

Artificial Intelligence in Advanced Polymer Manufacturing

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Abstract

Artificial intelligence (AI) is currently transforming the polymer lifecycle, from materials discovery and design to manufacturing and recycling processes. In this review, we will discuss the undergoing paradigm shift from conventional labor-intensive processes to machine learning and data driven automation, including the key machine learning models and techniques being applied across diverse polymer science application areas. Significant limitations and opportunities in AI-driven polymer manufacturing exist in data availability and model interpretability.

Keywords: AI, Polymer Manufacturing, Machine Learning, Additive Manufacturing, Sustainability.

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The global landscape of polymer manufacturing is currently undergoing a structural transformation, moving away from the empirical paradigm of Edisonian trial-and-error toward a data-driven framework known as polymer informatics.¹⁻³ This shift is necessitated by the inherent complexity of polymeric materials, which are defined by a stochastic and hierarchical architecture that spans from the molecular and nanostructure, self assembly, processing, to the macroscopic bulk property.^{4,5} As the demand for high-performance, sustainable, and functional polymers accelerates in sectors such as aerospace, automotive, energy storage, and biomedical engineering, the traditional and slow development cycle in polymer research and manufacturing has become an unsustainable bottleneck. Artificial intelligence (AI) and machine learning (ML), integrated with automated hardware and the Internet of Things (IoT), offer the primary mechanism to speed up such timelines, facilitating the rapid discovery of novel chemistries and optimizing advanced manufacturing processes.^{1,2,6,7}

Machine Learning (ML) with algorithm development and data training enables computers to adaptively learn from data and perform simulation and decision-making tasks while optimizing the process.^{4,6,8} ML can be categorized into Supervised Learning, and Unsupervised Learning, based on whether or not the data need to be labeled during the learning process.^{2,4,8,9} Focusing on decision-making via environmental feedback, Reinforcement Learning (RL) constitutes another major paradigm beyond these 2 categories, while Deep Learning (DL) is a specialized subfield within ML, utilizing Deep Neural Networks (DNNs) to perform both supervised and unsupervised tasks with high levels of abstraction.¹⁰⁻¹⁷ Eventually, supervised learning, deep learning, and reinforcement learning will encompass many fields in polymer research and advanced manufacturing. Figure 1 offers a timeline for AI and its subareas, and a classification with examples in polymer fields. Table 1 compares a number of common AI algorithms, highlighting their strengths, weaknesses, and evaluation metrics.

1. The Paradigm Shift in Polymers and Manufacturing

At the core of AI-driven polymer manufacturing is the field of polymer informatics, an interdisciplinary domain that leverages data science to establish quantitative relationships between chemical structures and macroscopic performance.^{4,8,18} Unlike small molecules, which can be easily represented using standard chemical descriptors, polymers present unique challenges due to their distribution of chain lengths (dispersity), branching patterns, and stereochemistry. The development of machine-readable descriptors that can accurately capture this stochastic nature is a critical area of ongoing research.^{4,19}

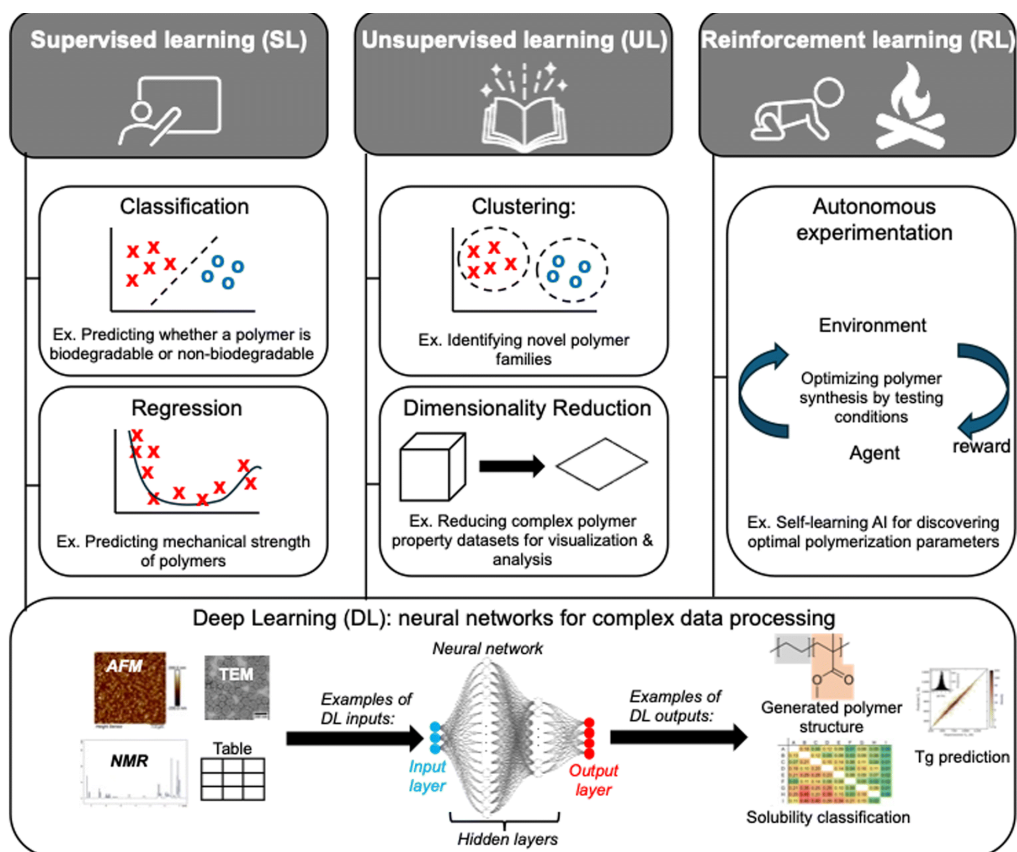
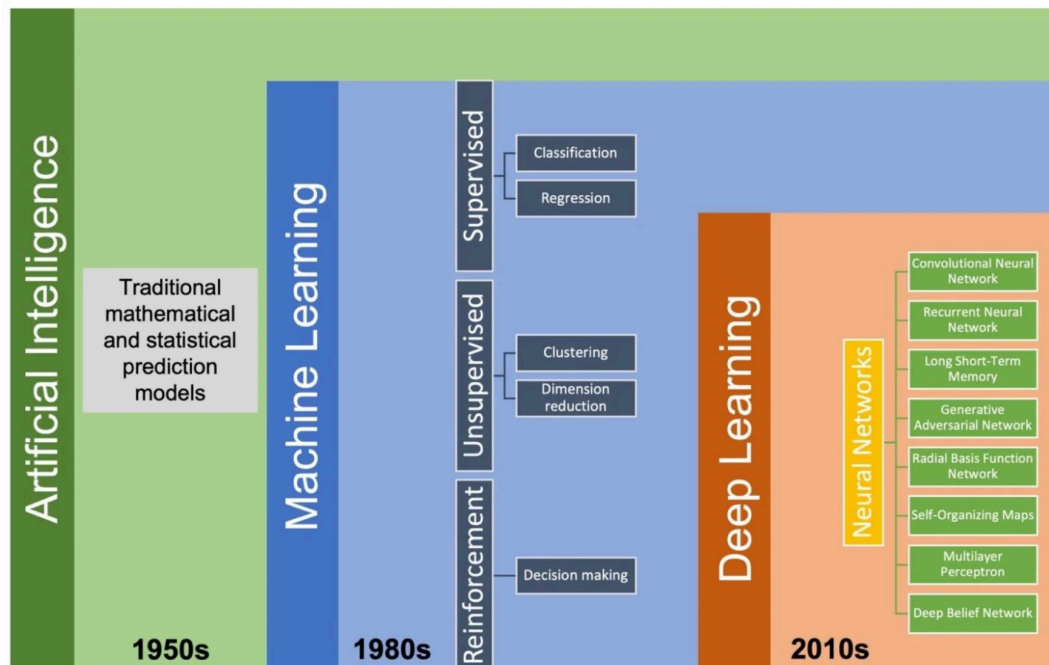


Figure 1. Top: The development timeline for AI and its subfields. (Figure and Caption from reference,²⁰ without change, under Creative Commons 4.0 license.²¹) Bottom: Overview of main machine learning methods and their applications in polymer science. Deep learning (DL) can be applied across all three categories (supervised, unsupervised, and

reinforcement learning) to analyze complex polymer data, predict properties, and optimize synthesis. Examples of experimental data sources used in ML driven polymer research include Atomic Force Microscopy (AFM), Transmission Electron Microscopy (TEM), and Nuclear Magnetic Resonance (NMR) spectroscopy. (Figure and Caption from reference,²² with change, under Creative Commons BY-NC 3.0 license.²³)

Theoretical Frameworks for Polymer Descriptors

To enable machine learning to process polymer data, the chemical, structural, or other information need to be translated into numerical vectors, which can involve proper identification of input features that can represent the monomeric units, the polymerization degree, the backbone or branch structures, and so on.^{24,25} Recent advances have seen the application of multitasking deep neural networks (DNNs) that can predict multiple properties—such as glass transition temperature (T_g), tensile strength, and gas permeability—simultaneously by learning shared representations across large datasets.^{4,26} The data scarcity remains as a significant hurdle, as the polymer research and manufacturing often operates with limited and to-be-better-curated datasets.^{19,26} One way to mitigate this challenge is to adopt transfer learning and data fusion techniques, which allow models trained on large, general material datasets to be fine-tuned on smaller datasets with improved accuracy for specialized applications.¹⁹

Physics- and Chemistry-Aware Modeling

The evolution of AI in science including polymer informatics also involved a shift from "black-box" models to physics- and chemistry- informed machine learning.^{2,27,28} By integrating fundamental physical laws and chemical theories into the machine learning and neural network

architectures, researchers can ensure that AI predictions remain within the boundaries of scientific reality. This is particularly relevant for predicting complex behaviors such as degradation pathways in biodegradable materials or multi-property trade-offs in energy storage materials.^{26,29} The integration of scientific domain knowledge, such as the Flory-Huggins solution theory or molecular dynamics simulations, allows algorithms to generalize better, even from smaller datasets.^{4,19}

Table 1. Comparing different AI Algorithms. Adapted from references.^{2,4,18,20,29}

Task	Examples	Advantages	Disadvantages	Evaluation Metrics
Regression	Linear, Lasso, Ridge regression, ANN	Easy implementation, handles high dimensions, fault tolerance	Overfitting, linearity assumptions, hardware demands	R ² , MSE, RMSE, MAE
Classification	K-Nearest Neighbors, Support Vector Machines, Random Forest, Naïve Bayes	Handles imbalance/outliers, fast predictions, scalable	Sensitive to noise/outliers, black-box, hyperparameter tuning	Accuracy, Precision/Recall, F1-score, Sensitivity/Specificity, ROC, Cohen's Kappa
Clustering	K-means, DBSCAN, Mean shift	Fast, robust to outliers, handles arbitrary shapes	Requires predefined clusters, poor in high dimensions	Typically internal metrics like silhouette score
Deep Learning / Image Analysis	ANN, CNN, RNN	High accuracy, feature detection, sequential modeling	High compute/data needs, vanishing gradients, poor explainability	Average Precision, Mean Average Precision, Pixel Accuracy, Dice Coefficient, Intersection-Over-Union (esp. for CNN)

2. AI Aided Additive Manufacturing and Self-Driving

Laboratories

AI in Additive Manufacturing

Additive manufacturing (AM), or commonly known as 3D printing (3DP) is an essential tool for innovation in many industries and R&D projects.^{18,30-32} The opportunities for academic

research, especially in the discovery of new polymer materials with optimized properties, may start at lower technical readiness levels (TRLs) but can easily achieve the right form-function factor with 3DP. The capability of 3D printing to fabricate complex objects quickly and cost-effectively makes it highly desirable compared to conventional manufacturing processes.³³ The use of stimuli-responsive materials adds a new dimension to functionality, with the appropriate field-effect giving it a new term called 4D printing.³⁴ For thermoplastics, thermosets, and elastomers, it is necessary to select the proper 3D printing method to address materials-processing challenges and meet the desired properties. Therefore, composites have been the materials of choice for achieving superior properties with nanocomposites, with a high strength-to-weight ratio.

Recent years have seen a rapid increase in research using 3D printing for applications like biomedical implants, membrane separation, sensors, aerospace and automotive applications, potentially revolutionizing these fields.³³ The emergence of new 3D printers with higher resolution, greater efficiency, faster speeds, and broader material applicability has garnered more interest and could potentially reshape research and development in many fields. AI/ML has also been applied for correlating 3D printing and art restoration. Statistics is foundational in the optimization process of 3D Printing which is key to the use of ML methods and algorithm development.³⁵

Artificial Intelligence (AI) and machine learning (ML) approaches are increasingly applied to various materials and fabrication methods to innovate designs with enhanced efficiencies and productivity, with much progress in polymer materials and discovery chemistry facilitated by AI/ML.^{2,9,18,36-39} Using AI/ML workflows can be a path forward for optimization of the materials, 3D printing methods, and characterization, including new methods for correlation. Large Language Models (LLMs) and algorithms, including simulation, can further augment this

field. Furthermore, the development of Self-Driving Labs (SDL) and AI/ML Workflows can be the norm. The end goal should be faster and better relationships among structure, composition, processing, and properties (SCPP). The goal is to equip computers and machines with human-like intelligence, or remove the human-in-the-loop. Figure 2 provides a classification of ML-driven manufacturing applications, along with an example architecture of artificial neural network (ANN) for predicting the dimensional changes in 3D-printed cylinders from features such as slice thickness, deposition angle and direction, bead width, raster-to-raster air gap, as well as shell number.⁴⁰

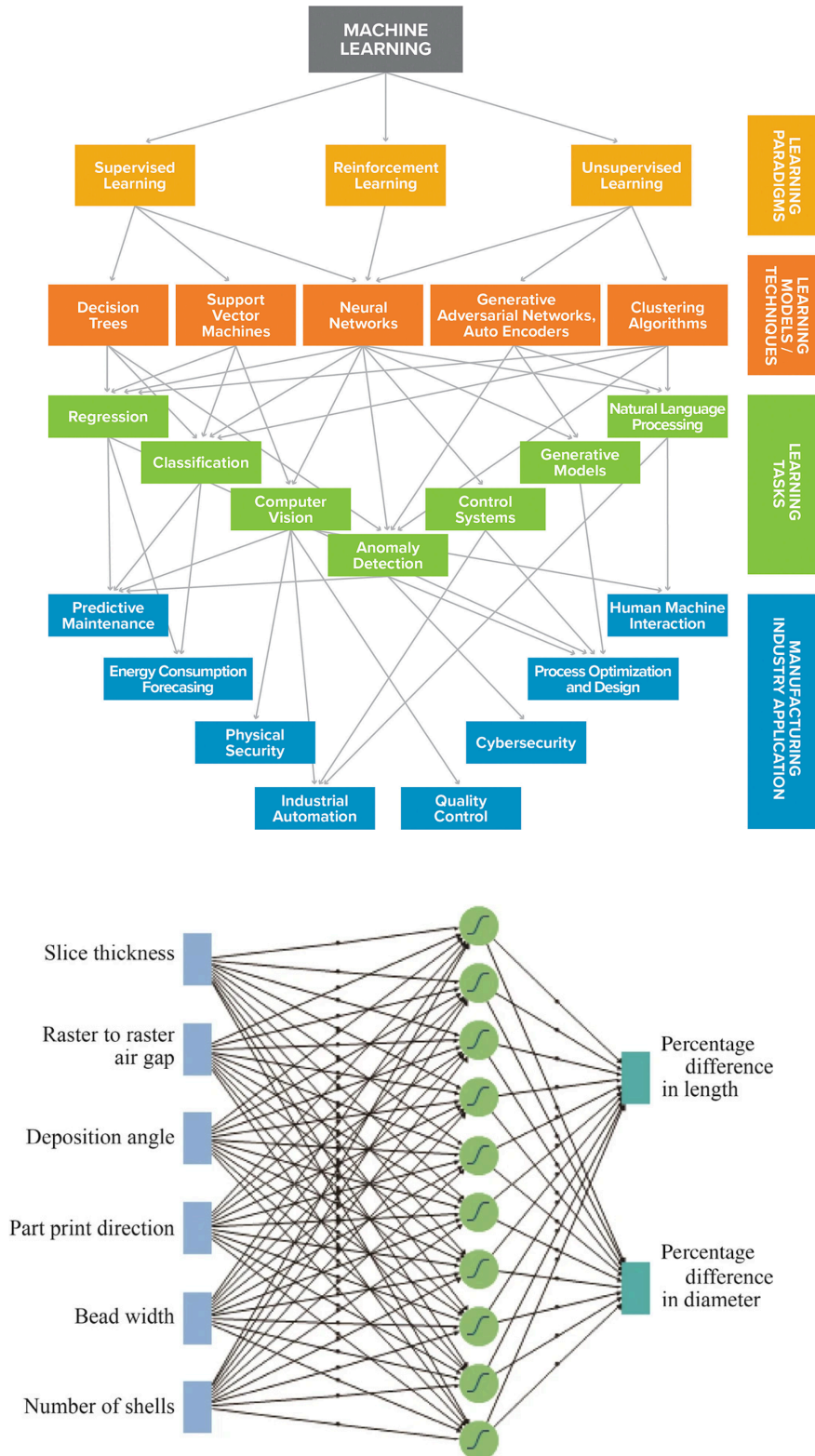


Figure 2. Top: Common categories for various aspects of machine learning, grouped into paradigms, techniques, tasks, and relevant manufacturing industry applications. (Figure and

Caption from reference,³ without change, under CC-BY 4.0 License.²¹) ; Bottom: Schematic example of the ANN (The image and caption are used without changes from the reference⁴⁰, under Creative Commons 4.0 License²¹).

AI/ML has vast potential to explore the large number of parameters in 3D printing polymers.^{18,38,39,41} Based on available databases, AI/ML can effectively optimize the materials synthesis and 3D printing process and automate the path to informed decision-making for optimization experiments, resulting in greater efficiency and faster product development. The benefits include, but are not limited to: 1) new high-performance materials, 2) enhanced recipe and process optimization on the method of choice, 3) efficient quality control, and 4) automated design and functionality development.

ML has been used to optimize the material and design of 3D printing.^{33,36,39} It is important to develop real-time methods for defect detection, which can be followed by a feedback loop mechanism for correction during 3D printing. This is to ensure the optimal process parameters that can be programmed or instructed on the printer itself.³⁰ Parameter optimization and in-situ monitoring will enable linking of process parameters and key elements such as melt pool characteristics, porosity, and mechanical properties.³⁹ The applications of AI/ML in the AM field also pose challenges related to the design of sensors, computational costs, eligibility criteria, and data collection techniques with the use of high-performance computing (HPC). Simulation and ML methods were demonstrated to augment the design and testing of sensor materials and composites.^{10,42,43}

Self Driving Labs

Significant advances in chemical and material synthesis are moving towards the use of the 'self-driving laboratory' (SDL).^{5,44} With an SDL, instead of human operators performing all

operations required for synthesizing, characterizing, and analyzing data, an alternative mode of operation is introduced wherein these steps are automated, and decision-making within the workflow is handled by machine learning-driven algorithms that suggest the next experimental parameter space for material and/or molecule optimization.⁴⁵ In an SDL operation, it is worth noting that the role of the human expert is not obsolete. Still, in some ways more important: their job is to determine the scientific questions to answer, constrain the regions of the parameter space, determine the suitable reaction protocols within which optimization can occur, and provide oversight on any automated analysis for membrane performance.

In a continuous-flow reactor synthesis, SDL operation involves reaction parameters such as temperature, residence time, or reagent equivalents.^{5,45,46} This has been demonstrated for copolymerization chemistries of a 3D printable material.⁴⁷ In a robotic system, if needed, liquid handlers (gantry robots) or switch valves allow the system to autonomously select different reagents, catalysts, additives, or reaction paths between each experiment. Precise control over field parameters, safety, efficiency, and scalability is essential for new 3D printing materials and methods.⁴⁸ For synthesis of new materials, the reagents are individually pumped through a mixing stage in a packed-bed or a plug flow column and subsequent reactor with an in-/online analytical module(s): high-pressure liquid chromatography (HPLC), infrared (IR), nuclear magnetic resonance (NMR), or ultraviolet (UV) directly monitoring the output. The feedback from the analytical module (e.g., yield) can then be returned to the AI agent, which selects conditions or set-point for the next experiment.

One of the core challenges in SDL development is facilitating information exchange among machines, AI, and human users in a universally understandable manner.^{45,47-49} Achieving this within the context of SDLs often requires a coordinator software to provide a (graphical) user interface (UI) for input from the human scientist, a hardware interface to translate experiment parameters into executable tasks, and an AI interface that translates the platform's data into an ML-optimized format. Implementation of a continuous feedback loop,

SDL set-up can accelerate membrane development.^{5,44} Expanding the large language model (LLM) suitable for AI/ML optimization is needed to categorize the media and solvent effects in process optimization.^{16,49} Demonstrations of flow chemistry and various optimization models will be set up, ranging from ML-driven algorithms to deep learning (DL) and more discovery-mode tasks. This task will support researchers in the analysis and interpretation of field data using real-time ML tools applicable at any stage of the optimization process and its sub-steps.

3.AI in Primary Polymer Manufacturing Processes

The impact of AI extends beyond the laboratory and into the heart of industrial production.³ Primary manufacturing processes, including injection molding, extrusion, and polymerization, are being revolutionized by real-time monitoring, predictive maintenance, and closed-loop process control.⁷

In plastic injection molding, AI is used to transform statistical process control into a fully automated inspection system.^{50,51} By leveraging pressure and temperature sensors embedded within the mold cavities, AI models can calculate critical product characteristics, such as dimensions and weight, for every single part produced in real-time.

A previous work on real-time intelligent modeling demonstrated that combining simulation models with fuzzy inferences allowed dynamic defect corrections during the molding.⁵¹ This minimizes material waste and energy consumption by optimizing injection speed, pressure, and cooling time for each specific cycle.⁵¹ Figure 3 depicts a system of using multilayer perceptrons to predict part quality from an injection molding system. Table 2 compares traditional and AI-driven quality control.

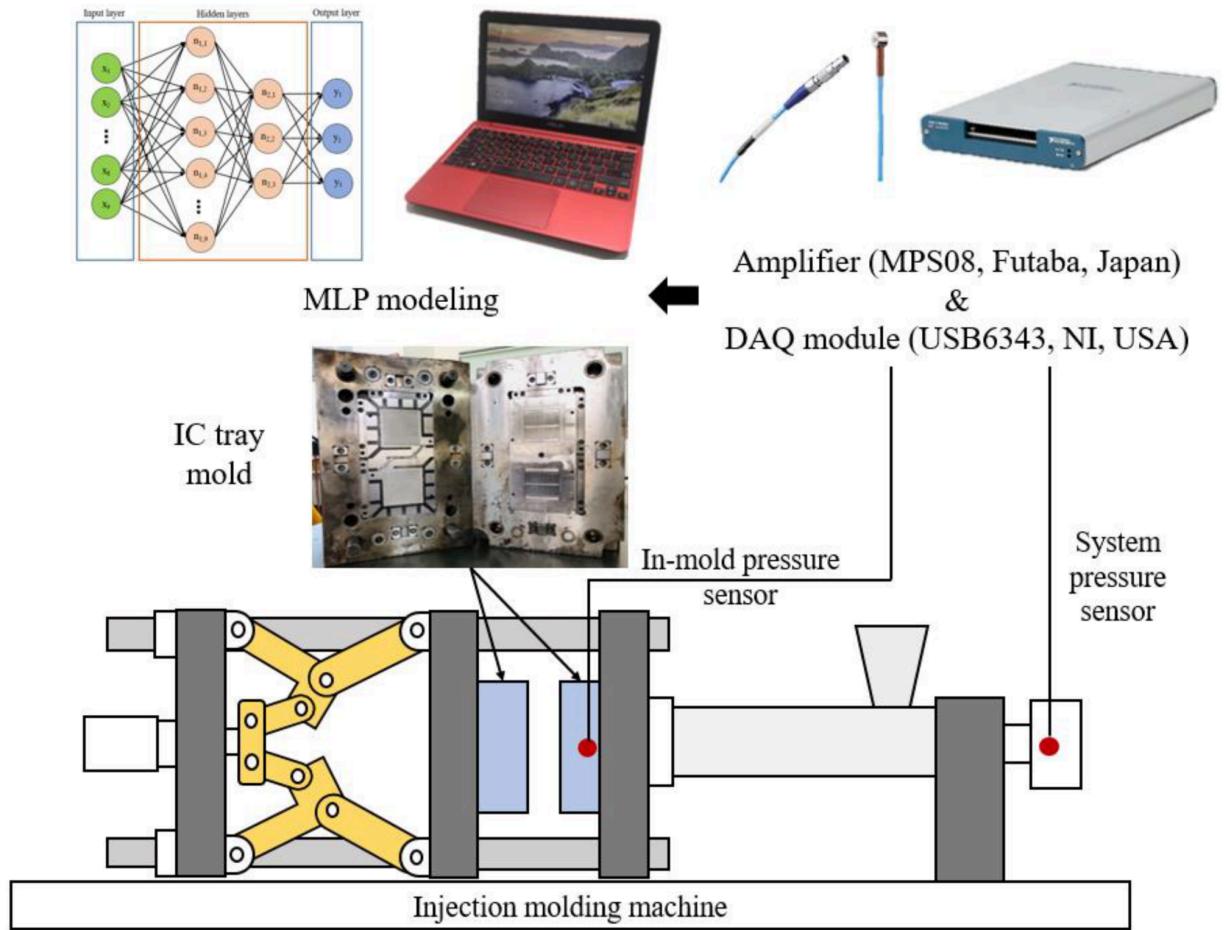


Figure 3. Schematic of the MLP inspection system. (Figure and Caption from reference,⁵⁰ without change, under Creative Commons 4.0 license.²¹) MLP refers to Multilayer Perceptrons.

Table 2. Comparing Traditional and AI-driven Quality Control

Feature	Traditional Quality Control	AI-Driven Quality Control
Inspection Type	Random sampling, statistical process control	Automated inspection of every part
Data Source	Post-production measurements	Real-time cavity pressure and temperature sensors
Defect Detection	Manual or optical after the fact	Prediction of characteristics like weight and dimensions mid-cycle
Traceability	Partial, batch-level	Full individual part-level documentation
Waste Reduction	Reactive rejection of faulty batches	Proactive parameter adjustment to prevent defects

Furthermore, polymer extrusion or reactive polymerization extrusion process is highly sensitive to fluctuations in temperature, pressure, and mixing speed.⁵²⁻⁵⁴ IoT-enabled sensors now provide real-time data streams for AI algorithms to analyze and adjust these parameters dynamically.⁷ Figure 4 illustrates a real-time surface defect monitoring system for polymer extrusion, which involves extruded polymer tubes passing through a monitoring system between a fan cooler and rolling machine.

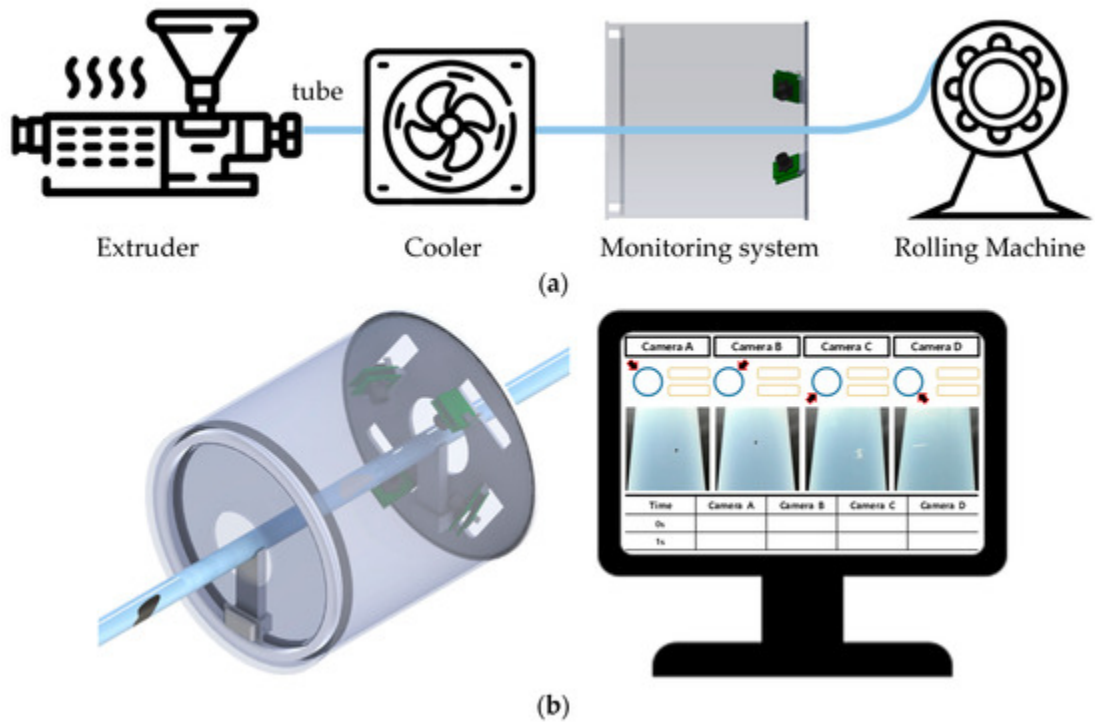


Figure 4. Schematic of a real-time monitoring system: (a) integrated into the production process; (b) defect detection notification screen. (Figure and Caption from reference,⁵² without change, under Creative Commons 4.0 license.²¹)

4. AI in Specialized Polymer Manufacturing

Specialized polymer manufacturing involving biomolecules, organic small molecules, and additives in multicomponent configurations can be important for cutting edge applications in energy and medicine.⁵⁵⁻⁶⁰ For example, in a polymer mediated ionic or molecular crystal system, the resultant complex structures have a strong dependency on the polymer-induced weak forces or chemical bonding that are exerted during their crystallization or self-assembly processes.^{56,58,61-63} In previous works, it is systematically shown that the assembled structures and optoelectronic behaviors of an organic small molecule is sensitive to the polymer additives' molecular weight, chain architectures, and other behaviors.^{56,62,64-66} To overcome the challenges posed by large processing parameter spaces involved, it is now possible to predict properties or phase structures via inverse engineering and physics-informed machine learning, even with a small dataset.^{4,67,68} In drug delivery systems, the fabrication and incorporation of a polymer matrix have a profound impact on the medical applications of organic small molecule drugs or nucleic acid therapy.^{61,69} AI algorithms are currently being used to predict therapeutic outcome, optimize patient-specific formulation, target specific tissue or organ with higher efficiency, and connect with real-time biosensors to drive automated drug delivery.^{58,70,71}

On the other hand, the manufacturing of high-performance polymer composites represents a complex engineering challenges due to the non-linear interactions between fibers, resins, and processing conditions.²⁹ Automated Fiber Placement (AFP) has emerged as a predominant approach for fabricating large, complex aerospace structures, such as fuselage sections and wing skins.^{72,73} AFP involves laying down multiple strips of carbon fiber prepreg onto a tool surface via a robotic arm. The quality of the final part is dictated by precise control over parameters such as the "nip-point" temperature at compaction pressure and lay-up speed. Inconsistencies in these variables can lead to lap-and-gap defects or out-of-plane buckling,

which can reduce the structural integrity of a component by as much as 30%.⁷³ Historically, identifying these defects has required manual visual inspection, which creates a significant bottleneck. In addition, AI is being integrated into AFP to automate path planning and provide real-time inspection.⁷²⁻⁷⁴ Machine learning and deep learning algorithms can analyze sensor data in live to identify irregularities or flaws with 95%+ accuracy.²⁹ In addition, ML-algorithm-based process planners are capable of handling complex and contoured structures by learning from historical data and simulations. Like a highly experienced human planner, these systems generate optimized fiber placement paths that minimize defects and maximize structural performance.⁷⁴ Table 3 compares traditional and Ai-driven AFP.

Table 3. Comparing traditional and Ai-driven AFP ⁷²

Metric	Hand Lay-up /Manual AFP	AI-Optimized AFP
Lay-up Rate	Variable, limited by human speed	Up to 50 m/min (high-speed systems)
Inspection Time	32% - 63% of total production time	Significantly reduced via in-situ AI monitoring
Productivity Gain	Baseline	Up to 450% improvement
Material Waste	High (often ~62%)	Reduced to ~6% through precise placement
Cost Reduction	Baseline	Up to 43% reduction in manufacturing costs

5.AI in Polymer Sustainability

AI-driven bioplastic screening is revolutionizing the development of alternatives to petroleum-based plastics.^{2,53} In a previous study, an informatics workflow identified single- and multi-layer replacements for food packaging by predicting eight key properties across a library of 7.4 million ring-opening polymerization (ROP) polymers.⁷⁵ By filtering for specific enthalpy of polymerization (ΔH_p) values (targeted at -10 to -20 kJ/mol), researchers identified candidates with 95% monomer recovery rates, ensuring high chemical recyclability.⁷⁵

On the other hand, chemical recycling -- a process that breaks down plastics into their molecular building blocks-- is a complex chemical process that benefits significantly from AI-driven optimization.⁷⁶ Machine learning models are used to facilitate chemical recycling in the

following aspects: (1). **Optimize Catalysis:** AI aids in designing more efficient enzyme catalysts for polymers like PET and identifying novel crosslinker molecules (mechanophores) that can make plastics more resistant to tearing.⁷⁷ Figure 5 illustrated an example of using AI to design Polyesters with desirable properties. (2). **Predict Reaction Kinetics:** Neural networks have been trained on comprehensive datasets (e.g., 942 data points across 44 variables) to predict PET hydrolysis conversion efficiency with an R^2 of 0.93.⁷⁶ (3). **Model Pyrolysis Oil Yields:** XGBoost models are being used to predict the oil yields from real waste compositions, allowing facilities to prioritize the most promising waste streams for chemical upcycling.^{78,79}

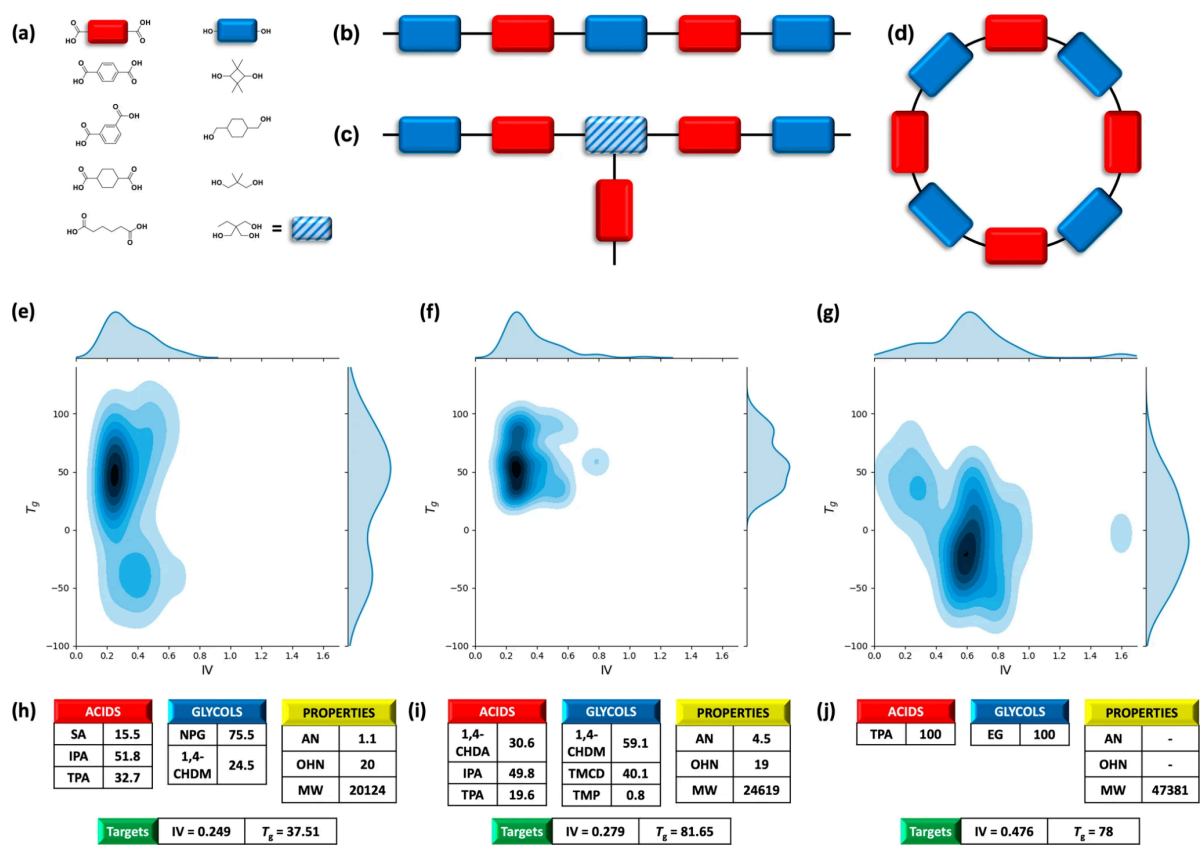


Figure 5. a Polyesters are composed by combinations of diacid (red) and glycol (blue) monomers, and they can form b linear, c branched, and d cyclic chains that are present in linear polyesters. For branched polyesters, a small amount of trimethylolpropane (TMP, blue/white striped monomer) is required. The distribution of T_g and experimentally refined IV values for the e linear, f branched, and g “cyclic” polyesters demonstrate the heterogeneity of the total database. Representative examples of input/output values of a h linear, i branched, and j “cyclic” polyester. Each sample consists of a set of acid and glycol monomers together with their corresponding percentage, and a vector of resin properties: end-group statistics (AN and OHN) and weight-average molecular weight (Mw). T_g in °C, IV in dL/g, Mw in g/mol. (Figure and Caption from reference,⁸⁰ without change, under Creative Commons 4.0 license.²¹)

6. Barriers and Future Directions

The shift toward AI-driven manufacturing is changing the nature of work in the polymer and manufacturing sector forever.^{3,12} Adaptability and the ability to work alongside AI systems have the modern operator acting as a "co-pilot," utilizing smart dashboards that not only show preferred set-point shifts in a plant or lab but also explain *why* those moves matter. This reduces mental /physical fatigue and allows the worker, researcher, or other workforce to focus on continuous improvement, compliance, and safety rather than routine parameter monitoring.

While the potential of AI in polymers is immense, several critical barriers hinder its universal adoption. The community remains heavily anchored in the traditional research paradigm, and moving to a fully data-driven model requires overcoming technical and cultural obstacles. To overcome such challenges, a major shift in perspective and paradigm is required, and a great starting point may be from adopting a data-driven approach to correlate desirable outcomes (properties, functions, or criteria) with important input features, either via descriptors, or other representations (images, spectra, structures and others).^{24,81}

A grand technical challenge is the lack of high-quality, diverse, and well-tagged datasets.^{47,67,70} Many key measurements rely on instruments from manufacturers that do not provide open interfaces, impeding the creation of unified databases.¹⁹ The industry is moving toward "FAIR" (Findable, Accessible, Interoperable, and Reusable) data standards to ensure that experimental results can be shared and utilized by machine learning models globally.^{2,4}

There is an increasing focus on Explainable AI (XAI) to ensure that models do not just find optimal materials, but also provide insight into the underlying mechanisms.^{19,29} This is essential for gaining the trust of engineers in high-stakes industries like aerospace and medical devices, where an unexplained prediction can lead to unacceptable risks.

The trajectory of AI and machine learning in the chemical and materials science market points toward a historical expansion. The future of polymer manufacturing is defined by the seamless fusion of digital twins and physical domains. As the current research trend continues to bridge the gap between algorithm benchmarks and industrial applications, a circular economy driven by machine-learning-automated designs and materials will likely become a technical reality through the sustained integration of artificial intelligence and advanced polymer manufacturing.

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Conflicts of Interest

The author declares no conflict of interest.

Author Contributions

RCA planned the layout, and drafted introduction and Section 2. JC drafted Section 1, 3-6, and contributed to the overall design and writing.

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