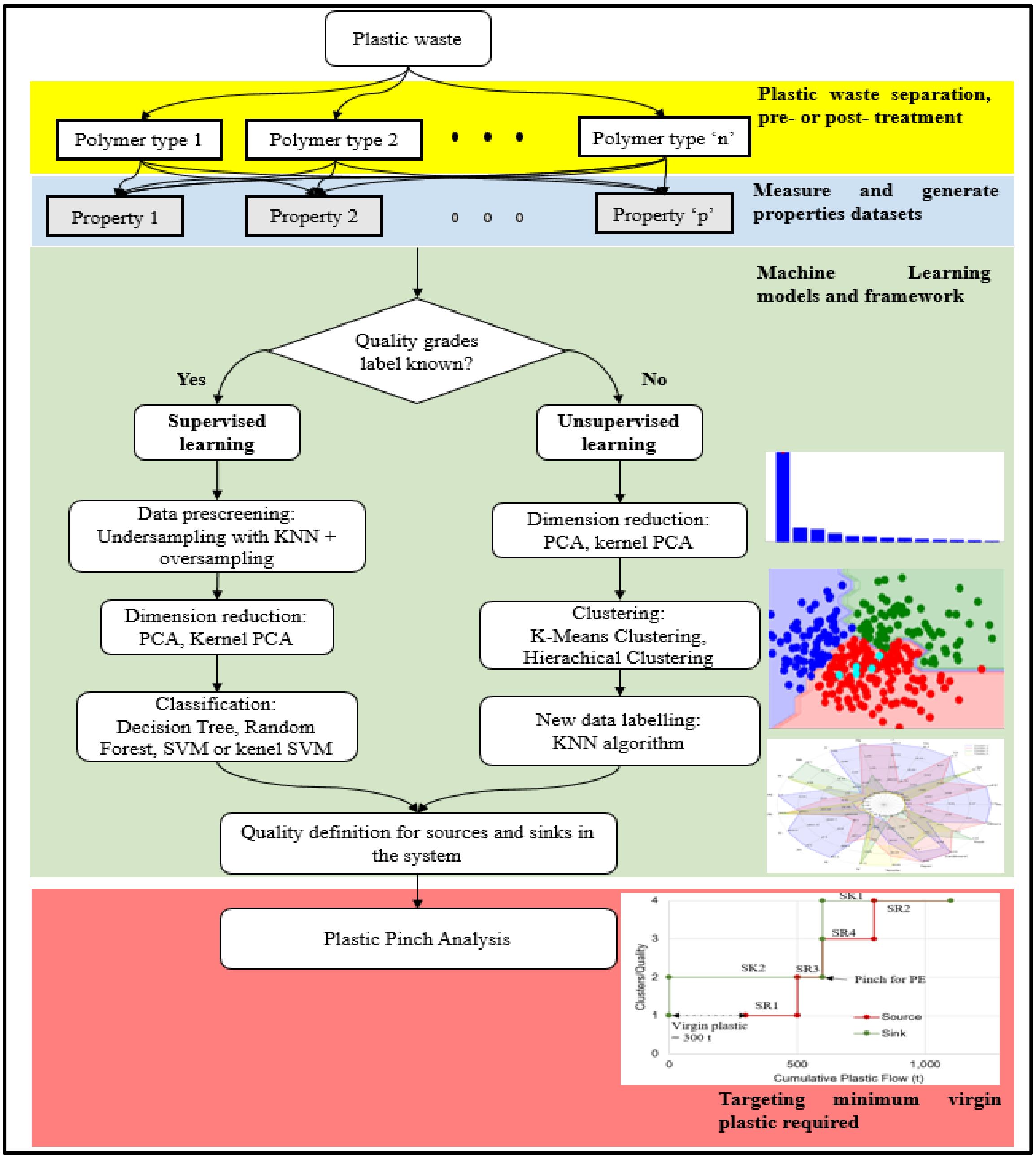
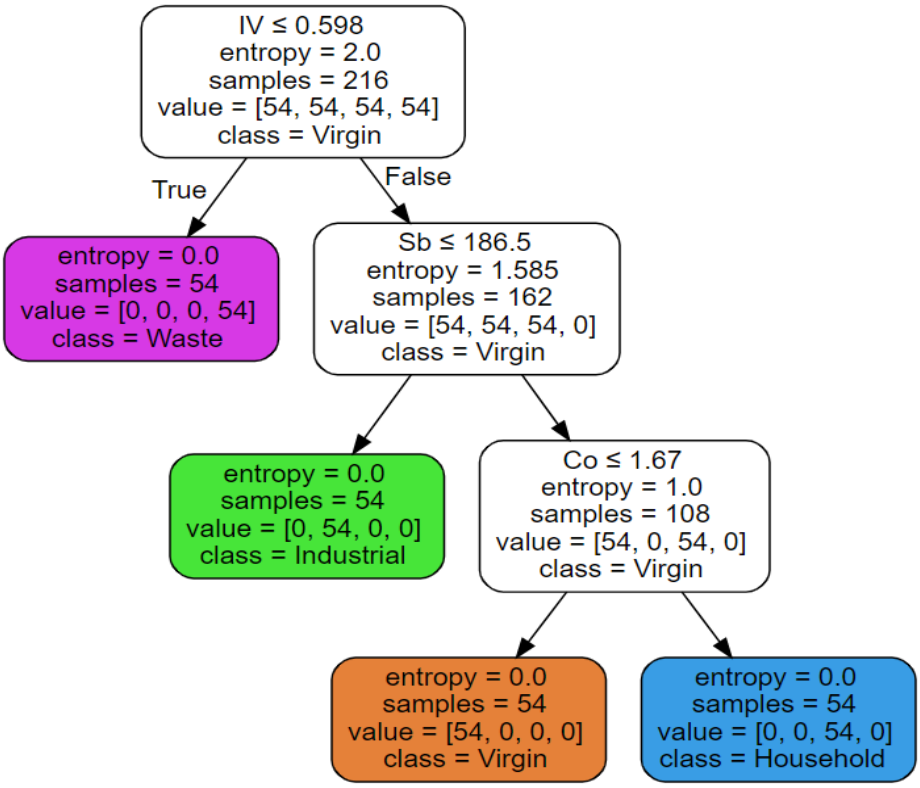


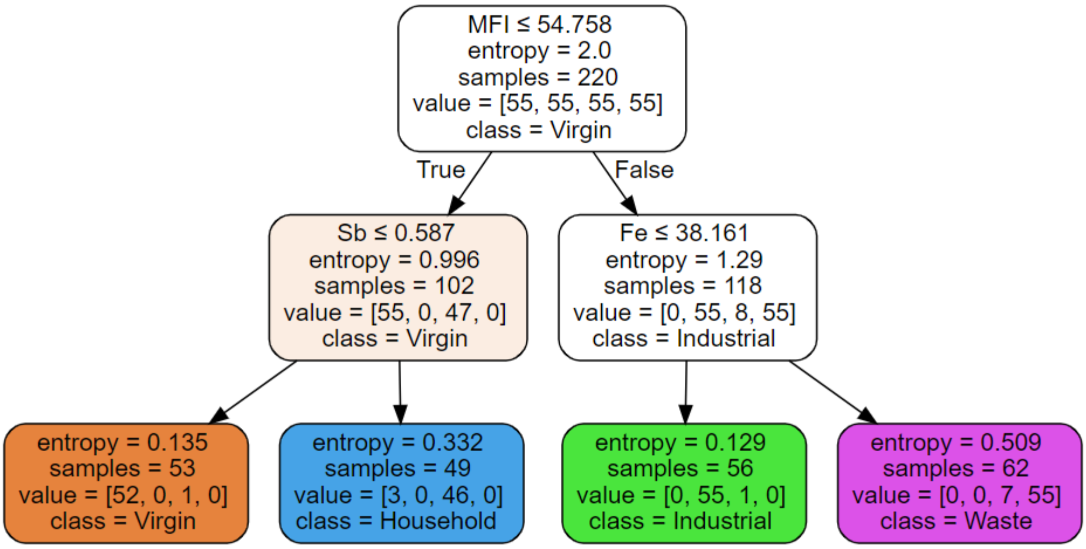
Fig. 4. A data-driven plastic pinch analysis framework.

The decision trees were trained on the data with known quality grades with 2-3 maximum tree depths to avoid overfitting, using the entropy method (Fig. 5). Accuracies on the decision tree model for PET, PP and PE are 99.9, 90.0 and 97.2%, with 2-3 levels with a maximum of two features per level after applying linear PCA to the data. The f1-scores, precisions and recalls are all over 90 % as well for all polymers. PET and PP require only two levels of depth for over 90 % accuracies prediction (Fig. 5(a-b)), while PE requires three levels of depth to achieve 97.2 % (Fig. 5(c)). The outputs suggested that the models predicted the correct categorisation of plastic waste for each polymer due to almost zero entropies at the child nodes. Even with two features and a maximum of three levels, the results underscore the connection between bulk properties to the quality of the plastic waste. Interestingly, the quantification starts with the degradation properties (IV and MFI) as the primary division for quality classification. The next division properties are mainly the metal contamination within the plastic waste streams.

(a) PET



(b) PP



(c) PE

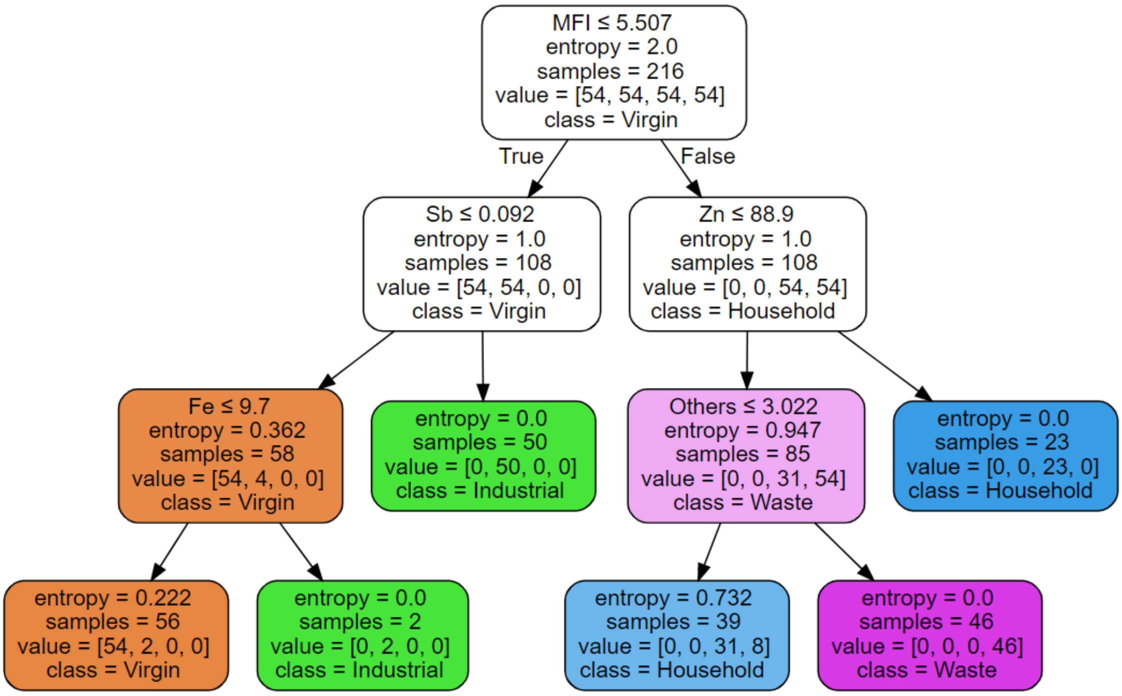


Fig. 5. Decision tree representation for each polymer types: (a) PET (b) PP (c) PE. Each box of tree, value = [a, b, c, d] corresponds to data [virgin, industrial, household, waste]. The units for the variables follow the units presented in Table S1 and S2.

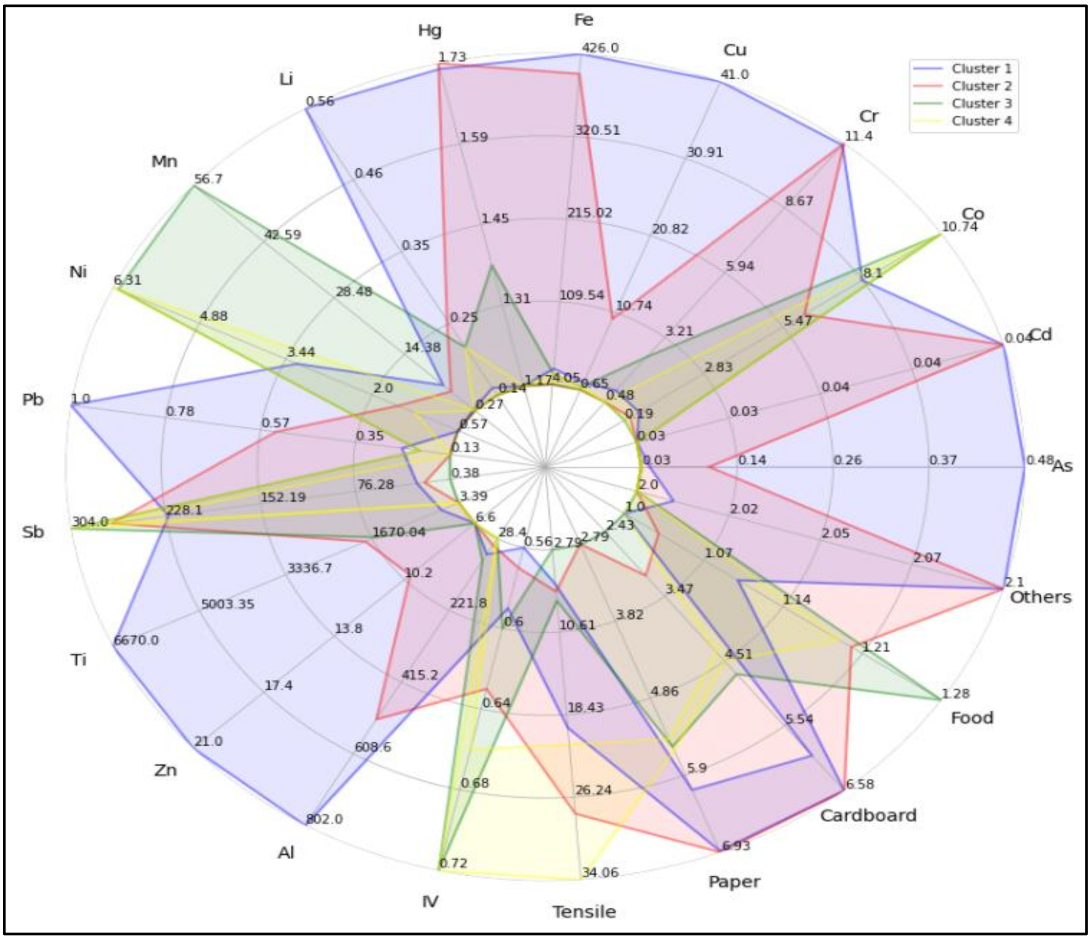
Going one step up, if the quality grades of the data samples are unknown, the unsupervised learning method is employed, namely, the K-means clustering algorithm or hierarchical clustering (HC) approaches. For an imbalanced dataset, the centroids estimated using K-means tends to be pulled towards the majority cluster, which creates more datasets that belong to other clusters. The Hierarchical Clustering method captures the latent structure of the imbalanced datasets better in this case, but still with quite different results from the classification. This work first reduces the dimensionality of the datasets using linear or kernel PCA and then applies the clustering approaches to the reduced dataset. The outcomes of the models include the clusters of the plastic datasets, which can be labelled as the quality grades of the plastic waste samples. Another K-Nearest Neighbor (KNN) algorithm is applied to the new data to classify it to the predicted clusters, which allows quality grading of the new plastic waste sample.

The results of clustering approaches are represented with radar charts presented in Fig. 6, showing the property ranges within each cluster. Using a dendrogram as a reference, the HC approach identifies the optimal cluster for PET and PP are 4, while for PE is 6. Based on Fig. 6(a) for PET, Clusters 1-3 have distinctive properties that differentiate them, except for Cluster

4, in which the most distinctive feature is the tensile strength. Cluster 1 has quite similar characteristics to Cluster 2, with Cluster 2 having a lower maximum limit for some metal contaminants (Co, Cu, Ti, Zn) that suggests cluster 2 may has a better grade than Cluster 1. Cluster 3 features a higher range of IV and a lower range of most of the metal contaminants and other residues, which suggests Cluster 3 should be the higher grade compared to Cluster 1 and 2. However, for Ti, Mn and food residues, Cluster 3 has higher limits. This can create ambiguity in the quality grade definition for the clusters. Depending on the importance of the properties in the system, the definition of the quality grades can differ. Cluster 3 and 4 are quite similar as well, but Cluster 4 has higher maximum tensile strength. This work assumes the higher tensile strength indicates better plastic quality, and considering degradation, Cluster 4 should be the highest grade.

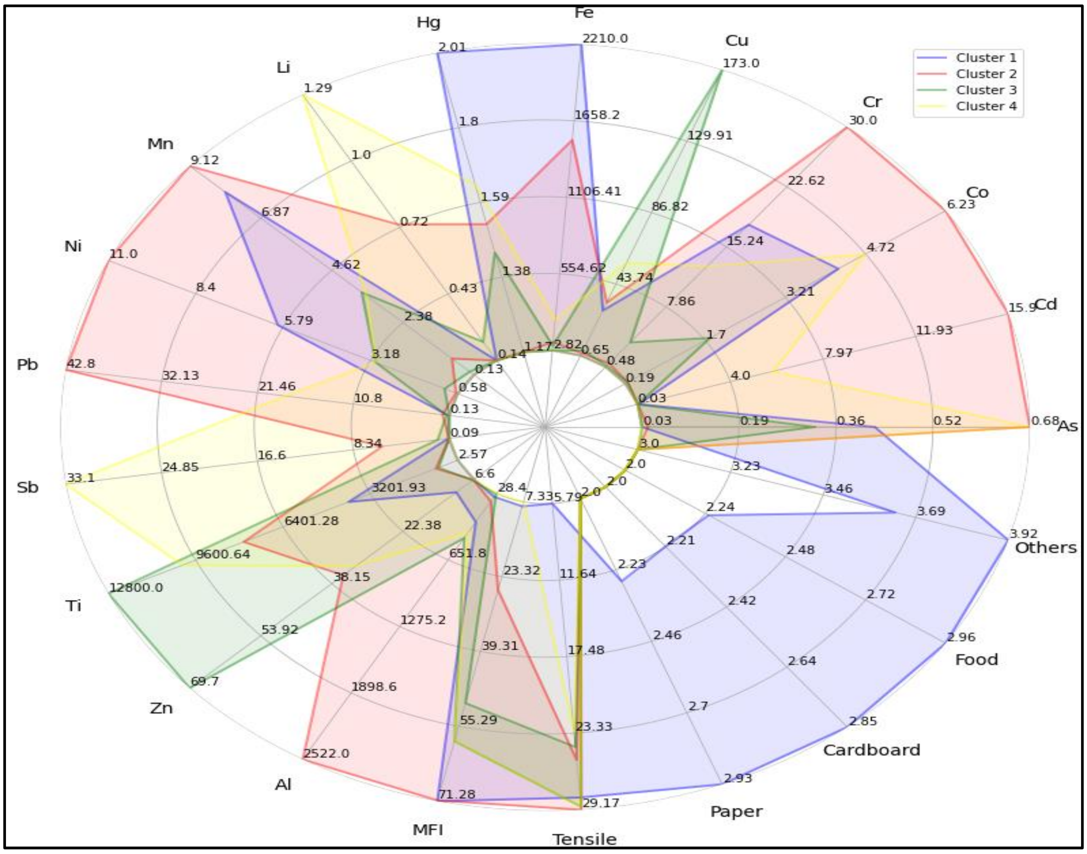
For polymer PP in Fig. 6(b), Clusters 1 and 2 each have higher maximum limits of contaminants/residues compared to each other. In terms of polymer degradation, Clusters 3 and 4 feature lower MFI, which suggests plastic in these categories is not degraded much. Cluster 4 has a lower maximum limit of MFI than Cluster 3. While for polymer PE in Fig. 6(c), the optimal cluster is 6, but only one sample is assigned to each Cluster 5, and 6 due to the maximum and minimum limits coinciding, as shown in Fig. 6(d). Both clusters have similar characteristics to Cluster 4 as well, except for some impurities: food residues, paper, cardboard, and others. This suggests the data may be overfitted, and four clusters are enough to make the plastic clustering for this polymer type.

(a) PET

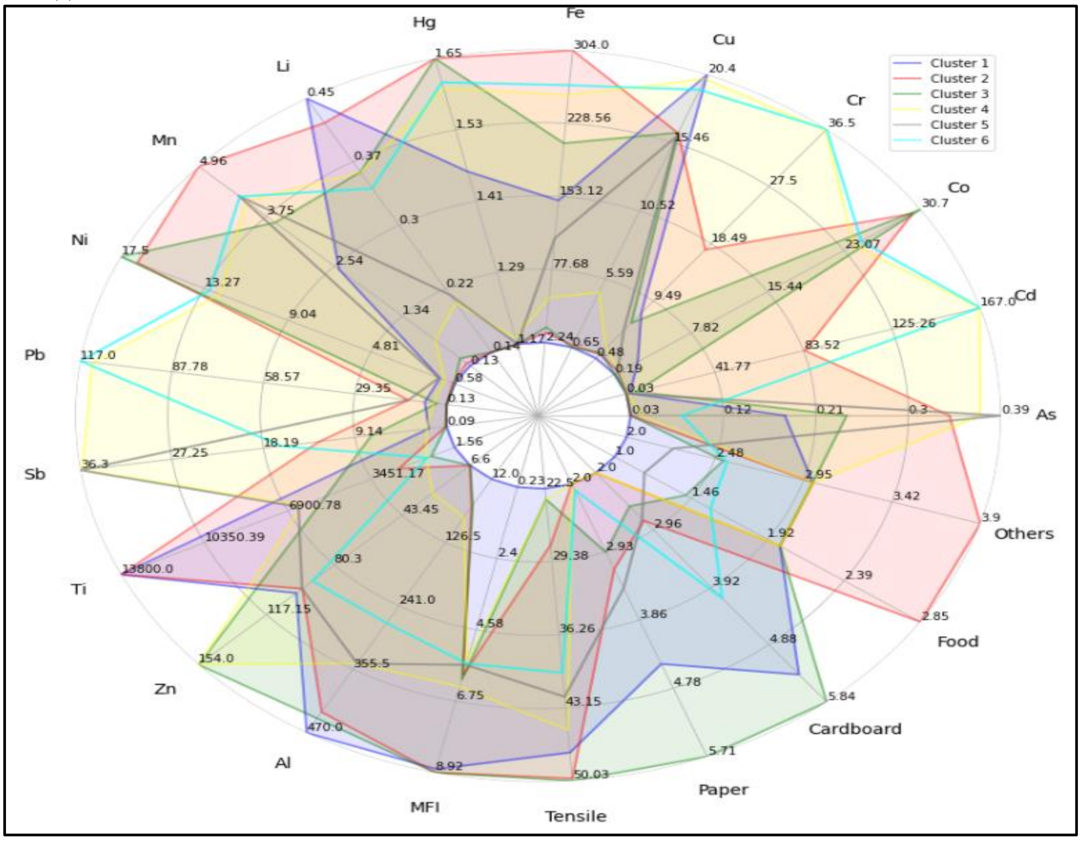


Cluster 1
Cluster 2
Cluster 3
Cluster 4
Fe
Cu
Cr
Co
Cd
As
Others
Food
Cardboard
Paper
Tensile
IV
Al
Zn
Ti
Sb
Pb
Ni
Mn
Li
Hg

(b) PP


Fe
Cu
Cr
Co
Cd
As
Others
Food
Cardboard
Paper
Tensile
MFI
Al
Zn
Ti
Sb
Pb
Ni
Mn
Li
Hg
Cluster 1
Cluster 2
Cluster 3
Cluster 4

(c) PE


Fe
Cu
Cr
Co
Cd
As
Others
Food
Cardboard
Paper
Tensile
MFI
Al
Zn
Ti
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Hg
Cluster 1
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Cluster 3
Cluster 4
Cluster 5
Cluster 6

(d) Clusters 4, 5 and 6 for PE

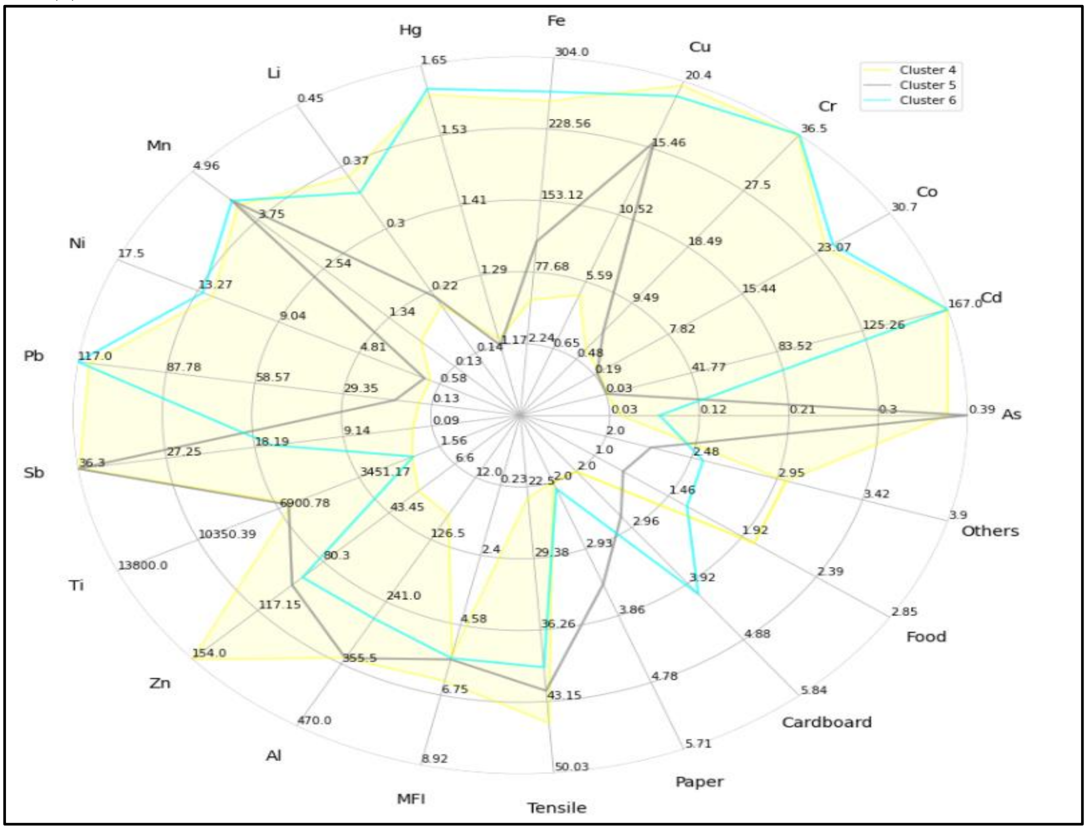


Fig. 6. Radar charts representation of property ranges for each property and for each polymer type (a) PET (b) PP (c) PE (d) Representation of Clusters 4,5 and 6 for PE. The units for the variables follow the units presented in Tables S1 and S2.

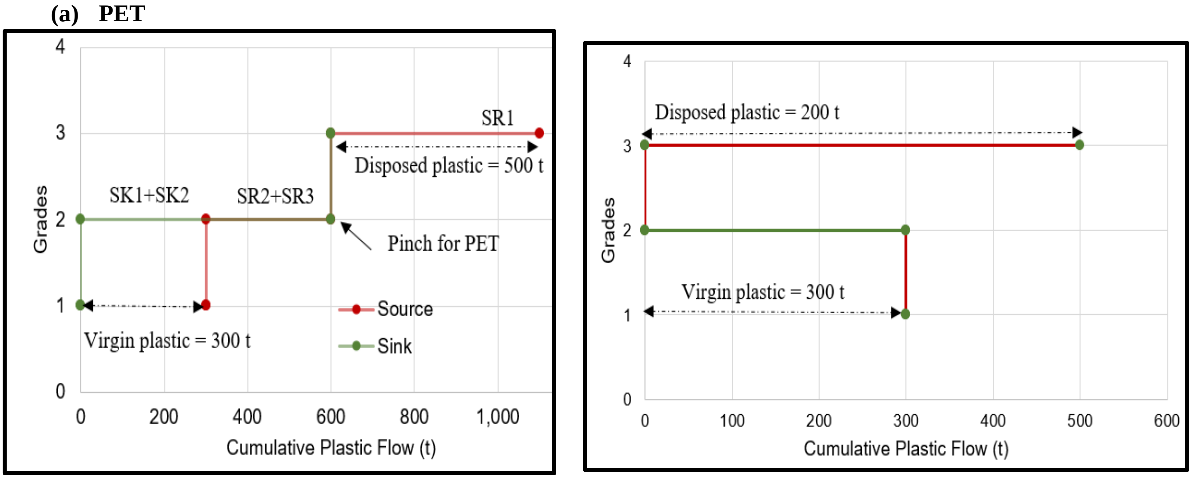
3.2 Recyclability quantifying from the AI-driven pinch analysis

After the quality grading system has been identified, the outcomes can be applied to any plastic recycling system to determine the plastic recyclability. The available regional plastic supplies/sources and demands/sinks streams are fitted into the trained Machine Learning algorithms to identify their respective clusters. The case studies data for all the polymers are given in Tables S1 and S2. Fig. 7 below shows the composite curves for all studied polymer types. The grading system in this work is assumed that the degradation property is prioritised. For PET polymer, Cluster 4 is determined as the highest grade, followed by Clusters 3, 2 and 1. For polymer PP, the grades for the clusters are ordered as {4 > 3 > 1 > 2}, while for polymer PE the grade is ordered as {4 > 1 > 3 > 2}- see Section 3.1 for explanation.

There are no available sources with quality grade ‘1’ but other qualities (Fig. 7(a)). Adjusting the source composite curve indicating a minimum amount of 300 t of external plastic with at least grade ‘2’ is required for the studied system. Some of SR2 and SR3 with quality grade ‘2’ can be directly recycled to SK1+SK2 with grade ‘2’ requirements, while others are to be disposed of, either landfilled or incinerated. The Pinch Point is at quality grade ‘2’. As for PP polymer (Fig. 7(b)), the available sources SR1, SR2, and SR4 are good enough quality to satisfy all the demands of SK1-SK4, with which about 100 t of waste is disposed of. The Pinch Point is at quality grade ‘3’ with an external plastic requirement of 400 t with at least grade ‘3’. For the last polymer type PE (Fig. 7(c)), a similar Pinch Analysis procedure is applied, and the problem is of ‘threshold’ Pinch type. This means that all of the sources are good enough quality to fulfil all the demands without disposal. External plastic required is about 300 t of grade ‘1’ PE.

The grand composite curves display the net plastic flow within each quality grade. It directly shows the cascading flow of the plastic from higher grade to lower grade. For example polymer PP, it shows that the plastic sources from grade ‘1’ can be recycled/reused for plastic demands of grades ‘2’ and ‘3’ since there are net deficit plastic flows for these categories. The clear representation of the cascading system allows users to identify the plastic recyclability potential within the system and shows the quality bottleneck of the current plastic waste. Analysing the Pinch Points helps to understand which plastic waste type or quality grade to improve so that virgin plastic production or generated waste can be reduced. For polymer PP, the disposed plastic above the Pinch Point can be upgraded to below the Pinch Point (grade ‘3’), and for PET the extra plastic waste can be upgraded to at least grade ‘2’, so that the virgin plastic can be reduced, while waste generation can be avoided for the studied system.

(a) PET



(b) PP

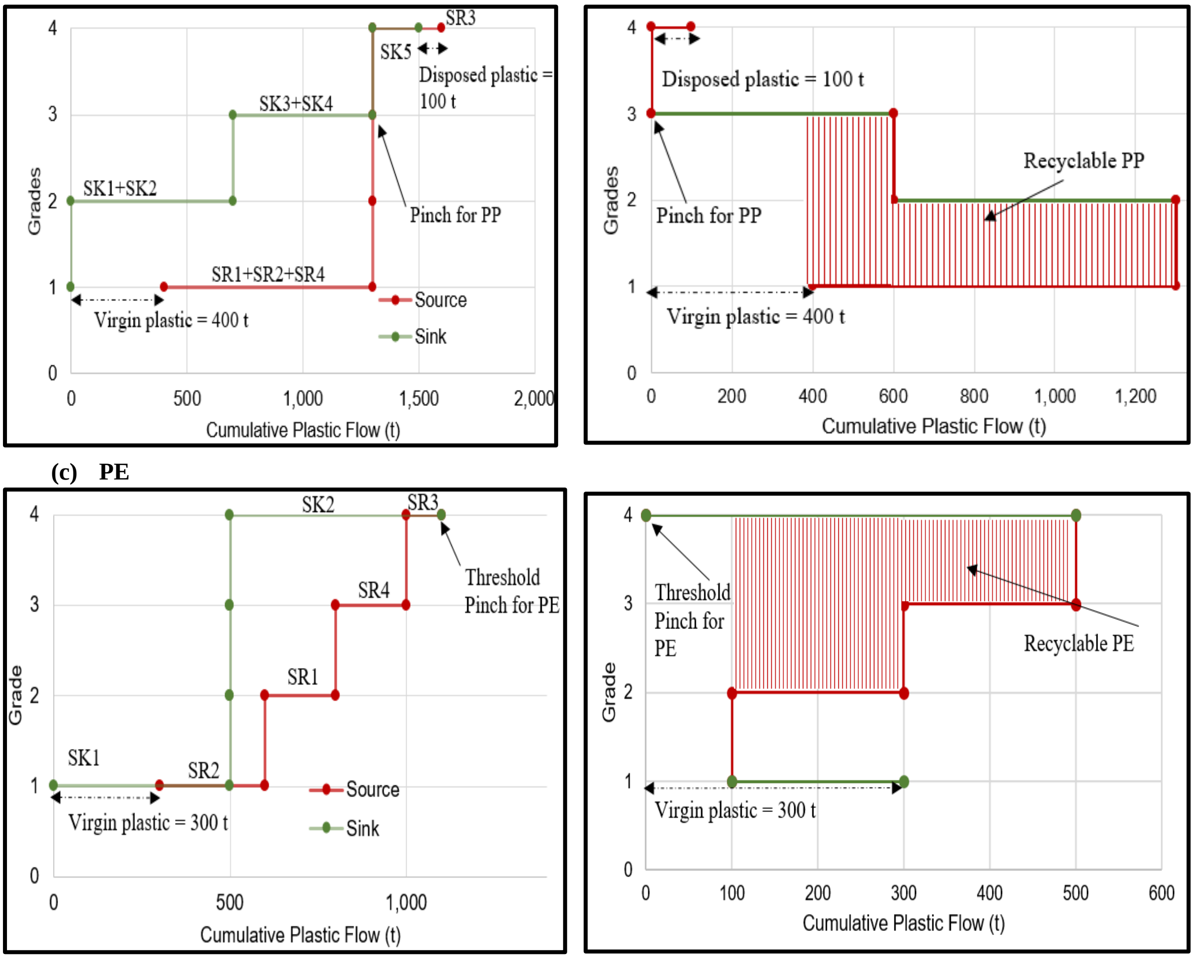


Fig. 7. Pinch analysis of the plastic waste recycling for each polymer type using composite curves (left) and grand composite curves (right) for; (a) PET, (b) PP and (c) PE.

The framework identifies the maximum PET recyclability is about 38 %, 100 % for PE and 92 % for PP. It suggests that for this specific case, the End-of-life (EOL) practice of PET can be strengthened to improve the plastic waste properties, especially SR1.

3.3 Trends of environmental impacts of plastic recycling

The carbon footprint analysis considering various percentages of recycled plastic is conducted to identify the environmental impacts of plastic recycling. The carbon emission footprint considered is the cradle-to-gate emission contributed by recycling, virgin plastic production, and landfill of disposed of plastic waste (net emission). Fig. 8 shows the carbon emission footprints for the polymers, indicating the breakdown of different components of the CO_2 emission with various percentages of recycled plastic, with data from Devasahayam et al. (2019) presented in Table S3.

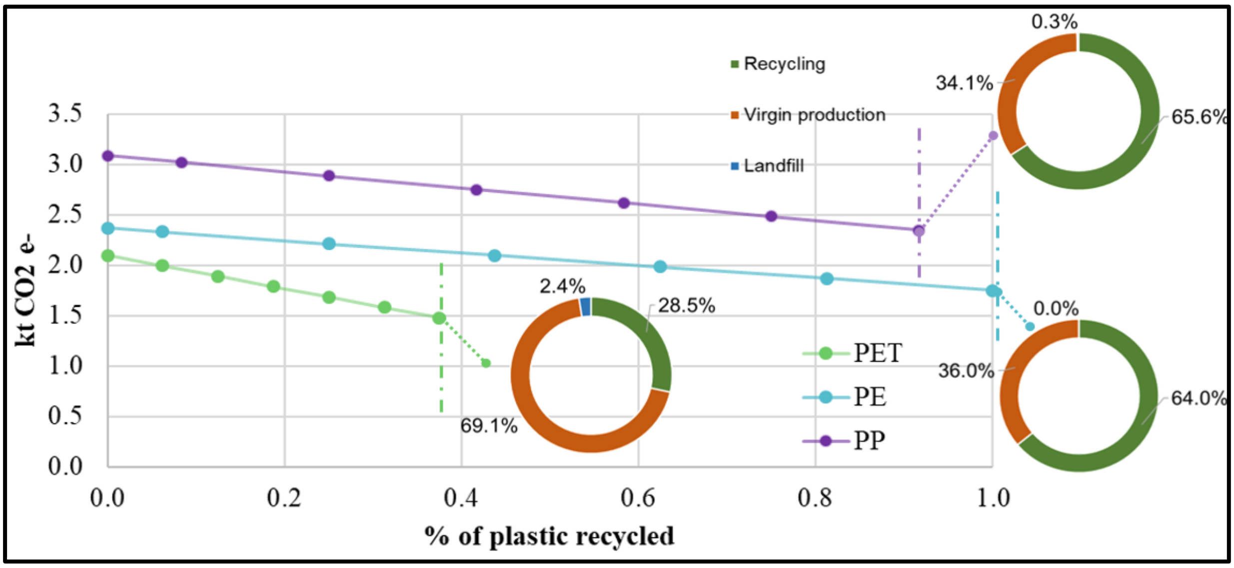


Fig. 8. Carbon emission footprint for different percentages of plastic recycled. Dotted lines represent the maximum percentage of plastic that can be recycled according to plastic pinch analysis.

It can be observed that the trend of footprint analysis drops when recycled plastic increases. This is due to the carbon emission factor for virgin plastic productions dominating the recycling process and landfills. The global warming potential of recycling plastic is just 1.4 CO_2e, as compared to virgin production of PET (3.4 CO_2e), PP (2.0 CO_2e) and PE (LDPE for 2.1 CO_2e). Since virgin plastic required is always more than the recycled plastic flow, the carbon emission footprint of virgin production is always higher than the recycling process. The maximum recycling percentage of plastic waste identified from Plastic Pinch Analysis provides the optimal solutions in terms of environmental impacts. Note that these results may differ depending on the carbon emission of the recycling technologies. Energy and water needed for plastic recycling are also less compared to the cradle-to-gate production of raw plastics, indicating recycling plastics could save more energy and water usage (see Table S3).

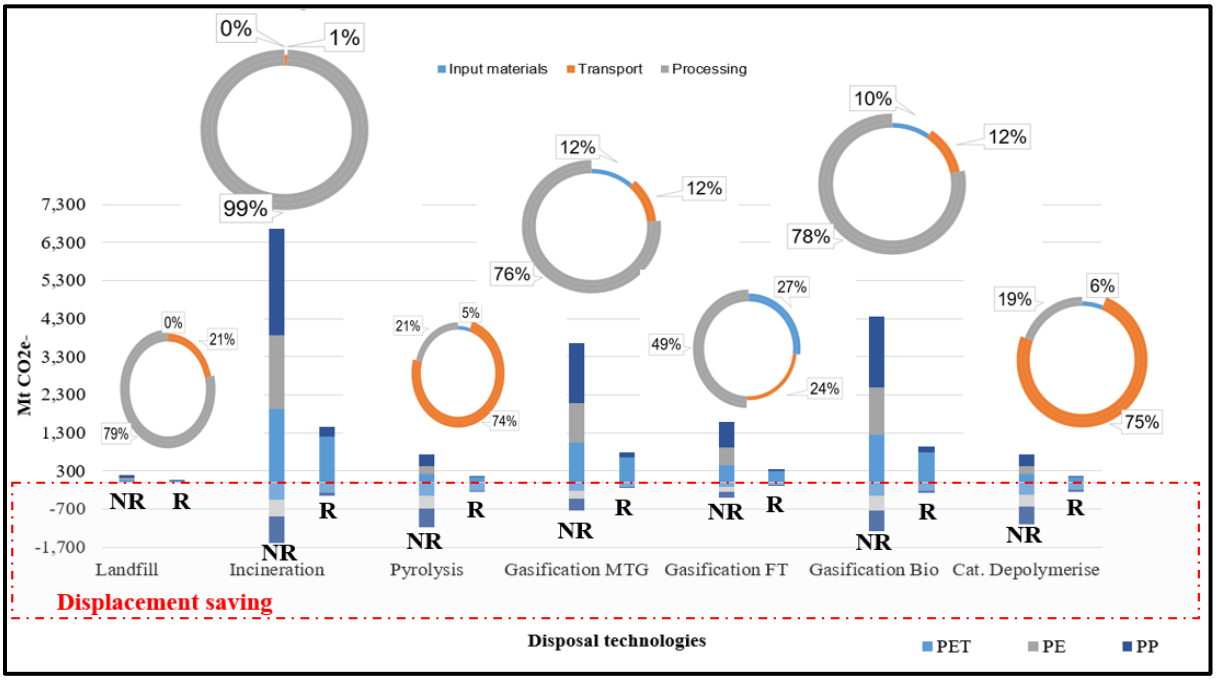


Fig. 9. Carbon emission footprint for different disposal technologies for each polymer type. 'NR' denotes the base case scenario where no recycling occurs, 'R' denotes for recycling scenario after Pinch Analysis

Various waste disposal technologies could yield different footprints due to the displacement savings of the carbon emission. Fig. 9 shows the carbon emission footprint for different recycling technologies, with data from Devasahayam et al. (2019) presented in Table S4. The landfill has no carbon emission footprint due to the assumption that the carbon footprint is returned to the environment, while a minority is generated from transportation and processing. Incineration consumes the largest amount of energy, which is indicated by about 99 % of the carbon emission from the processing unit. Even though it provides displacement savings, the net emission is still positive for incineration. Pyrolysis and catalytic depolymerisation offer negative net emission potential for disposing of plastic waste, indicating waste disposal may be a better option compared to recycling (if no displacement saving is considered for recycling). In this case, disposing of waste with these technologies may be better than recycling plastic waste (mechanical recycling). It can be seen that the recycling scenario definitely reduces the emission footprints of different recycling technologies.

4 Discussion and conclusion

The exploitation of natural resources should lead to irreversible ecological harm. Despite the strong emphasis on plastic recycling worldwide, industrial practitioners remain heavily reliant on raw plastic products. Other than the reasons for the cost-effectiveness of the recycling system, resource quality is the central driving force toward a sustainable circular economy. The complex properties of plastic waste are another hurdle for recycling, and the quality grading becomes difficult. This work has shown that utilising a machine learning framework to identify a quality grading system is effective for any plastic waste. The framework could account for the extensive properties of plastic waste, ranging from mechanical, degradation, and chemical properties which are measurable. The Machine Learning algorithms extract crucial intuitions based on the available data of plastic waste streams and categorise the waste streams into classes. Depending on the sampled sources or applications, these classes define the quality grades of the waste and aid in plastic recycling network optimisation. The use of Pinch Analysis tools allows users to visualise and identify the quality bottleneck that drives the plastic recyclability easily. Different case studies featuring different polymer types are formulated to showcase the novel concept. Using the data-driven quality grading system, the framework identifies maximum PET recyclability as about 38 %, 100 % for PE and 92 % for PP. Improving EOL treatment of PET could potentially increase the waste recycling rate. The results show that the concept is promising and effective in determining the qualities and optimising the recycling network. These initial prototyping steps have made a number of simplifying assumptions – such as having a homogeneous polymer composition of the treated plastic waste, unlimited availability of fresh plastic material, and simple material cascading.

This framework is subjected to variables in the method itself, including the clustering philosophies, maximum depth of decision trees, and overfitting or underfitting of the ML algorithms. These will affect the outcomes of the clustering/classification, which in turn affect the strategic planning of plastic recycling. The proper hyperparameter tuning should be conducted to all variables to ensure the optimal number of clusters is guaranteed or to avoid overfitting or underfitting. The plastic recyclability and deficit are also subject to uncertainties such as treatment technologies, cost and footprint, for which the strength of the Pinch framework is flexible to these factors and can be easily manipulated. Different clustering concepts can also be explored to compare the clustering results, which may bring insights to various AI-based quality grading systems.

However, it is to be noted that the compatibility of the sources mixture should be ensured before sending to the demands. The heterogeneous mixture of the polymers could incur problems of incompatibility between polymers and decrease the polymer strength. The method for compatibility estimation can be found in Huysman et al. (2017) through binary interfacial tension determination. The opportunities of different polymer types mixture (e.g. PET with PE or PP) are not considered, which could further improve the recycling rate if the polymer mix is homogeneous and fulfils the demand properties. For multiple polymers streams, the homogeneousity is difficult to estimate due to the limited accuracy of mixture interfacial tension estimations and requires accurate empirical verification. The main function of the Plastic Pinch Analysis tool is to allow users to strategically plan the plastic recycling and optimise the external virgin plastic required. Homogeneousity of plastic waste can be regarded as one of the key parameters during recycling planning or defining the quality grade.

This framework could output the recycling rates of the plastic polymers and can be compared with governmental regulation on the targeted recycling rates. The benefit of the Composite Curve is that the number of clusters can be adjusted so that the recycling rates can be manipulated easily as well, providing suggestions for practitioners to manage the plastic resources. In this case, various measures can be planned to meet the government requirements, e.g. waste treatment technologies can be set up to improve the quality grades of waste.

In this advanced technological era, the future trends would be the use of computerised systems and sensors for plastic trade flows. This is a necessity for managing the vast information flows efficiently and coordinating the recycling activities of circular economy. A property database on the globally available plastic waste can be constructed by measuring the properties, either pre-or post-treatment. Through Big Data Analytics, the patterns of various plastic waste can be identified that allow proper planning of the plastic waste. The data-driven tools can be enhanced as well, not just to apply to properties of plastic waste, the spectral analysis of the plastic can be integrated with property analysis to generate a globally or locally available plastic screening tool. The challenge of dataset scarcity can be coped with by generating similar datasets using generative models such as generative adversarial networks or the Gaussian mixture model. Despite the fact that the effective use of resources should be the main priority, different aspects of the recycling system's cost, energy usage, detailed life-cycle analysis or environmental footprint should be considered. The quality grading and Pinch concepts provided in this work can be complemented with advanced mathematical approaches to make a more accurate and business-informed recycling decision.

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