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Recycling of Thermoplastics with Machine Learning: A Review

*Rodrigo Q. Albuquerque, Florian Stephan, Annalena Pongratz, Christian Brütting, Katharina Krause, and Holger Ruckdäschel**

This critical review examines the transformative role of machine learning (ML) in revolutionizing thermoplastic recycling across mechanical, chemical, and biological pathways. As global plastic waste challenges intensify, sophisticated ML approaches are emerging as powerful tools to overcome traditional recycling limitations. Recent technological breakthroughs are systematically analyzed that leverage ML to optimize sorting precision, process efficiency, and quality assurance in recycled thermoplastics. The review presents a detailed analysis of feature engineering strategies that have proven most effective across diverse recycling applications. By identifying current implementation barriers and unexplored opportunities, a forward-looking research agenda is established for ML integration that can accelerate progress toward a truly circular thermoplastic economy. This interdisciplinary perspective bridges materials science, computer science, and sustainability to provide actionable insights for researchers and industry practitioners.

1. Introduction

Polymers are very important materials for modern societies and they can be used in a wide range of essential applications in the food, medical, automobile, and aerospace industries, just to cite a few. As a consequence, plastic has been generated in a very high rate, leading to many environmental problems. The very large amount of plastic waste in the planet (e.g., in landfills or oceans) calls for novel and more efficient recycling technologies. Since most polymers were not originally designed for recycling, but designed to exhibit specific thermo-mechanical properties, recycling them efficiently and at low cost is still a big challenge nowadays, demanding many efforts from scientists and engineers worldwide.

R. Q. Albuquerque, F. Stephan, A. Pongratz, C. Brütting, H. Ruckdäschel
University of Bayreuth
Universitätsstrasse 30, 95447 Bayreuth, Germany
E-mail: ruckdaeschel@uni-bayreuth.de
R. Q. Albuquerque, K. Krause, H. Ruckdäschel
Neue Materialien Bayreuth GmbH
Gottlieb-Keim-Straße 60, 95447 Bayreuth, Germany

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While polymers are found across composites, thermosets, and thermoplastics, the latter presents a particularly critical target for recycling efforts. Thermoplastics, due to their linear or branched molecular structures, possess the unique ability to be repeatedly melted and reshaped, offering a significant advantage for closed-loop recycling. This reversible processing capability stems from the absence of permanent crosslinks, allowing polymer chains to flow upon heating and solidify upon cooling without fundamental chemical changes. In contrast, thermosets, with their crosslinked networks, are inherently difficult to remelt and reprocess, limiting their recyclability. Furthermore, while composites offer valuable material properties, their complex multi-phase structures often pose significant challenges to efficient separation and recycling of the constituent polymers. Given the vast production volume and widespread application of thermoplastics in consumer goods, packaging, and various industries, their effective recycling is paramount to mitigating environmental impact, conserving resources, and fostering a circular economy.

Effective plastic recycling is a multistep process that begins with a rigorous pre-treatment phase designed to remove contaminants and segregate diverse polymer streams, as shown in **Figure 1**. During this initial stage, sorting employs advanced techniques–such as near-infrared (NIR) spectroscopy and automated sensor systems–to rapidly classify plastic types, while mechanical shredding reduces material size to facilitate subsequent washing and drying processes, which are critical for eliminating residual adhesives, labels, and dirt.[1,2] Once a clean, homogeneous feedstock is obtained, the recycling pathway diverges into two main approaches: material recycling and monomer/oligomer recycling. In the realm of material recycling, mechanical recycling involves melting and re-extruding the plastics. This process benefits significantly from improved thermal and mechanical processing conditions, which help maintain the polymer's original properties and ensure high product quality, as demonstrated in recent studies.[3,4] In parallel, solvent-based recycling leverages selective dissolution to separate and recover pure polymers from mixed waste streams, a method that overcomes limitations related to polymer degradation and mixed-material impurities.[5,6]

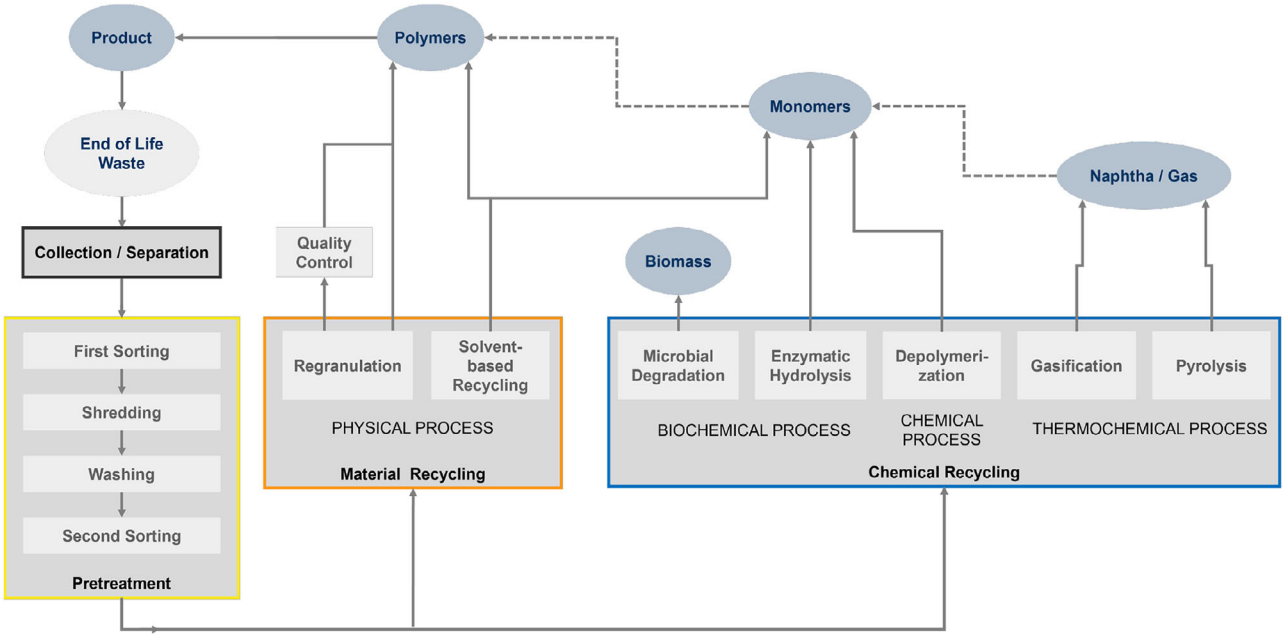

Figure 1. Overview of the mechanical and chemical recycling processes.

Building on these conventional approaches, chemical and biological recycling provide transformative alternatives by breaking down polymers into their constituent monomers and/or oligomers or converting them into value-added chemical intermediates.

Biological recycling refers to processes that employ biological entities to degrade polymers into monomers, biomass, or other reusable platform chemicals. While microbial degradation of polymers into biomass, water, biogas, and CO_2 can be considered a form of biological recycling,[7,8] this review will not focus on such approaches, as they typically do not yield readily usable monomeric units or platform chemicals. Instead, enzymatic hydrolysis is of particular interest, as it enables the recovery of monomers or other low-molecular-weight building blocks. Suitable biological catalysts for enzymatic hydrolysis are extracellular enzymes capable of cleaving hydrolysable functional groups such as ester, urethane, ether, or amide bonds.[9] Enzymatic hydrolysis follows a four-step process: (1) diffusion of the enzyme to the polymer surface, (2) adsorption and formation of an enzyme-substrate complex, (3) cleavage of chemical bonds via hydrolysis, and (4) release and diffusion of degradation products into the aqueous reaction solution, from which they can be recovered.[10] The feasibility and efficiency of this process largely depend on the substrate specificity of the enzyme. While this high specificity allows for selective recycling from mixed plastic waste, it also limits enzymatic recycling to a subset of polymers–such as Polylactic Acid (PLA), Polyethylene Terephthalate (PET), and certain PAs and PUs–for which suitable enzymes have been identified.[9]

In chemical recycling, depolymerization processes, which reverse the polymerization reaction, have been enhanced by novel catalytic systems and refined reaction conditions that maximize monomer recovery and purity.[11,12] Beyond these technological advancements, emerging research highlights the importance of aligning recycling strategies with circular economy principles, emphasizing process optimization and environmental impact assessments as key factors for long-term sustainability.[13–16] Additionally, gasification and pyrolysis offer thermochemical routes that transform plastic waste into synthesis gas, fuels, or other useful chemicals by subjecting the material to high temperatures in controlled atmospheres; these methods have recently benefitted from optimized reactor designs and process intensification strategies that improve energy efficiency and product yields.[17,18] Comprehensive reviews further underscore the potential of these chemical pathways by detailing advances in catalyst development, process integration, and lifecycle analysis, all of which contribute to a more sustainable and circular approach to plastic waste management.[19,20]

Digital tools like Machine Learning (ML) can become the perfect partner to help recycle thermoplastics, be it mechanically, chemically or biologically, as such digital techniques have already proven to enhance the sustainability of polymer engineering applications in general.[21–27] ML models are data-driven, where prediction accuracies strongly depend on the data used to train the model. After being appropriately trained, ML models can be used to 1) perform predictions of target properties for new experiments;[28] 2) suggest experiments with desired target property (aka, inverse design[29]), and 3) provide interpretation for the relation between the independent variables (or features) and target properties.[21] ML tools can help improve mechanical, chemical or biological recycling, as discussed below.

ML has emerged as a transformative approach in mechanical recycling, offering innovative solutions to longstanding challenges across multiple processing stages. Particularly in sorting, ML algorithms have demonstrated remarkable capabilities in detecting and classifying plastic waste with unprecedented precision, utilizing advanced techniques such as NIR, mid-infrared (MIR), and laser-induced breakdown spectroscopy (LIBS).[30–32] These techniques enable accurate identification and

separation of complex plastic streams, including challenging materials like black plastics, by analyzing molecular vibrations and chemical signatures. Beyond sorting, ML has shown promise in optimizing other critical recycling processes, such as predicting material degradation during regranulation[33] and managing batch quality in recycled polymer production.[34] Transfer learning techniques have further expanded these capabilities, offering more efficient predictive models for material properties with reduced training requirements,[35] ultimately contributing to more sustainable and technologically advanced recycling methodologies.

ML models also address critical challenges in chemical recycling across multiple domains: solvent efficiency,[36] process economics,[37] material design for ring-opening polymerization (ROP) polymers,[38] and identification accuracy in NIR sorting.[30,39,40] For effective chemical recycling, determining optimal solvents for polymer solubilization is essential. Solvent miscibility parameters provide this crucial information, and these parameters have been successfully predicted using ML models trained on experimental and quantum chemical data.[36] In a breakthrough approach, Ma et al.[37] developed a waste plastic pyrolysis oil hydrocracking (WPOH) process that integrates process simulation with deep learning for multi-objective optimization, achieving a 50.44% increase in net profit while addressing environmental concerns. Recent advances in NIR sorting–a critical pre-processing step for both chemical and mechanical recycling–demonstrate the potential of combining NIR spectroscopy with chemometrics and ML techniques.[30] These approaches enable accurate differentiation between Polypropylene (PP) and Polyethylene (PE), while also predicting key properties such as bulk density, crystallinity, and short-chain branching (SCB) in PEs from diverse sources. The combination of NIR and ML even allows for the correct identification of compostable polymers with high accuracy.[40] ML contributes to chemical recycling both directly and indirectly by facilitating the design of recyclable plastics.[38] This dual approach involves: (1) designing novel chemically recyclable polymers with targeted properties, and (2) optimizing chemical recycling processes for these materials at end-of-life. The integration of theoretical inputs from simulations and calculations as features in ML models represents an increasingly valuable strategy for enhancing model performance. Together, these innovations demonstrate the comprehensive capabilities of ML models in addressing the diverse challenges of chemical recycling.

While ML has demonstrated significant potential in various aspects of polymer science, a dedicated review synthesizing its application to the multifaceted challenge of mechanical, chemical and biological recycling of thermoplastics is lacking. This review addresses this gap by providing a critical analysis of how ML-driven solutions can overcome the intrinsic difficulties associated with these types of recycling processes, contributing to a more sustainable and circular material flow. We begin with an introduction to the pertinent ML techniques, followed by in-depth sections detailing their implementation in optimizing each recycling method. Subsequently, we highlight the main feature engineering strategies used in the reviewed literature and explore future directions and emerging trends, emphasizing the potential of ML to improve thermoplastic recycling.

2. ML Modeling

In this section, some of the most important ML models and techniques found in the reviewed literature are briefly described, and references are provided to get a deeper understanding of each method.

2.1. Artificial Neural Networks

Artificial Neural Networks (ANNs[41]) are computational models inspired by the human brain, employing interconnected "neurons" to process information. Each neuron calculates a weighted sum of its inputs, applies a non-linear activation function, and transmits the result to subsequent layers. This architecture enables ANNs to excel in diverse tasks, including image recognition and natural language processing. Several flavors of ANNs have been developed, as discussed below.

Deep Learning (DL[42]), a specialized branch of ANNs, leverages networks with more than two hidden layers to learn hierarchical representations of data. This "depth" allows DL models to capture elaborate patterns and automatically extract relevant features from raw data, a capability that distinguishes them from traditional ML approaches. Convolutional Neural Networks (CNNs) exemplify DL's power in computer vision, effectively processing image pixels to associate them with target properties. ANN/DL/CNN models can have millions of trainable parameters and become very complex, on one side potentially boosting model accuracy to successfully solve very challenging problems, but on the other side hindering interpretability.

Transformers[43] are powerful ANNs that revolutionized ML by using a mechanism called "self-attention." Unlike earlier models that process data sequentially, transformers can examine all parts of the input simultaneously, allowing them to understand relationships between distant elements in text or data. A key innovation is how transformers handle position information through special encodings that help the model understand sequence order. This design enables efficient parallel processing and exceptional scalability, making transformers the foundation for today's most advanced ML systems across language processing, image analysis, and many other applications.

Graph neural networks (GNNs,[44]) are a type of ANN designed to operate on graph-structured data, where relationships between entities are crucial. Unlike traditional neural networks that process data in grids or sequences, GNNs leverage the connections within a graph to learn representations. They achieve this by iteratively aggregating information from neighboring nodes, allowing each node to "learn" from its context within the network. This capability makes GNNs particularly effective in applications involving social networks, molecular structures, and knowledge graphs, where the relationships between data points hold significant meaning.

The multilayer perceptron (MLP[45]) is a fundamental type of ANN characterized by its feedforward architecture. It comprises interconnected neurons arranged in an input layer, one or more hidden layers, and an output layer, facilitating the sequential flow of data from input to output. When two or more hidden layers are present in a MLP, it can be called deep MLP or sometimes deep feedforward neural network.

The application of pretrained ANNs to address problems distinct from their original training objectives, known as transfer learning,[46] is a common practice in ML research. This approach involves preserving the learned features encoded in the initial hidden layers by freezing their parameters, and adapting the model to the new task by retraining only the final layers. Transfer learning offers substantial efficiency gains, enabling the rapid development of high-performance models compared to training ANNs from scratch, and thus has become increasingly prevalent in recent studies.

Physics-Informed Neural Networks (PINNs[47]) merge ANNs with physical principles by embedding governing equations directly into their loss functions. Unlike purely data-driven methods, PINNs are constrained by the physical laws expressed as differential equations, enabling physically consistent solutions even with limited or noisy data. This approach creates powerful models for complex phenomena across scientific and engineering fields and has gained popularity in recent years.

2.2. Support Vector Machines

Support Vector Machines (SVMs)[48] are a versatile class of supervised ML algorithms employed for both classification (Support Vector Classifier or SVC) and regression (Support Vector Regressor or SVR) tasks. For SVC, the fundamental principle is to identify an optimal hyperplane that effectively separates data points belonging to distinct classes within a potentially high-dimensional space. This hyperplane is chosen to maximize the margin, defined as the distance between the hyperplane and the closest data points from each class, termed support vectors. In contrast, SVR focuses on fitting a function to continuous-valued data. Rather than maximizing the margin between classes, SVR aims to find a function that deviates from the actual target values by no more than a specified tolerance, denoted as ϵ. This tolerance defines a hypertube around the predicted function. The goal is to fit as many training data points as possible within this ϵ-hypertube. Specifically, SVR optimizes the parameters of a function (often a hyperplane in high-dimensional space) to minimize the prediction error outside this ϵ-hypertube, while simultaneously ensuring the function's flatness. This balance between error minimization and model complexity is crucial for preventing overfitting. Both SVC and SVR can handle linear and non-linear decision boundaries or regression functions through the application of kernel functions. These kernels implicitly map the input data into higher-dimensional spaces, where linear separation or regression becomes feasible.

2.3. Random Forests

Random Forests (RF[49]) are an ensemble learning method widely used for both classification and regression tasks. They operate by constructing multiple decision trees during training and outputting the mode (for classification) or mean (for regression) of the predictions from individual trees. Each tree is trained on a random subset of the data and a random subset of features, a technique known as bagging, which reduces overfitting and improves generalization. Random Forests are particularly valued for their ability to handle high-dimensional data, missing values, and noisy datasets, while also providing insights into feature importance. The way new trees are chosen and trained to improve this ensemble model leads to different decision trees-based methods, like gradient boosting regressor (GBR[50]) or extreme gradient boosting (XGBoost[51]), which are very popular among diverse ML investigations.

2.4. K-Nearest Neighbors

The k-nearest neighbors (k-NN[52]) algorithm is a non-parametric method used for both classification and regression tasks. In classification, a query point is assigned the class most frequent among its k nearest neighbors in the training dataset. Distance metrics, such as Euclidean or Manhattan distance, determine proximity. For regression, the predicted value is typically the average (or median) of the target values of the k nearest neighbors. The choice of k significantly influences the model's performance; a small k can lead to noisy predictions and overfitting, while a large k can smooth decision boundaries and potentially underfit. The hyperparameter k can be easily optimized via cross validation, from where the best k is chosen based on the best performance achieved for predictions of different validation sets (smallest error or highest accuracy). The simplicity and versatility of k-NN make it a popular choice for baseline models, although its computational cost can be high for large datasets.

2.5. Logistic Regression

Logistic regression,[53] despite its name, is a classification algorithm used to predict the probability of a binary outcome. It models the relationship between a set of independent variables and the log-odds (i.e., the measure of how much more likely an event is to occur than not occur, expressed on a logarithmic scale) of the dependent variable using a logistic (sigmoid) function. This function transforms the linear combination of predictors into a probability between 0 and 1. The model's parameters are typically estimated using maximum likelihood estimation, aiming to maximize the likelihood of observing the given data. Then a threshold is applied to the predicted probabilities to assign data points to one of the two classes. Logistic regression is widely used due to its interpretability, as the coefficients can be used to assess the impact of each predictor on the log-odds of the outcome.

2.6. Principal Component Analysis

Principal Component Analysis (PCA[54]) is a dimensionality reduction technique belonging to the unsupervised learning subarea that transforms a set of correlated variables into a set of linearly uncorrelated variables called principal components. These components (e.g., PC1, PC2, ..., PCn) are ordered by the amount of variance they explain in the original data. PCA achieves this by finding orthogonal directions (eigenvectors) that maximize the variance (eigenvalues) of the projected data. The first principal component (PC1) captures the most variance, the second (PC2) the second most, and so on. By selecting a subset of the top principal components, one can reduce the dimensionality of the data

while retaining most of its essential information. This process simplifies data analysis, visualization, and modeling by removing redundant or less informative features. 2D visualization of high dimensional data becomes very simple using PCA, from where clustering analysis is generally performed. However, PCA transformations also serve as a preprocessing step to train different supervised learning ML models.

2.7. Reinforcement Learning

Reinforcement learning (RL[55]) is a paradigm where an agent learns to make optimal decisions in an environment through trial and error. The agent interacts with the environment, receiving rewards or penalties for its actions, and aims to maximize cumulative rewards over time. This learning process is formalized using Markov decision processes, where the agent's actions influence the environment's state transitions. Deep reinforcement learning (DRL[56]) extends traditional RL by incorporating deep neural networks to approximate value functions or policies, enabling the agent to handle high-dimensional state and action spaces. DRL has achieved remarkable success in complex tasks, such as playing Atari games and controlling robots, by leveraging the representational power of deep learning to learn elaborate patterns and decision-making strategies directly from raw sensory input.

2.8. Gaussian Processes

Gaussian Processes (GPs[57,58]) are commonly used as surrogate models, particularly in Bayesian optimization, due to their flexibility, interpretability, and ability to model complex functions. This is achieved by defining a distribution over possible functions, rather than a single, fixed-parameter function. GP models predict the target property of a new sample by evaluating the similarity between its features and those of samples with known target properties. This similarity is quantified using a kernel function, such as the radial basis function (RBF) kernel, which dictates the shape and smoothness of the predicted function. According to GPs, the more similar the features of two samples are, the more similar their target properties will be. Crucially, GPs, and thus Gaussian Process Regression (GPR), not only provide a prediction for the target property but also offer a measure of uncertainty associated with that prediction, making them valuable when dealing with complex, non-linear relationships and when quantifying uncertainty is essential.

2.9. Bayesian Optimization

Bayesian optimization (BO[59]) is a technique used to efficiently find the optimal settings for a process or system, especially when those settings are complex and expensive to evaluate. It works by building a statistical model like GPR of the relationship between the settings (e.g., processing parameters and/or material composition) and the desired outcome, which is the target property to maximize, minimize or simply tune. The BO approach is then used to intelligently select the next set of settings to try, balancing the need to explore new possibilities (exploration) with the desire to exploit the knowledge gained from previous evaluations (exploitation). In essence, it helps to navigate complex, multidimensional parameter spaces, minimizing the number of experiments required to achieve the best possible result.[23,29] The BO approach is efficient for a maximum of ca 10–20 parameters and is very sensitive to data quality and acquisition function adopted to suggest new experiments.

Table 1. Machine Learning abbreviations used in the review.

Abbreviation	Full Name
ANN	Artificial Neural Network
BO	Bayesian Optimization
CNN	Convolutional Neural Network
CVA	Canonical Variate Analysis
DA	Discriminant Analysis
DL	Deep Learning
DRL	Deep Reinforcement Learning
DRSN	Deep Residual Shrinkage Network
DT	Decision Tree
GBDT	Gradient Boosting Decision Tree
GBR	Gradient Boosting Regressor
GNB	Gaussian Naive Bayes
GNN	Graph Neural Network
GPs	Gaussian Processes
GPR	Gaussian Process Regression
HCA	Hierarchical Cluster Analysis
k-NN	k-Nearest Neighbors
LDA	Linear Discriminant Analysis
ML	Machine Learning
MLP	Multilayer Perceptron
MLPC	Multilayer Perceptron Classifier
PCA	Principal Component Analysis
PLS	Partial Least Square
PLS-DA	Partial Least Squares-Discriminant Analysis
QDA	Quadratic Discriminant Analysis
RF	Random Forests
RL	Reinforcement Learning
SAM	Spectral Angle Mapper
SIMCA	Soft Independent Modeling by Class Analogy
SVC	Support Vector Classifier
SVR	Support Vector Regressor
SVM	Support Vector Machine
XGBoost	Extreme Gradient Boosting
YOLO	You Only Look Once (classifier)

Table 1 describes the abbreviations of the ML models used in the reviewed literature.

3. Pretreatment

The pretreatment of plastic waste is a crucial step to ensure efficient and high-quality processing in mechanical, chemical and biological recycling. This includes sorting to separate different polymer types, shredding to reduce particle size and washing to

remove contaminants. These steps are essential for improving the purity of the material and enhancing its recyclability.

3.1. Sorting

ML can play a crucial role in improving the efficiency and accuracy of plastic waste sorting. Numerous studies have demonstrated the ability of ML to detect, classify and separate entire products with high precision.[30–32,39,60–75] An overview of all publications that focus on sorting, detection and classification of plastic waste using ML can be found in **Table 2**. Many scientific approaches utilize camera-based systems that analyze the waste stream in real time, identifying different polymer types based on their visual characteristics.[60,62–64,66] These AI-driven systems can be applied to a wide range of plastic waste, including general packaging materials and specific product categories such as beverage bottles.[62,64,66] With the help of ML, not only can plastic types be detected and classified, but materials can also be sorted by color.[65] This ensures that the material streams are both pure in type and color, greatly improving the quality of the recycled material and making it more suitable for reuse in various applications.

In addition to the imaging techniques described above, spectroscopic methods are also widely used. Among the most frequently discussed techniques in the literature is infrared spectroscopy. Infrared spectroscopy utilizes infrared light to measure the vibrations of molecular bonds. Each molecule absorbs specific wavelengths of infrared light, resulting in a unique absorption spectrum. This spectrum serves as a "fingerprint" of the molecule, enabling its identification and analysis. Infrared spectroscopy is particularly useful for the identification of polymers, as different polymer types exhibit distinct absorption patterns that allow for precise differentiation. It is typically divided into NIR spectroscopy,[30,61,63,67,71,72] SWIP (short-wave infrared spectroscopy),[68] and MIR spectroscopy,[31,72,75] depending on the wavelength range. Furthermore, ML-based sorting systems that utilize NIR are capable of accurately identifying complex waste materials, including different types of textiles, even under challenging conditions such as moisture interference, thereby enabling efficient and automatic classification.[76,77] Additionally, FTIR (Fourier-transform infrared spectroscopy) enhances measurement precision in both ranges by applying Fourier transformation. However, challenges persist, including the identification of specific components such as conductive textile traces (smart materials). This underscores the necessity for a more extensive array of specialized strategies beyond spectroscopic methods for comprehensive waste sorting.[78]

A study by Stavinski et al.[31] explored the potential of MIR spectroscopy paired with ML to enhance the sorting process of post-consumer plastic waste. A schematic representation of the study is illustrated in **Figure 2**.

The objective was to address the limitations of current optical screening technologies that operate in the visible (VIS) and NIR regions, which are often hindered by dyes and polymer additives. To this end, the researchers compiled a comprehensive MIR database encompassing both virgin and post-consumer recycled plastics across five economically significant types (PET, HDPE, LDPE, PP, and PS). They then analyzed the dataset using various ML algorithms, including RF, k-NN, SVM, and Logistic Regression. To further refine the classification process, autoencoders were applied as a preprocessing technique to improve model accuracy. The RF algorithm achieved perfect classification (100% accuracy) in the molecular fingerprint region as well as in specific MIR bands (e.g., C–H stretching vibrations), which remained unaffected by interfering additives. Additionally, the study provided evidence that MIR spectroscopy, when combined with ML, can reliably classify black plastics and distinguish between HDPE and LDPE. These insights could play a key role in advancing more precise and efficient sorting technologies for recycling facilities.

Sutliff et al.[30] (**Figure 3**) investigated the sorting of polyolefins (PP, LDPE, LLDPE, MDPE, HDPE, PP-co-PE) using NIR spectroscopy, employing a data-driven approach. The authors screened over 12 000 machine-learning pipelines, with various combinations of preprocessing steps (scattering corrections, detrending and mean centering, filtering, normalization, dimensionality reduction) and classification algorithms. The aim was to identify data pipelines capable of sorting polyolefins materials with over 95% accuracy. The most promising preprocessing steps were further optimized using a nested cross-validation approach and the RF classifier. The top-performing classifier was then evaluated using a leave-one-group-out cross-validation method to test its ability to classify individual polymers it was not trained on. The results demonstrated that multiple data pipelines are capable of sorting polyolefins materials with high accuracy (>90%), with a simple robust normal variate signal preprocessing, scattering correction and normalization operations sufficient to clean NIR spectra for accurate classification. The LinearSVC was selected as the preferred model due to its simplicity and high balanced accuracy scores (>95%). A detailed overview of the study workflow can be found in Figure 3.

There are also approaches that combine Raman spectroscopy with FTIR to improve material identification.[39] While FTIR is highly effective for detecting organic compounds and characterizing molecular structures, Raman spectroscopy provides complementary information by analyzing molecular vibrations through inelastic light scattering. The combination of both techniques allows for a more comprehensive analysis of plastic waste, improving the accuracy of polymer identification and enhancing sorting processes in mechanical recycling. The use of ML further enhances these experimental techniques by optimizing data interpretation, improving classification accuracy and enabling real-time adaptation to variations in material composition. AI-driven algorithms can process complex spectral data more efficiently than conventional methods, making automated sorting systems more reliable and scalable.

A particular challenge in plastic sorting is the classification of black plastics, as traditional NIR spectroscopy methods struggle to differentiate them due to the strong absorption of IR light by carbon black pigments. To address this, alternative spectroscopic techniques such as fluorescence spectroscopy or LIBS spectroscopy have been explored.[32,69,73,74] Fluorescence spectroscopy analyzes the light emitted by a material after exposure to ultraviolet or visible light. Since some polymers and additives exhibit characteristic fluorescence, this method can help distinguish black plastics where infrared-based techniques fail. It offers a useful approach for improving sorting efficiency and

Table 2. Overview of publications on sorting in combination with ML. The table contains information about the publications, the objects sorted in them, the object materials, the sensor technologies used and the ML models applied.

Refs.	Sorted objectives	Sorting technology	ML algorithm	Materials
[60]	Complete products	Camera	YOLO, DeepSORT (Deep Simple Online and Realtime Tracking), ShuffleNetV2 (CNN)	Different types of plastic packaging
[61]	Complete products	NIR Spectroscopy	PLS, CNN, PCA, DT, RF, SVM	Bottles (PE, PP, PET), Shrink sleeves (PET, PS (Polystyrene), PVC (Polyvinyl Chloride))
[62]	Complete products	Camera	CNN	PP, HDPE, PET, PS
[63]	Complete products	Camera + 6 Sensors (NIR, humidity, temperature, CO_2, CH_4, laser profile sensor)	CNN	PET, PVC, PP, LDPE (Low-Density Polyethylene), Residual waste, Other
[64]	Bottles	Polarization Camera	SVM	PET, PE, PP, PS
[65]	Bottles	Camera	ReliefF (Feature Selection), SVM	PET (different colors)
[66]	Bottles	Camera	SVM	PET, Non-PET
[39]	Materials	Raman, FTIR	Adapted CNN (with Inception net)	HDPE, LDPE, PET, PP, Other
[67]	Materials	NIR	PR (Polynomial Regression), RF, ANN	PET, PP, PE, PS
[68]	Materials	SWIR-HIS (Short-Wave Infrared Hyperspectral Imaging)	PCA, Hierarchical PLS-DA	All virgin and recycled, PP, LDPE, HDPE, PS, PVC
[69]	Materials	LIBS	PCA	PET, PE, PP, PS
[32]	Materials	LIBS	PCA, KNN, RDF (Random designed Forest), HCA	20 polymers
[70]	Materials	LIBS	SVM	PE, PP, PS, PMMA (Poly(Methyl Methacrylate)), PVC
[30]	Materials	NIR	SIMCA, PLS-DA, RandomForest, MLPC, LDA, QDA, LinearSVC (Linear support vector classifiers), RBF_SVC (radial basis function support vector classifier), GNB, KNN, AdaBoost	HDPE powder, HDPE pellet, PP pellet, MDPE (Medium-Density Polyethylene) pellet, LDPE pellet, LLDPE (Linear Low-Density Polyethylene) pellet, PP-co-PE (PP-PE Copolymer) pellet
[31]	Materials	MIR	RF, KNN, SVM, LR	PET, HDPE, LDPE, PP, PS
[71]	Materials	NIR	SAM, PLS-DA, PCA-LDA	PP, PS, ABS (Acrylonitrile Butadiene Styrene), ABS/PC (Polycarbonate Blend), ABS FR (Flame Retardant)
[72]	Materials	NIR, MWIR	Bernoulli NB, Gaussian NB, Decision Tree Classifier, Extra Trees Classifier, Random Forest Classifier, kNN Classifier, Linear SVC, Logistic Regression, Ridge Classifier, PLS-DA, MLP Classifier	PE, PET, PP, PS, PVC
[73]	Materials	Fluorescence spectroscopy	DA (linear discriminant analysis), CNN, KNN, Ensemble, SVM	SBR (Styrene-Butadiene Rubber), HDPE (High Density Polyethylene), PA6 (Polyamide 6), PA66 (Polyamide 66), PA66V0 (PA66 Flame Retardant V0 Grade), PBT (Polybutylene Terephthalate), POM (Polyoxymethylene), PP, PS, TEEE (Thermoplastic Elastomer Ester-Ester), TPE (Thermoplastic Elastomer), TPU (Thermoplastic Polyurethane)
[74]	Materials	LIF (Laser-induced fluorescence)	PCA, Hi-PLS-DA (Hierarchical partial least square-discriminant analysis)	EPS (Expanded Polystyrene), PS, HDPE, PP
[75]	Materials	MIR	CNN	PVC, PS, PP, PE and Blends of them
[76]	Waste textile	NIR	PLS, ANN, DT, RF, GBDT, Extra-tree, AdaBoost-tree, SVM, 1D-CNN, 1D-Inception-CNN	Polyester, Viscose
[77]	Waste textile	NIR	CNN, PCA, CVA	Natural, synthetic (polyester polyamide) and artificial fibers and binary mixtures

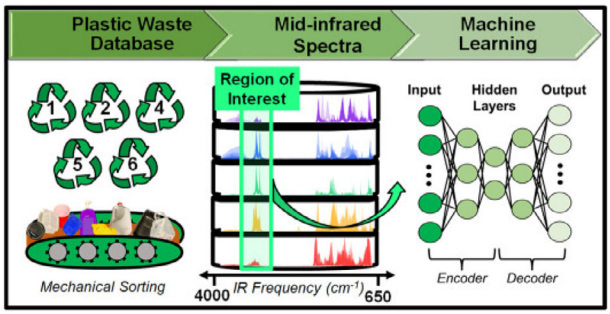

Figure 2. The study's workflow is presented in this schematic, demonstrating the utilization of MIR spectroscopy to analyze plastic waste samples and subsequent automated classification via ML algorithms. Reproduced with permission from ref. [31] (2023, Royal Society of Chemistry).

recyclability.[73,74] By integrating ML, fluorescence spectra can be analyzed with greater precision, allowing for more accurate differentiation between polymer types and improving automated sorting performance. LIBS is a laser-based technique that determines the elemental composition of plastics. Unlike infrared spectroscopy, it is not affected by carbon black pigments and can still identify different polymer types based on their chemical signatures. This makes LIBS a promising tool for sorting black plastics in recycling processes. The combination of LIBS with ML algorithms enhances its efficiency by enabling automated spectral pattern recognition, reducing classification errors and increasing processing speed. ML models trained on extensive spectral databases can refine LIBS-based sorting systems, improving their adaptability to real-world plastic waste streams.[32,69,70]

Gajarska et al.[32] explored the use of LIBS spectroscopy and chemometrics to identify 20 different virgin polymer types. The study involved a variety of polymer samples, including polymer thin films and embedded polymer pellets. Furthermore, the study examined the impact of common additives such as carbon black, antioxidants, flame retardants and UV absorbers on polymer identification. Samples were analyzed under different experimental conditions, with systematic variations in laser energy, gate delay and atmosphere. To extract chemically relevant information from the LIBS spectra, the authors employed "spectral descriptors" as features. Multivariate data analysis, including PCA, k-NN, HCA and an in-house designed RF experiment, was utilized for data processing and analysis. Through PCA, the original 10D dataset was reduced to a 2D representation, enabling clearer interpretation of the data. The authors were able to effectively discriminate among the 20 polymer types, as shown in **Figure 4**, even in the presence of additives (**Figure 5**), by employing a two-step optimization process using ML algorithms.

In view of the great number of papers found for sorting, as compared with shredding and washing, an overview of the literature revised for sorting is shown in Table 2, from where one sees some interesting trends. First, there is a clear evolution from traditional camera-based systems to more sophisticated sensor technologies, with NIR spectroscopy emerging as a dominant technique especially for material identification. Second, the ML algorithms demonstrate a progression from simpler classification methods (SVM, PCA) to more advanced deep learning approaches (CNN, YOLO) particularly for complete product sorting. Third, there is a notable distinction between studies focusing on complete products versus material-level sorting, with the latter typically employing more specialized spectroscopic techniques (LIBS, MIR, FTIR). Additionally, most studies concentrate on common plastic types (PET, PP, PE, PS, PVC), with fewer addressing complex polymer blends or recycled materials. The combination of multiple sensor technologies and ensemble ML models appears to be an emerging trend for improving sorting accuracy, as seen in more recent publications. This collective research demonstrates the field's movement toward more sophisticated, multi-modal approaches to address the challenges of plastic waste sorting.

3.2. Shredding

In the context of recycling, the shredding of recycled polymers constitutes a fundamental step, given its role in material processing and enhancing the efficiency of the subsequent recycling steps. The shredding process enables the targeted separation of diverse materials, particularly in the case of components comprising multiple plastics (i.e., multi-plastic parts). The mechanical effects, including cutting, shearing or grinding, break the polymers down into smaller particles, thereby facilitating the separation of these materials by their respective types. The entire process is highly dependent on the material properties of the plastics, the technical specifications of the shredding machines and the selected process parameters such as cutting speed, degree of grinding and energy input. Particle size distribution resulting from the shredding process significantly impacts downstream operations, with smaller and more uniform particles generally leading to more efficient sorting and purification. Furthermore, the shredding methodology must account for various polymer characteristics including brittleness, elasticity and thermal properties to prevent material degradation while maintaining throughput. Advanced shredding technologies now incorporate sensor-based controls to optimize energy consumption and reduce wear on machinery components, particularly critical when processing contaminated waste streams or plastics containing additives and fillers. These technological improvements address key challenges in plastic recycling infrastructure, namely the handling of mixed plastic waste and maintaining material integrity throughout the mechanical recycling process. The objective is to maximize material recovery and minimize environmental impact.[79]

Rojek et al.[80] explored the application of ML techniques to optimize the mechanical shredding process of polymer recyclates, with a particular focus on predicting energy efficiency and product quality. To achieve this, PLA was shredded using a multi-edge shredder, while the resulting process data was recorded and compiled into a comprehensive dataset. This dataset served as the foundation for training a variety of ML algorithms. Following an initial evaluation based on predictive accuracy, the five most promising algorithms were selected for further refinement. Subsequently, a hyperparameter optimization was performed to enhance the performance of these selected algorithms. **Figure 6** presents the results of the cross-validation, demonstrating that the hyperparameters–and consequently, the accuracy–varied for algorithms of the same type. The robustness of the findings was

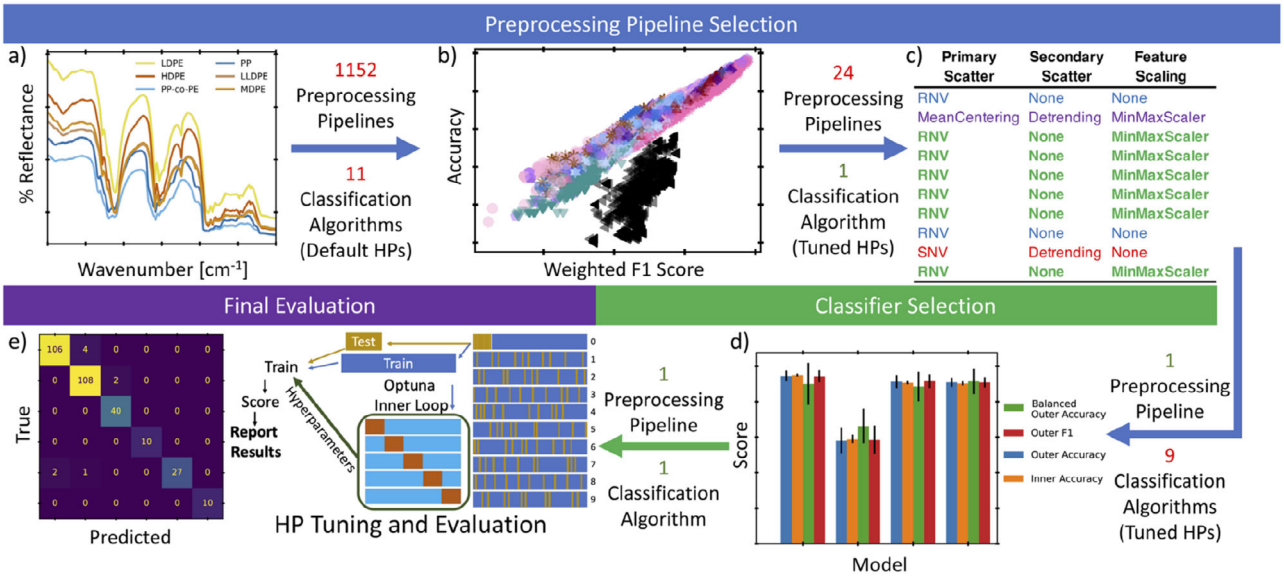

Figure 3. Overview of the study methodology: a) Initial NIR data collection from polyolefin samples. b) Screening of 11 different classification algorithms. c) Evaluation of different preprocessing combinations and optimal pipeline selection. d) Hyperparameter tuning and best-performing classifier selection. e) Final evaluation with leave-one-group-out nested cross-validation. Reproduced with permission from ref. [30] (2024, Royal Society of Chemistry).

ensured through cross-validation. The study revealed that the logistic regression-based one-vs-all classifier outperformed the other models, achieving an accuracy of approximately 93%. This algorithm effectively predicts target outcomes using a logistic regression framework, while its computational efficiency further enhances its practical applicability.

3.3. Washing

After plastic waste has been shredded into smaller pieces, it needs to be thoroughly cleaned. Washing removes dirt, adhesives and other residues that could affect the quality of the recycled material. This step is especially important for producing high-quality recyclates. In food-grade recycling, strict cleaning standards must be met to ensure the material is safe for reuse.

To date, no approaches have been reported that utilize ML to enhance plastic waste washing processes. This represents a significant research gap, especially given the crucial role of cleaning in achieving high-quality recycled plastics and even more so for meeting food-grade requirements. The absence of such studies suggests an untapped potential for ML technologies to significantly improve the efficiency, thoroughness and sustainability of these essential washing procedures.

4. Mechanical Recycling

Mechanical recycling is the most widely used method for processing thermoplastics due to its cost-effectiveness, simplicity, and

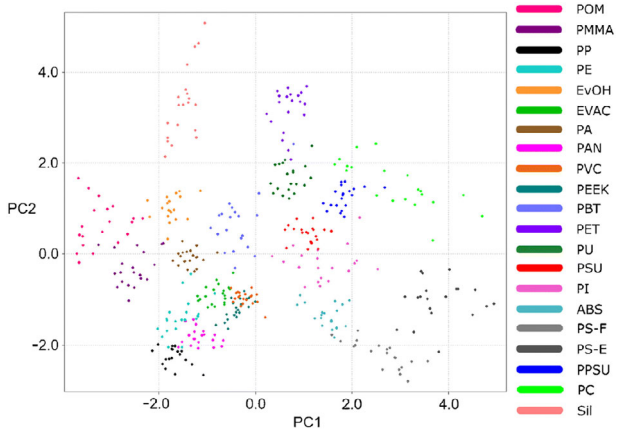

Figure 4. Representation of the separation of 20 polymer clusters in the space of the first two principal components (PC1 and PC2), based on an optimized set of spectral descriptors. Reproduced with permission from ref. [32] (2021, Springer Nature).

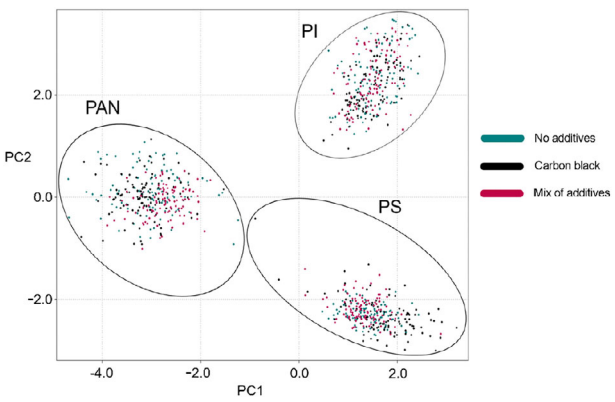

Figure 5. PCA representation of PAN (Polyacrylonitrile), PI (Polyimide) and PS samples with different additives (no additives, carbon black and a mix of additives). Reproduced with permission from ref. [32] (2021, Springer Nature).

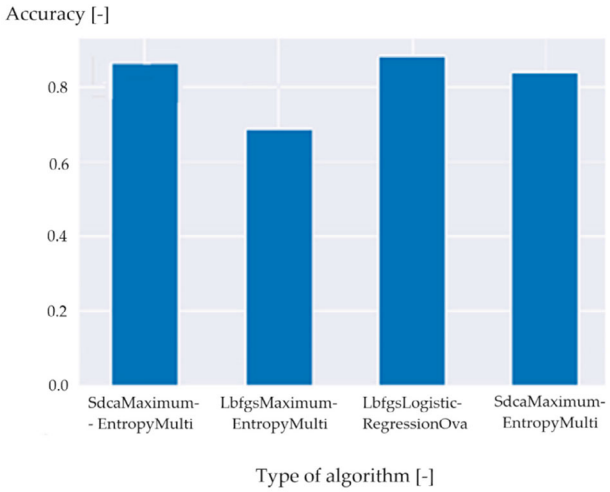

Figure 6. Results of the cross-validation of four different algorithm. The accuracy of the LbfgsLogisticRegressionOva is the highest. Reproduced with permission from ref. [80] (2024, MDPI).

scalability. Unlike chemical recycling, which requires high energy input and complex processing, mechanical recycling offers an efficient and economically viable solution for reducing plastic waste and conserving resources. However, challenges such as material degradation, contamination and limited applicability of mechanical recycling to mixed or heavily used plastics must be addressed to enhance its sustainability and effectiveness. In this context, ML represents a promising approach for optimizing various stages of the recycling process and the quality control of recycled material, as described below.

4.1. Regranulation

Regranulation is the final step in the mechanical recycling of polymer waste, after sorting, shredding and washing. In this process, the shredded plastic material is melted and homogenized before being cooled and solidified into uniform-sized pellets or granules. These granules can then be reused in manufacturing, transforming the plastic into a form that is compatible with various processing techniques and making it easier to integrate into the production of new products. Regranulation also helps standardize the properties of the recycled polymer, ensuring consistency and quality.

During the regranulation process, the polymer material undergoes thermal and mechanical shear forces, which can lead to the degradation of its properties.[81–84] The heat applied during melting and the shear forces generated by the mechanical processing can break down the polymer chains, causing a reduction in molecular weight. This degradation can result in a loss of mechanical strength, flexibility and overall performance of the recycled material. Lopez et al. processed PET several times to simulate degradation effects on PET samples under thermo-mechanical recycling.[83] They were able to reproduce a reduction in molecular weight, rheological properties and toughness. Similar results were obtained by Kim et al.[84] who were able to confirm the reduction in rheological and mechanical properties after repeated reprocessing of PET. The processing parameters and the screw configuration influence the degree of degradation.[85,86] Therefore, careful control of processing parameters such as temperature and shear rate is crucial to minimize the extent of degradation and maintain the quality of the regranulated material. For this reason, minimizing degradation during regranulation is essential. Research efforts are also being conducted to develop strategies that reduce polymer degradation and improve the quality of recycled materials. Since degradation leads to a decrease in molecular weight and viscosity, approaches are being explored to predict these changes using ML.[33,87]

The study by Castéran et al.[33] investigated the thermo-mechanical degradation of PE using a twin-screw extrusion process at high temperatures. The goal was to control the degradation process and develop data-driven models to predict material properties. HDPE and Ultra-High Molecular Weight Polyethylene (UHMWPE) were extruded in an intermeshing co-rotating twin-screw extruder at 350–420 °C under varying flow rates and screw speeds to induce molecular weight reduction. The ML models were trained using process parameters (temperature, screw speed and flow rate) as features to predict material properties such as molecular weight and zero-shear viscosity as targets. The rheological behavior of the extruded materials was analyzed offline with a stress-controlled rheometer and molecular weight distributions were determined using high-temperature size-exclusion chromatography (HT-SEC). A numerical approach based on the Carreau–Yasuda model predicted rheological behavior from in-line pressure measurements, validated against offline viscosity data and molecular weight estimations. SVR and the sparsed proper generalized decomposition (sPGD) method were tested for predicting process outputs and material properties. The results confirmed that SVR and sPGD effectively predicted molecular weights and zero-shear viscosity, with sPGD providing better viscosity predictions. A graphical comparison in **Figure 7** shows the agreement between predicted and actual values for both ML models. To address inaccuracies in data-driven models due to measurement errors, a stochastic approach was tested with SVR on HDPE extruded at 390 °C. Despite the limited dataset, the method produced satisfactory results, suggesting potential applications for different polymers, temperatures and additional properties such as viscosity and molecular weight. This study demonstrates that data-driven modeling can optimize the twin-screw extrusion process, offering a promising approach for predicting degradation in PE recycling and extending the lifecycle of recycled materials.

4.2. Quality Control and Property Prediction

As previously discussed, the inherent nature of mechanical recycling processes induces significant alterations in the polymer matrix, notably a reduction in molecular weight and modifications to the crystallization behavior. This inherently degrades polymers, altering crystallization, which negatively impacts and increases the variability of material properties due to inconsistent input from diverse recycling streams. To address these challenges, emerging approaches are exploring the use of ML for process optimization and property prediction. Examples include ML for improved batch management in rPP,[34] VOC control in PET recycling[88] and enhanced injection molding of recycled plastics

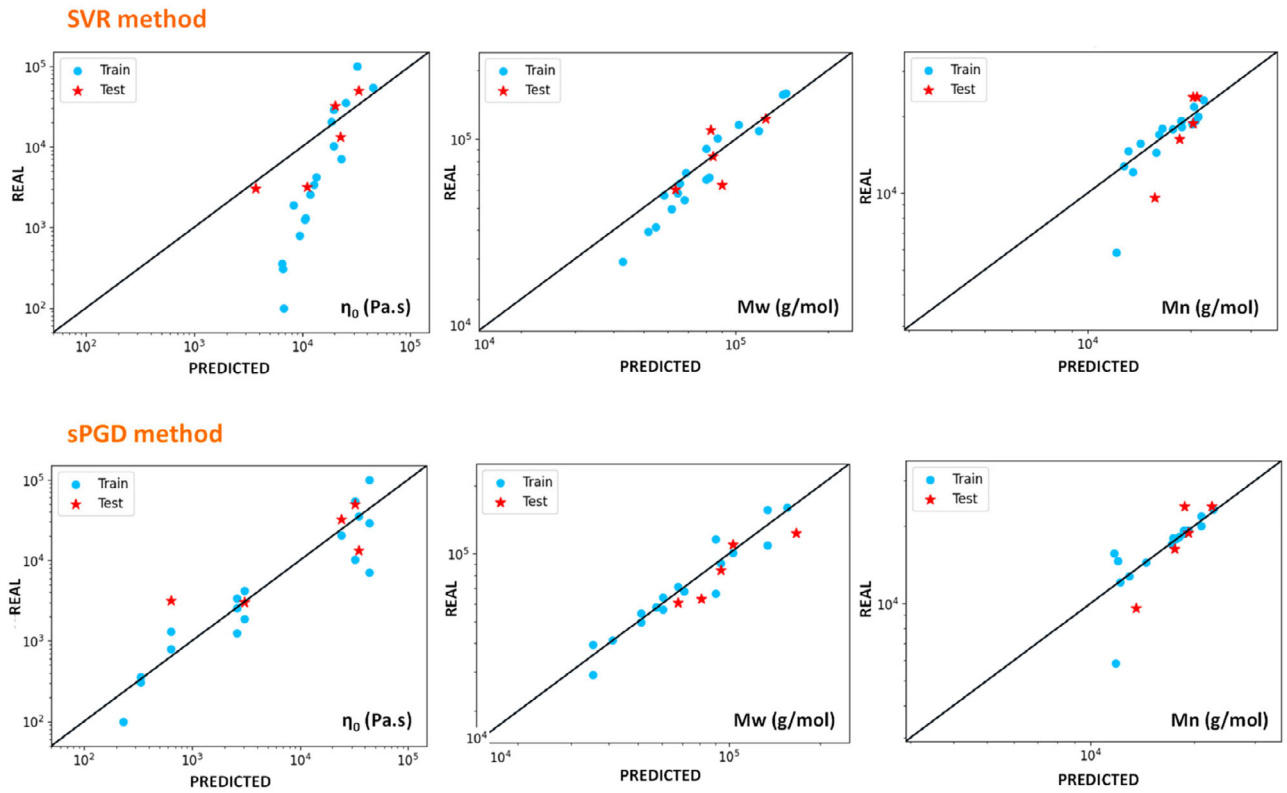

Figure 7. Comparison of the prediction performance of SVR and SPGD models for viscosity, molecular weight (Mw) and number average molecular weight (Mn). The plots show the real values versus the predicted values for training and test data. The solid line in each plot represents perfect prediction, with points close to the line indicating good model performance. Reproduced with permission from ref. [33] (2022, MDPI).

using Transfer Learning.[35] These studies demonstrate the growing potential of ML to enhance the quality and consistency of mechanically recycled polymers.

In their study, Chen and Huang[35] investigated how Transfer Learning (TL) can enhance the prediction accuracy of quality in recycled materials within the plastic injection molding process (**Figure 8**). The primary aim was to adapt a model initially trained on virgin material data to recycled materials. Process parameters such as pressure, temperature and flow rate were used as features, while quality indices such as dimensional accuracy and surface quality served as targets for the model. A ANN, pretrained on virgin material data, was adapted to the specific characteristics of recycled material using Transfer Learning. Compared to conventional training, TL showed significant advantages: it resulted in faster convergence and reduced training times, as there was no need for repeated hyperparameter searches. The model achieved better predictive performance with notably lower loss values, fewer iterations and quicker convergence. Furthermore, both the average and maximum test errors were reduced, indicating improved generalization and robustness of the model. Predictions from the TL model were more consistent and showed less underfitting, leading to more stable performance even with limited training data.

Altarazi et al. [89] conducted a comprehensive investigation into the utility of various ML algorithms for the prediction and classification of the tensile strength of polymeric films. The scope of their study encompassed films fabricated using distinct production processes, specifically compression molding and extrusion-blow molding. The research utilized a variety of polymer types and compositions, including both virgin and recycled polymers, as inputs for their models. The study's findings, derived from developing and evaluating nine distinct algorithms (including prominent methods like SVM, ANN and RF), demonstrated the superior predictive capability of the SVM algorithm. Specifically, for extrusion-blown films, SVM attained an R^2 of 0.96. This work underscores the significant potential of machine learning to precisely forecast critical material properties based on their respective processing parameters, offering a powerful tool for quality control and process optimization across various material streams.

Altarazi et al. [90] investigated the potential of ANNs in modeling the complex properties of extruded PVC composites. The objective of the study was twofold: first, to recognize the inherent nonlinear relationship between a composite's composition and its resulting post-production properties; and second, to accurately predict and optimize three key mechanical characteristics: tensile strength, ductility, and density. The research systematically varied the weight percentages of critical constituents, including virgin PVC, recycled PVC, calcium carbonate ($CaCO_3$) and plasticizers. The experimental design and subsequent analysis confirmed the effectiveness of ANN models in accurately estimating these nonlinear relationships. In addition, the findings indicated that ANNs can be utilized as a strategic tool to determine the optimal compositional blend necessary to achieve the desired

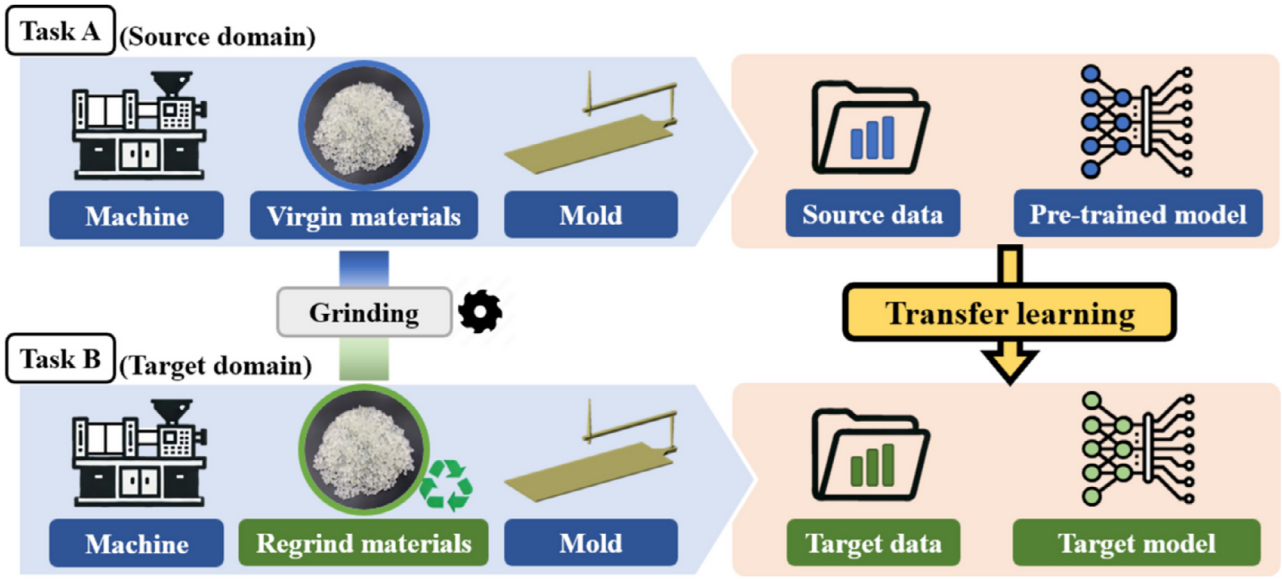

Figure 8. Overview of the transfer learning (TL) to improve the quality prediction in plastic injection molding with recycled materials. Task A represents the pre-training of the model with virgin material data. Task B represents the adaptation of the pre-trained model to recycled material data for enhanced prediction accuracy and efficiency. Reproduced with permission from ref. [35] (2024, Springer Nature).

material properties. This provides a robust framework for material design and quality enhancement in PVC composite manufacturing, particularly emphasizing the successful integration of recycled content.

The study of Teruel et al. [34] presents a ML-based approach to optimize recycled PP mixtures, aiming to reduce property variability through a batch management algorithm. Using historical production data, a predictive model based on non-linear mixing rules was trained to estimate the final material properties. The input features included the proportions and properties of different PP waste sources - melt flow index (MFI), Izod impact strength, shrinkage and ash content - while the targets were the same properties in the final blend. **Figure 9** shows a comparison between the predicted and actual results for the recycled PP blends. Validation showed a strong correlation, with most deviations within ±6%, except for impact strength, which deviated by up to 18%. Simulations using four years of data tested different property constraints and a parameter balancing quality and production volume. The results showed a significant reduction in variability - over 46% for most properties and 22% for impact strength - but tighter constraints limited production flexibility. By using ML, the batch management tool increases sourcing flexibility while ensuring more stable recycled PP properties.

5. Chemical Recycling

Chemical recycling encompasses a range of techniques, each targeting specific polymer types and offering varying degrees of selectivity and efficiency. The fundamental principle involves depolymerization, where long polymer chains are cleaved into smaller molecules through chemical reactions. Common methods include pyrolysis, solvolysis (e.g., hydrolysis, methanolysis, glycolysis), and gasification. Pyrolysis involves thermal degradation in the absence of oxygen, yielding a mixture of hydrocarbons that can be further refined. Solvolysis utilizes solvents and catalysts to selectively break polymer bonds, producing monomers or oligomers. Gasification converts plastic waste into syngas, a mixture of carbon monoxide and hydrogen, which can be used as a feedstock for various chemical syntheses.

Despite its potential, chemical recycling faces several significant challenges. The complexity of mixed plastic waste streams necessitates efficient separation and pre-treatment processes, which can be energy-intensive and costly. The development of robust and selective catalysts is crucial for achieving high yields and purity of recycled monomers. Furthermore, the energy requirements and environmental impact of chemical recycling processes must be carefully evaluated to ensure their sustainability. Economic viability remains a critical factor, requiring optimization of process parameters and integration with existing chemical infrastructure. Overcoming these challenges is essential for the widespread adoption of chemical recycling as a viable solution for mitigating plastic waste and fostering a circular economy. ML has been successfully used to address some of these problems, as described below.

5.1. Pyrolysis

Achieving high-quality pyrolysis oil directly from processing is essential to minimize downstream purification and associated costs. Hydrocracking, a specific pyrolysis technique, utilizes high-pressure catalysts and hydrogen to break down heavy hydrocarbon molecules. This process aims to maximize the yield of light, valuable products suitable for producing quasi-virgin polymers. In a recent study, Ma et al.[37] explored optimizing hydrocracking through a hybrid approach combining DRL with DRSN. Leveraging 398 different experiments, their method effectively

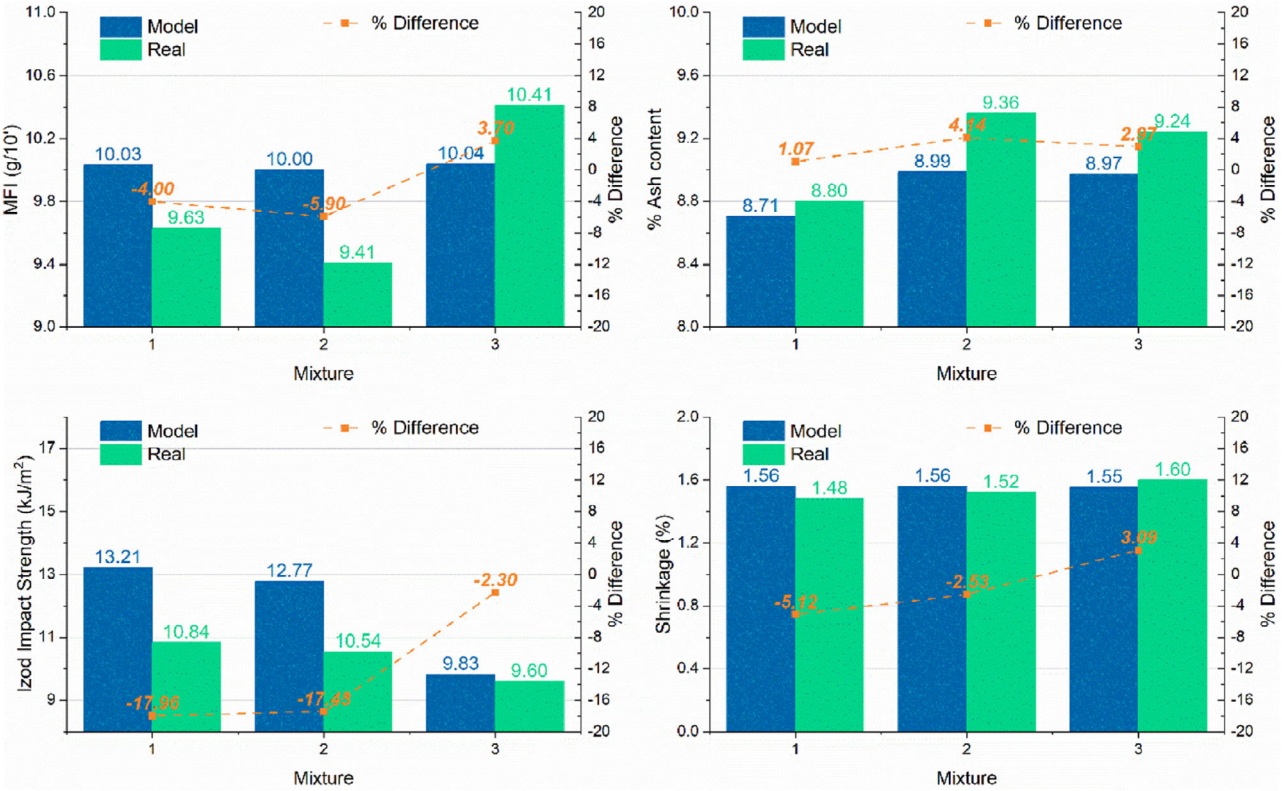

Figure 9. Comparison of model predictions and actual values for recycled PP mixtures. Graphs show the melt flow index (MFI), ash content, Izod impact strength and shrinkage. Reproduced with permission from ref. [34] (2024, Elsevier).

tuned critical process parameters, resulting in a reported increase in light product yield exceeding 50%.

Cheng et al.[91] investigated the application of various ML algorithms, including decision trees, ANNs, SVMs, and GPs, for pyrolysis analysis. Utilizing a dataset compiled from 93 recent publications, the study aimed to predict total mass balance, gas composition, and liquid product distribution. A decision tree-based ensemble model demonstrated superior performance, achieving an R^2 of 0.984 for liquid yield prediction. **Figure 10** presents the model's predictions and feature importance for wax, aromatic, gasoline, and diesel yields. The analysis revealed that reactor conditions, specifically feed intake, reaction temperature, and vapor residence time, significantly influenced wax production. For diesel yields, particle size, vapor residence time, and

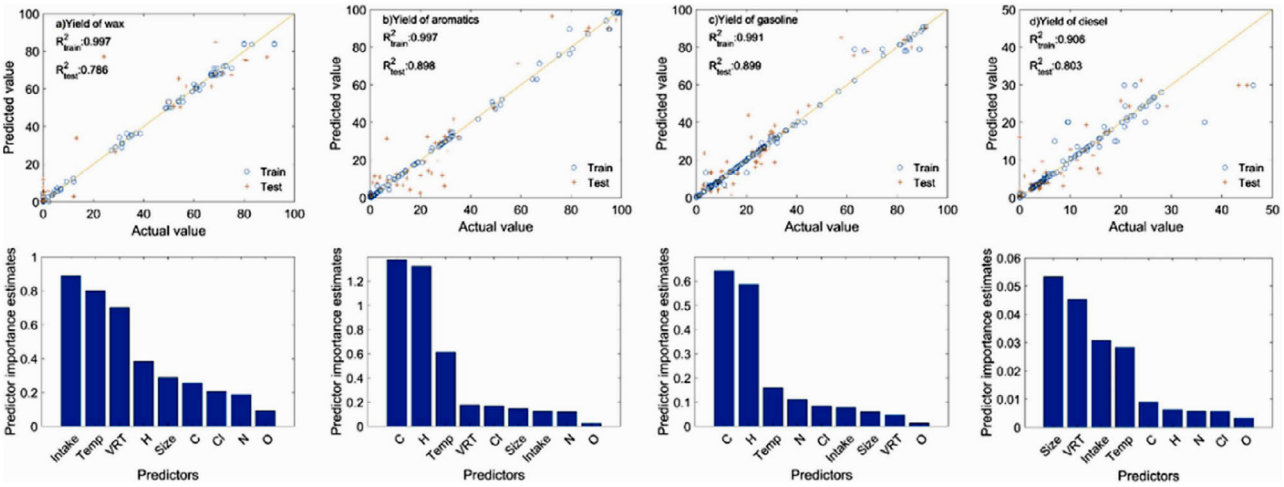

Figure 10. Actual and predicted values for a composition analysis obtained from a filtrensemble model regarding the wax, aromatics, gasoline and diesel yields. Reproduced with permission from ref. [91] (2023, Elsevier).

feed intake were identified as critical factors. Physical properties exhibited greater importance in predicting mid-carbon number products, while elemental ratios (carbon and hydrogen) were crucial for low-carbon products like gasoline and aromatics. Reactor conditions primarily affected high-carbon product yields (e.g., wax), whereas feedstock chemical properties predominantly determined the formation of specific chemical species like aromatics.

Qi et al.[92] employed ML to model and analyze the catalytic co-pyrolysis of polymers and biomass, investigating the impact of various parameters on product yields and oxygenate concentrations in pyrolysis oil. Utilizing a compiled dataset, the authors performed feature analysis and trained several ML models, including GBR, XGBoost, RF, and Histogram-based GBR (HGBR). The GBR model demonstrated robust predictive performance, achieving an R^2 of 0.98 for training and 0.87 for testing. The study revealed that catalysts, especially zeolites, significantly influenced product distribution, promoting gas production while reducing oil yield and oxygenate content. However, limitations were identified, including data scarcity, challenges in catalyst characterization, and the inherent nature of ML, which focuses on input-output relationships without elucidating underlying reaction mechanisms.

Ahmad et al.[93] investigated the optimization of LDPE pyrolysis for maximizing bio-oil production. This study aimed to identify optimal process parameters to enhance bio-oil yield while minimizing biochar and syngas byproducts. Seven ML models, including GBR and RF, were employed for predictive modeling and process optimization. The GBR model exhibited the highest predictive accuracy. Feature importance analysis, utilizing Mutual Information, revealed reactor temperature as the most influential parameter and nitrogen flow rate as the least. Optimal process conditions were determined to be 450°C, a residence time of 2 h, a nitrogen flow rate of 250 mL/min, and a catalyst loading of 6%, yielding 72.20% bio-oil, 6.35% biochar, and 23.48% syngas. The produced bio-oil presents a viable renewable fuel alternative, while biochar and syngas can be utilized for energy generation, heating, and industrial applications. This research demonstrates the potential of LDPE pyrolysis for sustainable energy recovery from plastic waste. Future studies should focus on process scale-up, catalyst optimization, and long-term stability testing. Furthermore, exploring biochar applications in agriculture and carbon sequestration could further enhance the process's sustainability.

Further research utilizes diverse ML models to address various aspects of plastic (co-)pyrolysis, including process optimization through condition identification[94] and comprehensive process analysis.[95,96]

5.2. Gasification

Hasanzdeh and Azdast[97] investigated the application of ML to model and optimize the air gasification of PET waste, focusing on predicting syngas composition (H2/CO ratio), lower heating value (LHV), and cold gas efficiency (CGE). The study begins with validating an equilibrium constant method for syngas prediction against existing data, demonstrating good agreement, as shown in **Figure 11**. A full factorial design with 121 trials, varying equivalence ratio and gasifier temperature, was employed and the data

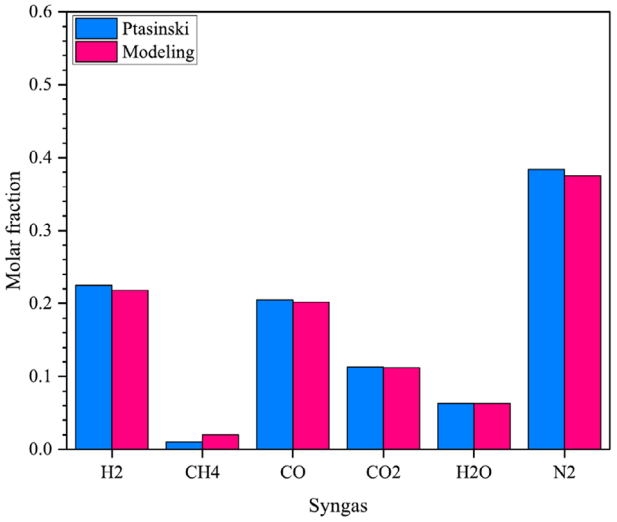

Figure 11. Comparison between the theoretical (red bars) and experimental values (blue bars) syngas composition. Reproduced with permission from ref. [97] (2024, Elsevier).

was modelled by a polynomial regression with cross terms. Residual analysis of the ML models revealed high accuracy, particularly for LHV and CGE, with R^2 values exceeding 0.99. While the H2/CO model showed slightly lower accuracy ($R^2 > 0.90$), it still exhibited significant predictive capabilities. The models' ability to predict new observations was also strong, with high predicted R^2 values. The research concludes that ML is a promising tool for optimizing PET waste gasification, offering potential for developing advanced control systems and contributing to sustainable waste management and clean energy production.

Qi et al.[98] analyzed the co-gasification process of biomass and municipal solid waste (MSW) by employing four advanced tree-based ML models (**Figure 12**). This research aimed to predict key performance parameters, including syngas composition, lower heating value, char yield, and carbon conversion efficiency, using 255 valid data points from literature. The study involved analyzing 18 input and 9 output features. The GBR model demonstrated high accuracy in predicting hydrogen yield (RMSE = 1.6), while the histogram-based Gradient Boosting model excelled in carbon monoxide prediction (RMSE = 1.2). SHAP analysis identified equivalence ratio, steam/fuel ratio, and biomass composition as the most influential features. To reduce dimensionality, PCA was performed, revealing that the first three principal components captured 66.2% of the data, emphasizing the importance of feedstock composition. The study acknowledged limitations, including the exclusion of catalysts and certain gasification methods like plasma and hydrothermal gasification.

Ayodele et al. [99] explored the use of Radial Basis Function (RBF) and MLP neural networks to model hydrogen production from the co-gasification of rubber and plastic waste. The researchers optimized the ANNs by determining the ideal number of hidden neurons, leading to specific network architectures for each model. Through analysis of the input parameters (RSS particle size, HDPE particle size, gasification temperature, and plastic waste amount), they found nonlinear relationships with hydrogen production. Notably, a one-layer MLP model

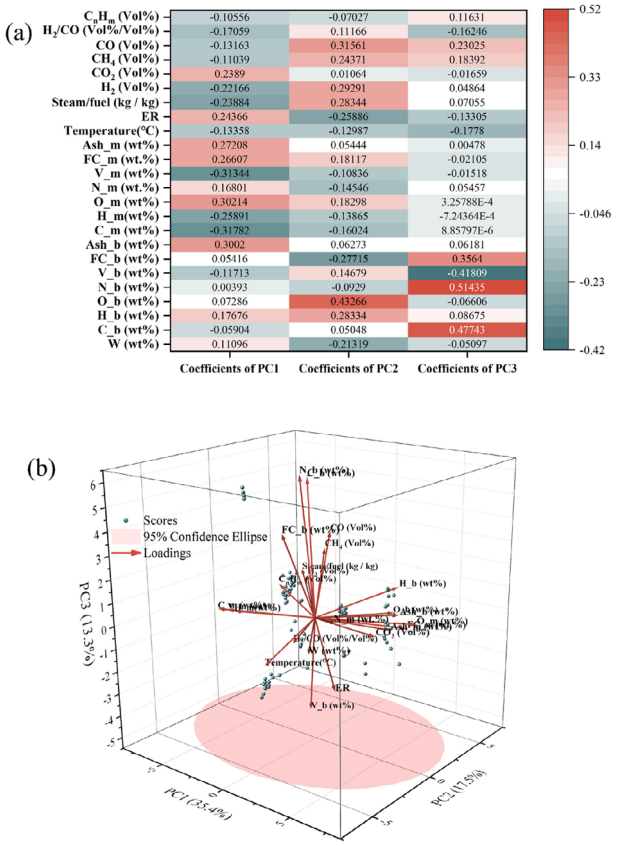

Figure 12. PCA investigation. a) Coefficient analysis. b) Distribution of data in the information space. Reproduced with permission from ref. [98] (2024, Elsevier).

demonstrated the highest predictive accuracy, achieving an R^2 of 0.990, highlighting the significant influence of all input parameters on hydrogen yield. The study concluded that ANNs, particularly the one-layer MLP, are effective tools for modeling and optimizing hydrogen production from co-gasification, offering valuable insights for future scale-up and process design.

Devasahayam et al.[100] investigated the prediction of hydrogen yield from plastic feedstock using ML algorithms, specifically decision tree and ensemble models such as boosting and RF. Utilizing a dataset of 30 data points, the study optimized tree-based models via GridSearchCV and evaluated their performance using cross-validation and train-test splits. The analysis identified temperature, particle sizes, and feedstock composition as critical factors influencing hydrogen production. The GBR emerged as the best performing model. The study further revealed that hydrogen yield is primarily surface-reaction controlled, exhibiting minimal temperature dependence above 500°C due to dominant high-temperature reactions.

Supercritical water gasification, an advanced technique involving the decomposition of organic material in water at elevated temperatures and pressures, offers an alternative route for hydrogen production. Azadvar et al.[101] recently investigated the prediction of hydrogen yield from this process using various ML algorithms, including decision trees, ensemble learning trees, SVMs, GBR, and Differential Evolution Optimization (DEO). Utilizing 246 experimental data points, the study aimed to identify optimal operating conditions for maximizing hydrogen yield. The ensemble learning tree model, enhanced by DEO, demonstrated superior performance, achieving an R^2 of 0.95 and an RMSE of 0.091. The validated model provided specific recommendations for catalysts and operating conditions based on feedstock composition. Further applications of ML to optimize hydrogen production from plastic waste gasification are comprehensively reviewed in Sofian et al.[102]

5.3. Depolymerization and Solvolysis

A significant research gap exists in the application of ML to recycling processes involving depolymerization and solvolysis. To date, no studies directly employing ML for these methods have been identified. This absence highlights the considerable potential for ML to advance chemical recycling research and development, especially in these two key sub-areas.

6. Biological Recycling

Similarly to chemical recycling, biological recycling via enzymatic hydrolysis enables true closed-loop recycling by breaking down polymers into their monomeric building blocks or other valuable platform chemicals. In this process, extracellular enzymes cleave covalent bonds within hydrolysable functional groups of the polymer. For complete depolymerization, these hydrolysable covalent bonds must be present within the main chain of the polymer. The chain scission proceeds through four consecutive steps: (1) diffusion of the enzyme to the polymer surface, (2) adsorption and formation of an enzyme-substrate complex, (3) cleavage of chemical bonds via hydrolysis, and (4) release and diffusion of degradation products into the aqueous reaction solution, from which they can be recovered.[10] Enzymatic degradation typically occurs in aqueous buffer solutions under mild conditions, usually at temperatures below 80 °C. Compared to chemical recycling, this approach avoids the need for harsh chemicals or high temperatures, thereby improving process sustainability while reducing energy consumption and environmental impact.[9] As enzymes are highly substrate-specific, a given enzyme variant typically cleaves only a single type of polymer. This specificity limits the applicability of enzymatic hydrolysis to polymers for which suitable enzyme candidates have already been identified. These are typically aliphatic polymers with low degrees of crystallinity, as increased chain rigidity and packing density in aromatic and crystalline regions impede enzyme access and hinder alignment of the polymer chain with the enzyme's active site. As a result, most studied substrates include aliphatic polyesters, polyamides, and polyurethanes. A prominent exception is PET, which, despite being a semi-aromatic polyester, can undergo complete enzymatic degradation once its crystallinity is sufficiently reduced.[103–105] While the substrate selectivity currently limits the applicability of enzymatic degradation to only few polymers, selectivity can also be advantageous when targeting specific polymers within mixed plastic waste streams. However, since the substrate specificity restricts the current applicability of enzymatic degradation to only a few polymer types, ongoing research aims to broaden the spectrum of degradable polymers by developing new and improved

enzyme variants. In this context, research efforts aim to achieve higher hydrolysis rates for both existing and novel polymer substrates, while enhancing enzyme stability with respect to temperature, pH, and other reaction conditions. Additionally, reaction parameters such as pH, temperature, buffer composition, and enzyme concentration are systematically optimized for each specific substrate-enzyme system.

In these areas, machine learning (ML) is playing an increasingly important role. It is employed for efficient enzyme discovery and engineering. Moreover, ML supports process optimization and facilitates the prediction of enzyme-substrate interactions and degradation rates, which are critical factors for advancing efficient and scalable enzymatic recycling technologies.[106,107]

6.1. Enzyme Design

Although the substrate specificity of enzymes can be advantageous for the selective recycling of plastics from mixed waste streams, it also limits the applicability of enzymatic recycling to only a few polymers. For enzymatic degradation to occur, the polymer must contain hydrolyzable functional groups in its backbone while also adhering to the "key-lock principle"–meaning that the polymer's chain structure must align with the active site of the enzyme. To enhance the efficiency of enzymatic degradation and expand its applicability to a broader range of polymers, ongoing research focuses on engineering enzyme variants with faster degradation rates, improved thermal stability, and activity toward previously non-degradable polymeric substrates.[9,109,110] To efficiently utilize the extensive sequence data available from literature and databases, ML models have been developed to identify patterns and predict promising enzyme variants with enhanced substrate activity. This approach significantly reduces the need for time-consuming and costly experimental screening trials, while accelerating the optimization of enzyme structures. The ML models employed in this process include 3D CNN, GNN, logistic regression, Bayesian optimization, SVM, RF, k-NN, MLP, and others. These diverse techniques enable a more accurate and faster identification of enzyme candidates with superior substrate activity, higher thermostability, or increased selectivity.

In addition, several studies have adopted a combinatory approach, integrating traditional methods such as structure-based rational design and directed evolution with ML techniques. This hybrid approach has proven to be a powerful tool for achieving fast and effective improvements in enzyme structure, further enhancing the potential for scalable and efficient enzymatic recycling.[106,108,111–120]

Lu et al.[108] utilized the 3D self-supervised CNN "MutCompute" [121] to systematically enhance the stability and activity of PET-hydrolyzing enzymes (**Figure 13**).

Trained on a large dataset of protein structures from the Protein Data Bank (PDB),[122] MutCompute evaluated local chemical microenvironments to predict stabilizing amino acid substitutions in wild-type PETase and ThermoPETase. Through an in silico mutagenesis scan, the model identified key mutations that significantly improved enzyme performance. In wild-type PETase variants, the most effective mutation exhibited a 29-fold increase in PET-hydrolytic activity at 40°C compared to the unmodified enzyme. Similarly, in the ThermoPETase scaffold, the most promising variant achieved a 38-fold increase in activity at 50°C, while also demonstrating an expanded temperature range of functionality. These enhancements underscore the potential of ML-driven approaches to optimize enzyme stability and catalytic efficiency. Figure 13 illustrates the ML approach and highlights the key findings of this study.

In another study by Ciu et al.[116] a transformer-based protein language model in combination with energy-based computational tools was used to identify amino acid residues that were non-beneficial for substrate binding in PET degrading enzymes. The transformer model was chosen based on its increased efficiency and its ability to capture long-range interactions. Unlike conventional ANNs that require manual feature engineering or predefined rules, transformer models are able to learn patterns autonomously from large datasets. This helps prevent bias of the model. Further, the self-attention mechanism of transformer models is ideal in the use of enzyme engineering as the catalytic efficiency of enzymes often depends on residues that are far apart in the linear protein sequence, but close in the folded structure. Transformers enable the model to consider dependencies between such distant residues. This approach led to the discovery of a novel enzyme variant, TurboPETase, which exhibited significantly improved PET depolymerization activity.

6.2. Interaction, Process Parameter and Degradation Rate Predictions

While the previously mentioned studies utilized ML to enhance enzyme activity and stability, other research groups have focused on predicting diverse enzyme and process properties. ML models have been employed to estimate key parameters for enzymatic activity, such as turnover number and the Michaelis constant, as well as properties like selectivity, thermostability, and solubility. Various ML approaches have been applied in this field, including GNN and CNN, language models, SVM, and decision trees.[123–129] The prediction approach can be advantageous to an experimental determination of these properties in terms of time, data availability and data quality. As an example, experimentally determined turnover numbers are often noisy and data availability is limited. ML approaches are thus helpful for high-throughput property prediction and thus efficient than conventional lab trials.[123,125] Further efforts have been made to predict optimal process parameters for respective enzyme variants, such as pH or temperature. Prediction and thus identification of suitable and optimal process conditions is crucial in realizing catalytic activity of the enzyme and exploiting its maximum efficiency. For this, ML approaches comprising multiple different regression and large language models as well as neural networks have been employed.[130–133] Lastly, prediction of enzyme-substrate interactions have been carried out via ML models.[134,135]

A recent study by Jiang et al.[129] presents a novel ML-based framework for predicting an enzyme's ability to degrade specific plastics by analyzing protein sequences. Thereby, the Plastic Enzymatic Degradation (PED) framework is developed, which leverages ML models to recognize sequence-function relationships in enzymes. An overview of this PED is shown in **Figure 14**.

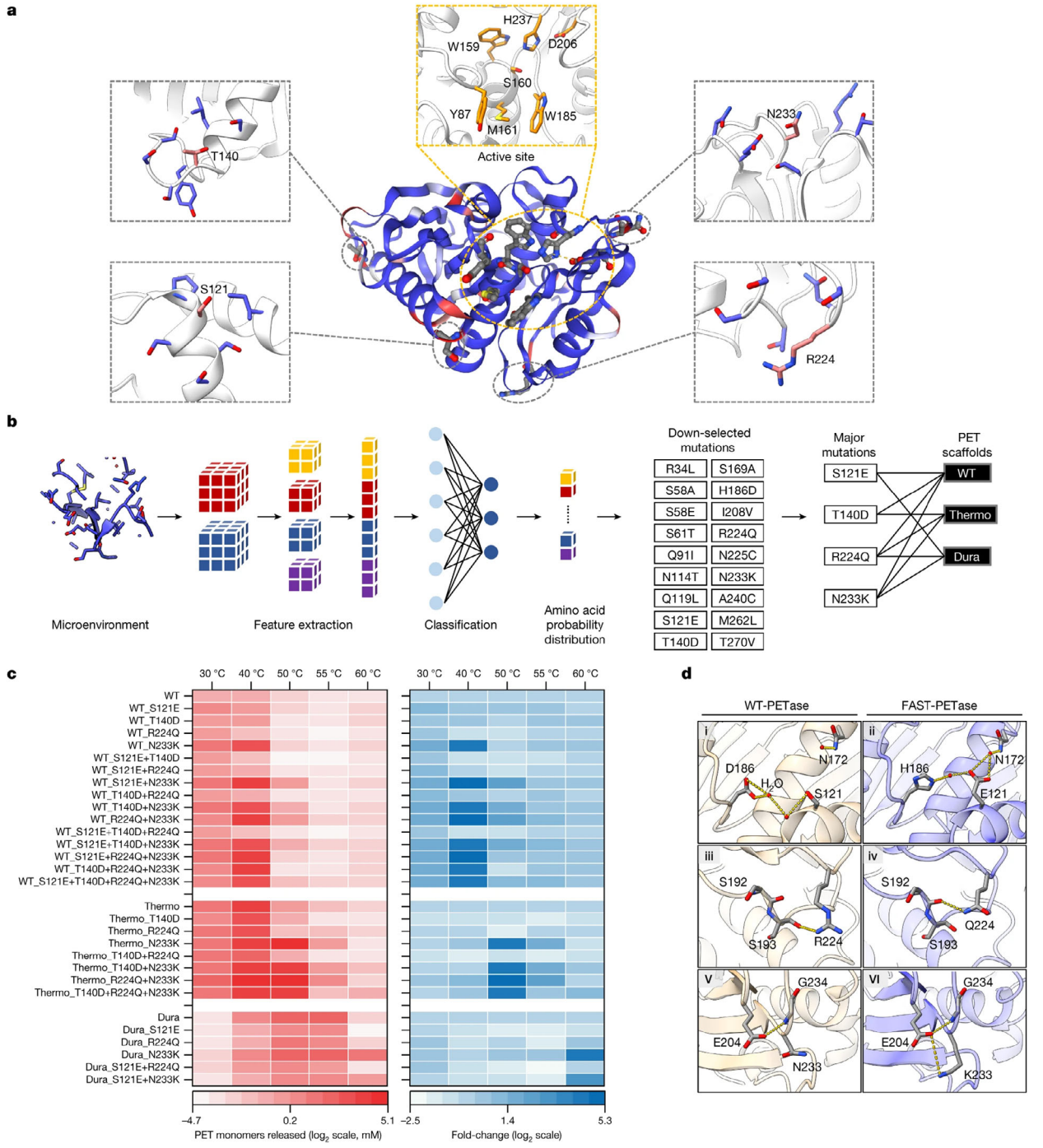

Figure 13. Overview of the key findings: a) Structure of wild-type PETase rendered by MutCompute b) ML workflow for the prediction of promising mutations based on the microenvironment of the base enzymes c) PET-hydrolytic activity (red) and fold change of activity (blue) of original enzymes and their mutations at various temperatures d) Structural comparison of wild-type PETase and the promising variant FAST-PETase. Reproduced with permission from ref. [108] (2022, Springer Nature).

A context-aware enzyme sequence representation (CESR) approach was introduced, enabling the extraction of both local amino acid-level and global sequence-level features. This method significantly improves the prediction of enzyme-substrate interactions, facilitating the identification of promising plastic-degrading enzymes. To build a reliable predictive model, the authors compiled a comprehensive dataset of experimentally validated enzyme-substrate pairs and tested various ML algorithms. Among the thirteen models evaluated, XGBoost demonstrated the highest accuracy (90.2%), outperforming other approaches such as RF, SVM and deep neural networks. The study also identified key sequence motifs and functional regions crucial for

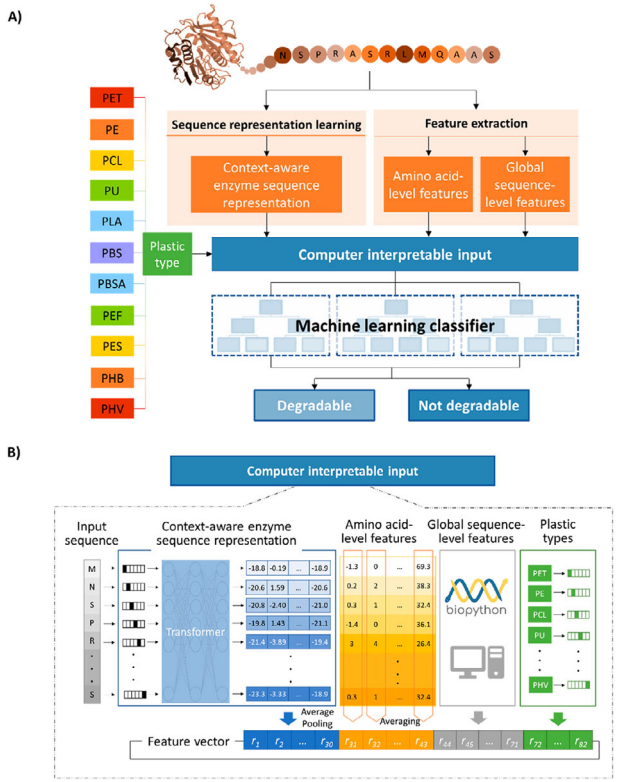

Figure 14. Overview of the plastic enzymatic degradation framework: A) Key components, input and output parameter. B) Computer interpretable input constructed by the feature vector. Reproduced with permission from ref. [129] (2023, ACS Publications).

enzymatic degradation, providing insights into enzyme engineering for improved degradation efficiency.

In another study, Zaretckii et al.[132] employed a transformer-based large language model (LLM), OphPred, to analyze protein sequences and predict their optimal pH levels. Since enzymatic activity is highly dependent on pH, optimizing this parameter is crucial for maximizing enzyme efficiency. The ability of LLMs to autonomously detect patterns, even across long-range dependencies, enabled OphPred to outperform traditional methods in predicting optimal pH levels. To ensure the robustness of the model, the study employed multiple dataset-splitting strategies, including homology-based, random, enzyme commission-based, and PFAM-based splitting.[136] Notably, the model demonstrated high predictive accuracy even for proteins with low sequence similarity to the training data, highlighting the effectiveness of LLM-based approaches in protein function prediction.

6.3. Process Optimization

While there are no known publications on ML-aided process optimization specifically for enzymatic plastic degradation, related fields have seen significant advancements. Researchers have employed ML techniques to optimize reaction parameters such as temperature, reaction time, and substrate and enzyme concentrations. Notably, Bayesian Optimization (BO) algorithms have been utilized to enhance these processes. When employing BO, process optimization can be reached in only a few trials. This makes BO ideally suitable when experimental determination of the target property is time consuming, costly or when limited resources are present.[137–139]

Tachibana et al.[137] utilized a customized Bayesian Optimization Algorithm (BOA) to efficiently optimize continuous reaction parameters–specifically temperature, reaction time, and the concentration of reactants and enzymes–in enzyme-catalyzed reactions, aiming to maximize catalytic performance under limited time and resources. **Figure 15** illustrates the modifications made to the standard BOA to create two customized versions. The original BOA, as depicted in Figure 15, tends to prioritize exploiting conditions within the existing data to achieve high performance metrics, potentially neglecting unexplored regions of the experimental space. To address this, BOA-1 was modified to exclude measurement point suggestions close to existing data, promoting better exploration of these untested areas. BOA-2 further customized the acquisition function to prioritize regions significantly distant from existing data points. This strategy aimed to achieve a more comprehensive exploration of the entire experimental range and accelerate the identification of global optimum conditions. Comparative analysis of these customized BOAs against a standard BOA and a traditional Design of Experiments (DoE) approach demonstrated significant improvements. In two biocatalytic reactions–C–C bond formation and amination–the customized BOAs achieved up to an 80% increase in turnover number compared to DoE and a remarkable 360% increase compared to the standard BOA.

In summary, ML is revolutionizing biological recycling by enhancing enzyme discovery, design, and process efficiency. ML models, including neural networks, decision trees, and Bayesian optimization, accelerate enzyme engineering by predicting substrate interactions, degradation rates, and key process parameters. These approaches improve enzyme stability, catalytic efficiency, and substrate specificity, leading to the development of more effective plastic-degrading enzymes. ML also aids in optimizing reaction conditions, such as temperature and pH, refining enzymatic recycling processes. Additionally, ML-driven process optimization enhances reaction efficiency and scalability, streamlining screening efforts. By integrating ML techniques, enzymatic recycling can become a more viable and scalable solution for plastic waste management, offering a sustainable and efficient approach to polymer degradation.

7. Feature Engineering Strategies

ML applications in polymer recycling rely heavily on effective feature engineering to transform raw data into meaningful inputs that capture the essential characteristics of polymers and recycling processes. This section discusses key feature engineering strategies employed across the mechanical, chemical, and biological recycling domains discussed in the reviewed literature.

7.1. Spectroscopic Data Preprocessing

Spectroscopic data preprocessing is critical for sorting applications where infrared, Raman, fluorescence, or LIBS spectra serve

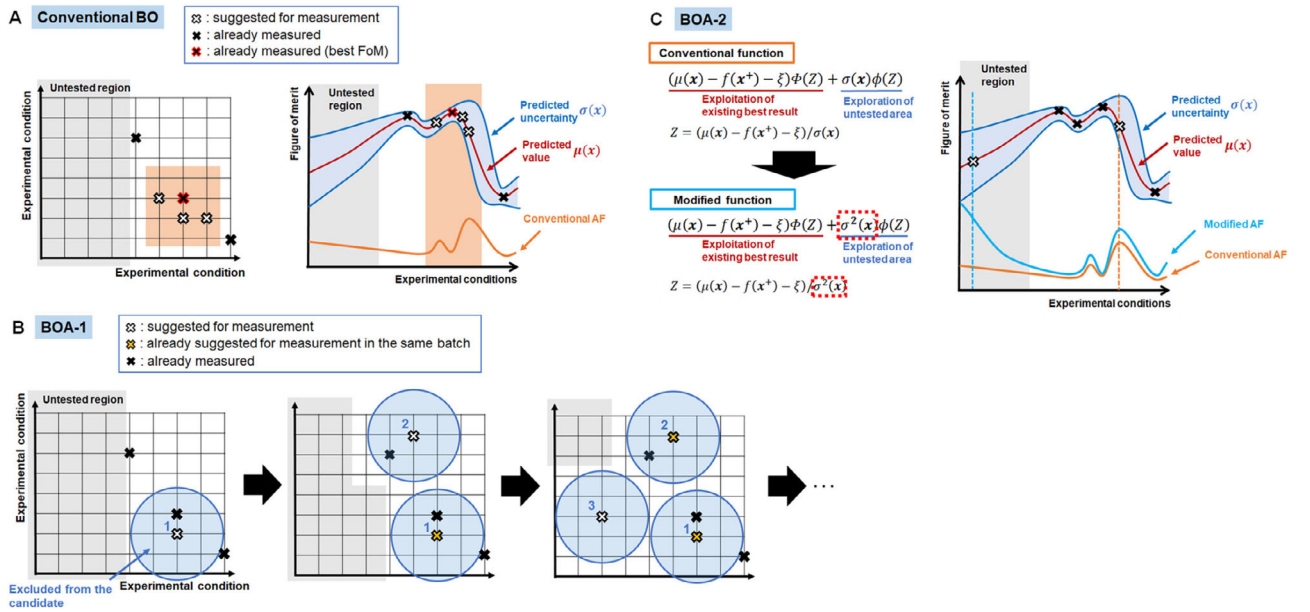

Figure 15. Overview of the modification of the BOA and acquisition function in customized BOA-1 and BOA-2 compared to a conventional BOA. Reproduced with permission from ref. [137] (2023, ACS Publications).

as primary inputs for polymer identification. As demonstrated by Sutliff et al.,[30] effective preprocessing can significantly enhance classification accuracy. Common preprocessing techniques include:

- *Scattering corrections*: Preprocessing methods such as robust normal variate help eliminate noise and baseline variations in NIR spectra, improving signal quality for polymer classification.
- *Normalization*: Normalizing spectral intensity ranges makes spectra from different samples comparable.
- *Dimensionality reduction*: PCA, as used by Gajarska et al.[32] in LIBS spectroscopy, reduces high-dimensional spectral data to lower-dimensional representations while preserving essential information (variance).
- *Spectral descriptors*: These targeted features extract chemically relevant information from complex spectra, focusing models on the most discriminative aspects of the data.

The choice of preprocessing pipeline significantly impacts model performance, as evidenced by Sutliff et al.'s[30] systematic evaluation of over 12 000 ML pipelines for polyolefin classification.

7.2. Process Parameter Representation

Recycling processes involve multiple interrelated parameters that must be appropriately represented for ML models. Key feature engineering approaches include:

- *Parameter normalization*: Standardizing process parameters with different units and scales (temperature, pressure, flow rate) enables fair contribution to model predictions, as seen in Castéran et al.'s[33] work on predicting polymer degradation during extrusion.
- *Temporal feature extraction*: For time-dependent processes like pyrolysis or gasification, features derived from time-series data (rates of change, cumulative yields) provide valuable process insights, as demonstrated in studies by Ma et al.[37] and Cheng et al.[91]
- *Interaction terms*: Capturing non-linear relationships between process parameters through multiplicative or polynomial terms, as used by Hasanzadeh and Azdast[97] in their polynomial regression models for gasification.

7.3. Polymer Property Representation

Effectively representing polymer properties requires domain-specific feature engineering strategies:

- *Molecular descriptors*: Numerical representations of polymer molecular structure, including molecular weight distributions, branching indices, and functional group prevalence, as utilized by Teruel et al.[34] in recycled PP property prediction.
- *Rheological parameters*: Features derived from viscosity measurements and flow behaviors provide insights into polymer processability and degradation, as shown by Castéran et al.[33]
- *Thermal properties*: Features extracted from DSC (Differential Scanning Calorimetry) or TGA (Thermogravimetric Analysis) data, capturing crystallization behavior, melting points, and thermal stability.

7.4. Biological Sequence Representation

For biological recycling applications, representing enzyme sequences requires specialized approaches:

- *Sequence embeddings*: Transforming amino acid sequences into numerical vectors that capture evolutionary relationships and functional properties, as implemented by Lu et al.[108] and Cui et al.[116] for PET-degrading enzymes.
- *Structure-based features*: Extracting features from 3D protein structures, including binding pocket geometry, surface properties, and electrostatic potentials.
- *Context-aware representations*: As demonstrated by Jiang et al.,[129] integrating both local amino acid-level and global sequence-level features improves prediction of enzyme-substrate interactions.

The Context-aware Enzyme Sequence Representation (CESR) approach developed by Jiang et al.[129] is particularly noteworthy for capturing the complex relationships between enzyme sequence features and plastic degradation capabilities.

7.5. Feature Selection and Importance Analysis

Across recycling domains, feature selection and importance analysis help identify the most relevant variables:

- *Mutual Information*: Used by Ahmad et al.[93] to identify reactor temperature as the most influential factor in LDPE pyrolysis, enabling targeted process optimization.
- *Tree-based importance metrics*: Studies like Qi et al.[98] and Cheng et al.[91] utilized feature importance from tree-based models to understand key factors in gasification and pyrolysis processes.
- *SHAP (SHapley Additive exPlanations)*: Provides interpretable feature importance values that clarify how specific variables contribute to model predictions, enhancing process understanding.

The PCA investigation performed by Qi et al.[98] (Figure 12) exemplifies how dimensionality reduction techniques can identify key relationships in complex datasets while preserving most of the original information.

7.6. Transfer Learning Approaches

Transfer learning represents an advanced feature engineering strategy where knowledge is transferred between related tasks:

- *Domain adaptation*: As demonstrated by Chen and Huang,[35] models trained on virgin materials can be adapted to recycled materials, reducing data requirements and improving prediction accuracy.
- *Pre-trained embeddings*: Transformer-based models pre-trained on large protein databases provide rich feature representations for enzyme engineering tasks, as shown by Zaretckii et al.[132] and Cui et al.[116]

The success of transfer learning approaches in recycling applications highlights the value of leveraging knowledge across related domains, particularly when dealing with limited datasets for specific recycling processes.

In conclusion, effective feature engineering is fundamental to the successful application of ML in polymer recycling. The strategies outlined above transform raw process data, spectroscopic measurements, polymer properties, and biological sequences into meaningful features that enable accurate predictions and process optimizations. These approaches address the unique challenges of each recycling domain while maximizing the value extracted from available data.

8. Perspectives and Trends

The accuracy of ML models is increasingly enhanced by integrating theoretical insights from simulations, quantum chemical calculations, and physical equations into datasets. Recent advancements in the speed and accuracy of these theoretical models, often accelerated by ML itself, position them as critical components in developing high-performance recycling technologies. Besides this clear trend towards physics-informed ML, perspectives and trends are shown for different topics, as well as challenges and future directions.

8.1. Technological Integration and Market Competitiveness

While ML has improved efficiency in specific recycling processes, such as NIR-based sorting, many equipment types, including extruders, injection molding machines, and their attachments, have yet to fully benefit. Integrating pre-trained ML models into the operational systems of these devices is crucial for advancing recycling technology. Companies adopting this strategy are likely to gain a competitive advantage in the recycling equipment market.

8.2. Holistic Data-Driven Approach

Leveraging comprehensive data from individual recycling stages to train deep learning models can provide a holistic and precise understanding of the recycling process. This approach promises significant savings in material, energy, and time, thereby enhancing overall efficiency. The data required includes, among others 1) processing parameters, ii) inline and offline measurements, and iii) final product quality metrics.

Although training and optimizing these models is relatively straightforward, the online acquisition, time synchronization, and storage of data from diverse equipment remain significant challenges for plastic recycling companies. However, substantial progress is being made in this area.

8.3. Talent and Digital Transformation

The shortage of ML scientists with expertise in recycling or polymer engineering may drive companies to adopt offline large language models for ML and data science tasks, as well as to invest in training existing employees in digital domains. This talent gap is also fostering the growth of digital companies that offer user-friendly ML and data science solutions, which will ultimately contribute to the advancement of recycling technologies.

8.4. Challenges and Future Directions

Data Limitations. Most current studies rely on relatively small datasets, which limits the generalizability of ML models. Future research should focus on:

- Developing larger, more comprehensive datasets across different recycling technologies through multiple complementary approaches: (1) implementing general inline characterization systems for continuous data collection during industrial operations, (2) leveraging advanced simulation techniques to generate synthetic training data that captures process variability, and (3) integrating physics-informed ML approaches that incorporate fundamental recycling principles to reduce data requirements while improving model robustness. Each of these strategies represents a significant research challenge in its own right, requiring interdisciplinary collaboration between materials scientists, process engineers, and data scientists to establish scalable data generation frameworks that can adequately represent the complexity of industrial recycling environments.
- Creating standardized data collection and reporting protocols
- Encouraging open-source data sharing in the recycling research community

Interdisciplinary Collaboration. Effective plastic recycling requires collaboration between materials scientists, computer scientists, chemists, and engineers. ML serves as a powerful interdisciplinary tool to bridge these domains.

Sustainability Considerations. Although ML offers promising solutions, researchers must continuously evaluate the environmental and economic sustainability of proposed recycling techniques.

Chemical recycling. While mechanical recycling dominates current practices, the application of ML to chemical recycling, particularly depolymerization and solvolysis, remains significantly underexplored. This represents a critical research gap, hindering the full realization of chemical recycling's potential for sustainable thermoplastics management.

Transferability. Additionally, the transferability of results to other polymer classes is only partially feasible, as the recycling technologies employed may differ slightly. In the case of vitrimers, common recycling approaches include mechanical grinding followed by reshaping at elevated temperatures, or chemical recycling using suitable solvents. While these technologies are generally similar, the inherent differences between polymer types limit the direct applicability of results across systems. Nevertheless, the application of machine learning to enhance recycling processes is broadly relevant and can be applied across various recycling strategies.[140]

Despite the promising applications of ML in thermoplastic recycling shown in this review, several fundamental limitations must be still acknowledged, besides the challenges already discussed above, when translating research findings to industrial contexts. *Dataset biases* represent a significant concern, as many ML models are trained on laboratory-generated data that may not adequately represent the heterogeneity of real-world plastic waste streams, which vary considerably in contamination levels, polymer blends, and degradation states across different geographic regions and collection systems. *Generalizability* issues emerge when models trained on specific plastic types, processing conditions, or equipment configurations fail to perform effectively across diverse industrial settings, particularly given the substantial differences between controlled laboratory environments and the dynamic, multi-variable nature of industrial recycling facilities. *Overfitting* remains a persistent challenge, especially when working with limited datasets common in recycling research, where models may perform exceptionally well on training data but demonstrate poor predictive capability when confronted with novel plastic compositions or processing scenarios not represented in the original dataset. These limitations underscore the critical need for more comprehensive, industry-representative datasets and robust validation protocols that better simulate real-world variability before ML approaches can be reliably implemented at industrial scales in thermoplastic recycling operations.

9. Conclusion

ML has demonstrated significant potential across all stages of thermoplastics recycling, from sorting and processing to quality control. By enabling more precise material identification, predicting process parameters, and optimizing complex recycling workflows, ML technologies are emerging as critical tools in addressing global plastic waste challenges. The material waste stream, the differing nature of the processes,[141] and the variety of materials involved result in a very complex overall process, which is why a generalized comparison of the different recycling strategies is not meaningful. The main points observed in the reviewed literature are subdivided below into the three main areas.

Mechanical Recycling. ML algorithms have revolutionized sorting processes, achieving over 95% accuracy in identifying and separating different plastic types using various spectroscopic techniques. Advanced image recognition and spectral analysis techniques can now distinguish complex material streams, including challenging cases like black plastics. ML helps optimize energy efficiency and product quality during processes like shredding and regranulation.

Chemical Recycling. ML models have been successfully applied to pyrolysis, gasification, and other chemical recycling techniques. Researchers have used ML to predict product yields, optimize reaction conditions, and analyze complex transformation processes. Gradient Boosting and ensemble learning models have shown particularly promising results in predicting chemical recycling outcomes.

Biological Recycling. ML is transforming enzymatic plastic degradation through multiple innovations. ML algorithms (3D CNNs, GNNs, transformer models) have identified mutations yielding up to 38-fold increases in PET-hydrolytic activity with improved temperature stability. ML frameworks predict enzyme-substrate compatibility with exceptional accuracy (90.2% using XGBoost), enabling efficient identification of polymer-specific biocatalysts. Transformer-based language models accurately predict optimal parameters like pH across diverse protein sequences. For process optimization, customized Bayesian optimization outperforms traditional approaches by improving turnover numbers up to 80% while thoroughly exploring parameter spaces.

As highlighted in this review, ML is not just a technological enhancement but a transformative approach that could fundamentally reshape thermoplastics recycling. By providing unprecedented insights, predictive capabilities, and optimization strategies, ML technologies are helping to address one of the most pressing environmental challenges of our time. It is important to emphasize that ML is not intended to replace recycling techniques, but rather to enhance them. Recycling can only be carried out through physical experiments; ML serves as a complementary tool to optimize and guide these processes more efficiently.

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Conflict of Interest

The authors declare no conflict of interest.

Author Contributions

R.Q.A., F.S., A.P., C.B., and K.K. contributed to the writing of the original draft, participated in discussions, and made corrections. H.R. was involved in paper correction and discussion.

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biological recycling, chemical recycling, machine learning, mechanical recycling, thermoplastics

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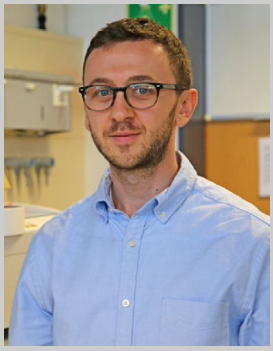
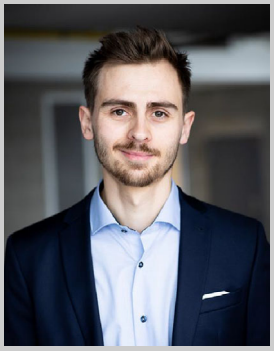
Rodrigo Q. Albuquerque has done his PhD in Theoretical Chemistry in Brazil and has worked as a researcher in Switzerland, Germany and England, where he investigated different materials (e.g. supramolecular polymers, nanoparticles, coordination compounds) by means of computational chemistry and molecular dynamics. After being guest lecturer at Technical University of Munich to teach and apply ML techniques, he became Senior Expert Digitalization at the Department of Polymer Engineering in Bayreuth, where he applies ML models to different problems and provides hands-on training on the same topic.



Florian Stephan M.Sc. has been working as a research assistant at the Chair of Polymeric Materials since November 2023. In the Functional Thermoplastics and Manufacturing working group, he is working on the development of PET recycling strategies using machine learning models. From 2017 to 2021, Florian Stephan studied mechanical engineering (B.Eng.) at Rosenheim University of Applied Sciences and wrote his bachelor's thesis on the design of a project planning tool for designing drive axles. With the subsequent Master's degree in Sports Technology (M.Sc.) at the University of Bayreuth, he deepened his knowledge in the field of additive manufacturing and completed his studies with a Master's thesis on the vibration characteristics of additively manufactured lightweight structures.

Annalena Pongratz, M.Sc. is a research associate at the Chair of Polymer Engineering at the University of Bayreuth, where she has been part of the Functional Thermoplastics and Manufacturing group since February 2023. Her current research focuses on the enzymatic degradation mechanisms of semi-aromatic polyesters, with a particular emphasis on the material properties that influence biodegradation and the associated degradation pathways. She earned her Bachelor of Science in Polymer and Colloid Chemistry in 2020 and subsequently completed a Master of Science in Polymer Science at the University of Bayreuth. During her studies, she developed a strong foundation in the synthesis, processing, and characterization of polymeric materials. Her master's thesis focused on the development of biocompatible polymer foams for applications in medical technology.



Christian Brütting has been working at the Department of Polymer Engineering in the Group of Polymer Foams since June 2018. From October 2020 to December 2023, Christian Brütting functioned as Research Manager in the Group of Polymer Foams. Since January 2024 he has been operating as chief engineer at the Department. As part of his scientific work, he is investigating the processing behavior of Polylactide (PLA)-based particle foams. From 2012 to 2015, Christian Brütting studied mechanical engineering (B. Eng.) at the Baden-Württemberg Cooperative State University (DHBW) Mosbach. In his subsequent master's degree (M. Sc.) in "Materials Science and Engineering" at the University of Bayreuth, he focused on lightweight construction and polymer materials. He successfully completed his studies with a master's thesis on "Investigation of epoxy-based resins for a novel additive manufacturing process". He successfully completed his PhD study in June 2024.

Katharina Krause studied Environmental Engineering and obtained a PhD in Materials Science with a focus on polymer processing at the University of Bayreuth. She currently works as an expert in sustainability and circular economy at Neue Materialien Bayreuth GmbH. In this position, she applies her academic background and research experience to advance the development of sustainable material solutions——an endeavor that reflects both her professional expertise and personal commitment.

Holger Ruckdäschel has been head of the Chair of Polymer Materials at the Faculty of Engineering at the University of Bayreuth since January 1, 2021. After studying materials science, he earned his doctorate in 2009 at the Chair of Polymeric Materials under Prof. Altstädt in Bayreuth. After 13 years of industrial experience at BASF, he thus returned to his academic roots. At BASF, he was involved in a wide range of topics and most recently headed the digital strategy of the plastics division. His other positions include polymer research and senior global roles in wind energy research and plastics additives. In recent years, he also drove digital innovations and new business models for the plastics industry with his team.