*Research Article*

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# Various Deep Learning Techniques for Applications in Polymer, Polymer Composite Chemistry, Structures and Processing

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ABSTRACT

Polymers and polymer composites possess a wide range of applications in chemical, material, and biomedical fields. Although conventional techniques to the design and processing of these significant materials have been successful, they have faced critical problems. Their synthesis is not only time-consuming, but it is also costly for polymer industries. In recent years, there has been a regenerated hype regarding deep learning, as an approach based on artificial neural networks. Due to the importance of both polymer chemistry and artificial intelligence systems in the academic research and industry, it is a requirement to present approaches combining these two promising fields. This paper aims to categorize various deep learning approaches used in the field of the polymer science. We expect that this can expand the polymer chemistry community engagement with artificial intelligence, especially deep learning and accelerate the improvement in the data-driven techniques for the synthesis and application of polymers.

## 1. Introduction

Machine Learning (ML) is a technique that enables computers to address challenges via data learning [1]. Deep structural learning (deep learning), as a part of a larger machine learning family, is based on the artificial neural networks (ANN) with representation learning. The relationship between Artificial intelligence (AI), machine learning, and deep learning (DL) has been shown in Figure 1 [2].

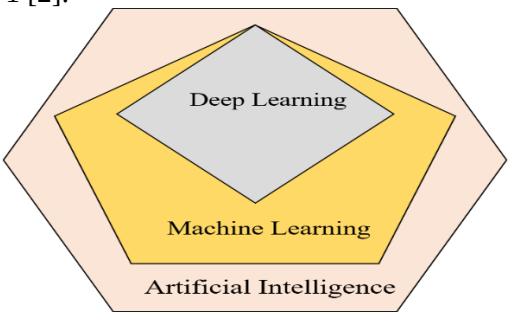


**Figure 1.** deep learning as a subset of machine learning and machine learning as a subset of artificial intelligence [2]

The majority of works in this area can be categorized into three main classifications (i.e., supervised, unsupervised, and semi-supervised) [3]–[5]. Figure 2 shows their architectures which apply in various fields such as speech and audio recognition, machine and computer vision, natural language processing, drug design, material inspection, medical image analysis, game programs, social network filtering, and bioinformatics. In these applications, DL produces results near to human expert performance and, surprisingly, the results in some examples are better than them [6], [7].

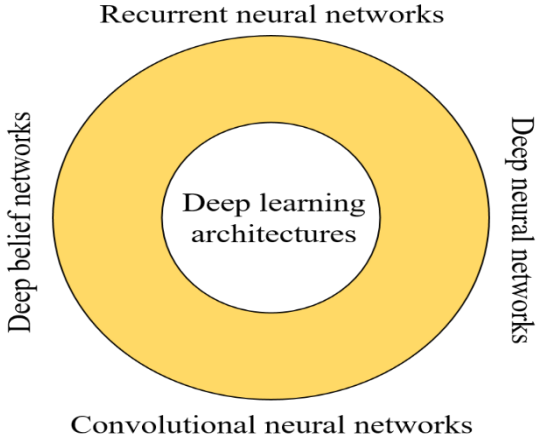


**Figure 2.** The architectures of deep learning [6], [7]

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In a broad problem range such as density, viscosity, band gap, atomization energy, and glass transition temperature, ANN-based techniques have displayed promising results after the beginning of this technique in the 1950s [8]. The main difference between biological brains and ANNs is that the first one is analog and dynamic, while the other one is symbolic and stationary [9]. Researchers used DL approach in a broad chemical challenge, including materials and drug design, synthesis planning, and computational chemistry development. In computational chemistry development, Siadati et al. [10-13] and Vessally et al. [14] have achieved successful results. Using the hierarchical recombination of properties, DL can extract relevant information and learns the represented patterns in the data. Mater et al. [1] also reviewed the various applications of deep learning in chemistry to encourage the broad chemical society to engage with this modern field. The "deep" adjective in the deep learning technique originates from the usage of multiple layers in the system. As a novel variation, DL not only allows an optimized implementation and a practical application but also is able to retain the hypothetical universality under mild conditions. This technique applies various layers to extract high-level characterizations from the raw input. This can be revealed in the image-processing field, where low layers can recognize edges and high layers can recognize human-related features, including letters, faces, or digits [15]. Moreover, during recent decades, convolutional neural networks (CNN) have achieved popularity as a strong approach to solve different technical problems such as driverless cars, style transfer, medical image recognition, and face recognition. Coupled with special activation functions and fully connected layers (FCL), ANNs have the ability to extract the important data (characterizations) from a determined dataset and then fit them to the desired feature as output during training. Following this, these networks can generalize the result of the other input information, which was formerly unrevealed. [8] Many repeated units, namely monomers, can be connected to build polymers, as one of the most significant materials in the modern society whose applications are diverse, from plastic bottles and bags to structural and electronic components in aerospace industries. Polymer design consists of three steps, including the monomer design, microstructure design, and material processing. These three steps can be called polymerization, crystallization, and manufacturing, respectively [16]. The majority of traditional design techniques to synthesize polymeric materials are experimentally driven. The AI-based digitalization of the design and synthesis optimization of polymer metals and their composites is the beginning of the way. Moreover, the material design using AI is a promising tool to expand breakthroughs in the bioengineering of polymer composites/nanocomposites (PCs /PNCs). As special ANNs, deep neural networks (DNNs) can offer a reasonable design for secure and more effective PCs [17]. The progress of better mechanical features, as well as variable functionalities, is a necessity for modern engineering applications. Hence, the composite design with superior efficiency can be considered as an essential factor in the material development sector. The combination of two or more raw materials in special architectures can lead to the production of composite with distinctive and spatially different features. Different traditional composite designs are not able to guarantee the global optimized design because of the immense numbers of freedom degrees and their various computational limitations. ML, which employs different probabilistic, statistical, and optimization approaches, enables computers to learn from the previous experience and recognize hard-distinguished patterns from complicated, noisy, and large data sets. Using this technique, researchers can overcome the limitations regarding conventional composite designs. In spite of the recent widespread influence and extensive application of ML, only a limited use of this technique for composite design has been recently reported [18].

## 2. DEEP LEARNING APPLICATIONS IN POLYMER AND POLYMER COMPOSITE FIELD

There have been some comprehensive review papers regarding AI-based applications in polymer technology [19-21]. However, we try to focus on the DL-based ones and cover the PCs in this study due to their importance in modern technology. Moreover, we categorized every related application of the DL in the polymer and PC field in one DL technique. This would help researchers realize the importance of every technique based on the mentioned applications and, more importantly, they can find which DL technique can outperform the other techniques according to the demand. These categorizations are introduced in Figure 3 and the most important DL applications in polymer and PC field are outlined in Figure 4. Moreover, the system characterizations of some referenced researches, including dataset, libraries/ platforms, input and output layer nodes, hidden layer numbers, activation, loss function, dataset size (training and validation test), accuracy and their optimizer are outlined in Table 1.

### *2.1. Deep neural network*

It is found that there are more than thousands of connections between tens of millions of neurons in the human brain. The NN consists of the input, hidden and output layer in which each layer is composed of different neurons, and the hidden layer is composed of many layers (Figure 5). The number of neurons numbers in the output layer of the NNs can be different based on various task kinds. In a three-classified problem, for example, there are three neurons in the output layer, each of which can represent the possibility of belonging to a specific classification.

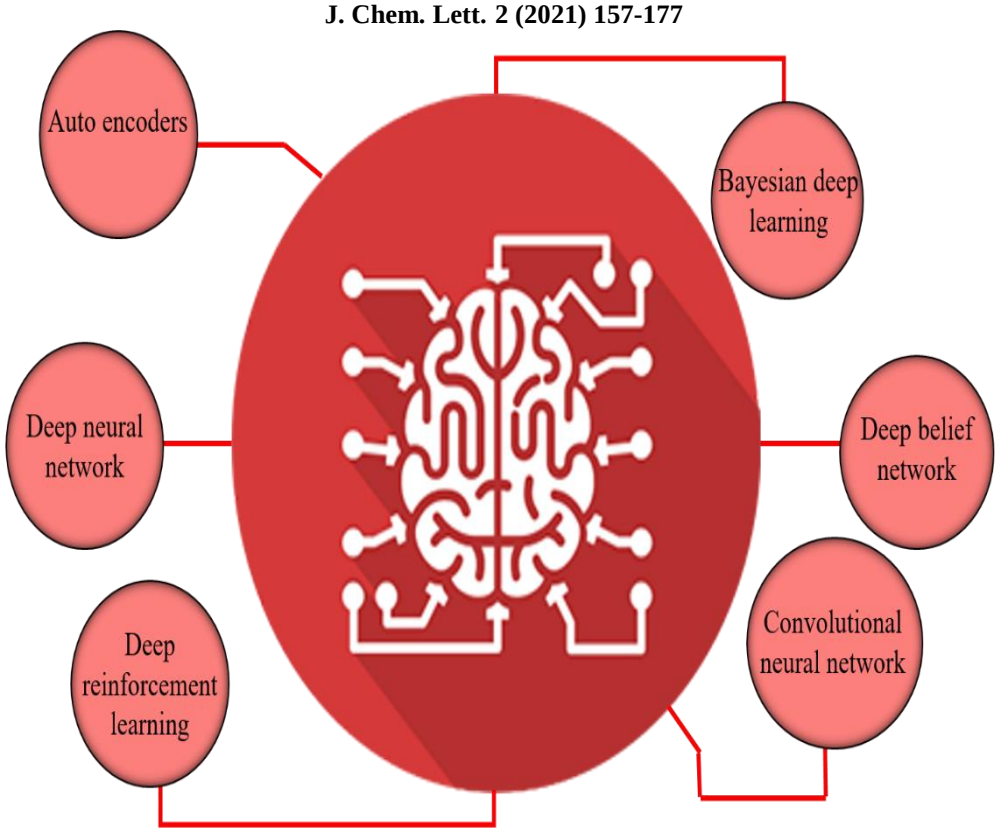



**Figure 3.** Different deep learning techniques used for polymer and polymer composite materials

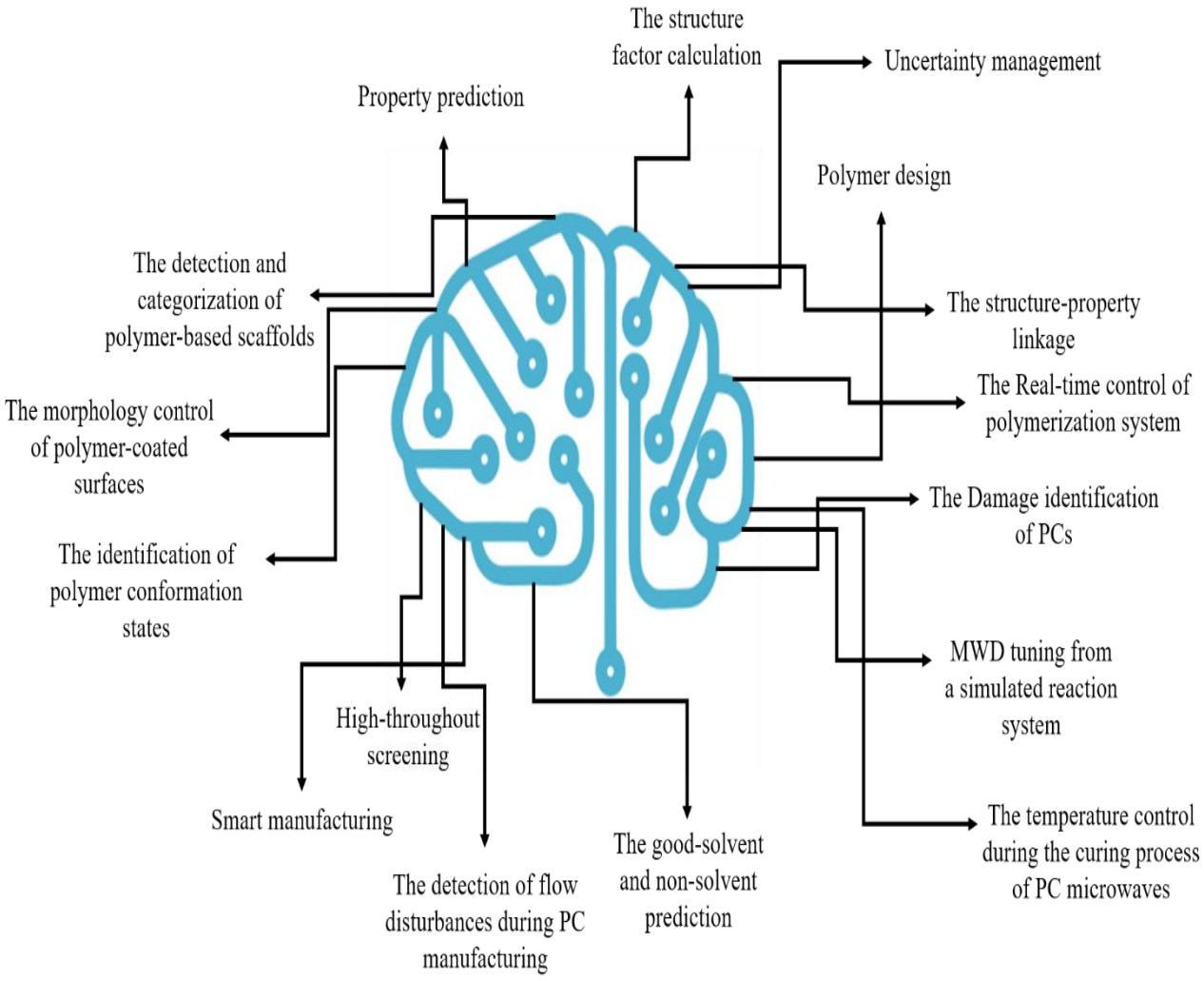



**Figure 4**. Deep learning in polymer and polymer composite technology

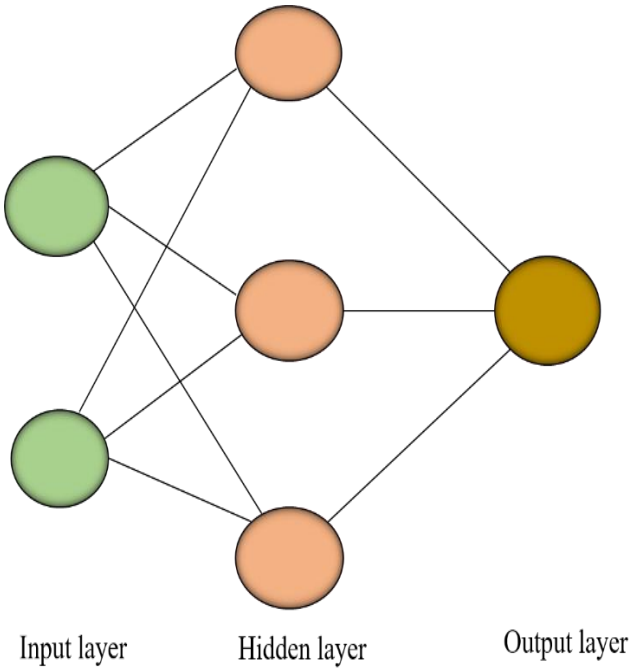



**Figure 5.** A NN architecture consisting of the input, hidden and output layers [22]

The calculation of a neuron in the hidden layer, as an example, is displayed in Figure 6.

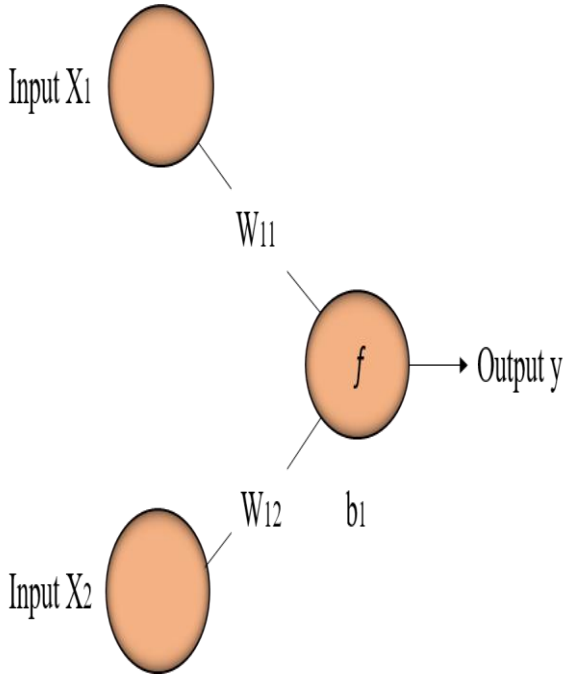



**Figure 6.** Equation for the neuron calculation: y=f(∑jwijxj∗)

Y:the output of the neuron, wij: the weight of the jth input and the ith neuron, xj: the jth input of the neuron, bi: the bias of the ith neuron, f: the activation function to fulfil a nonlinear transformation on the neuron output. ReLU, softmax, tanh, etc. can be considered as the most common activation function. [22]

NNs enable us to classify and cluster the means that we can consider as a classification and clustering layer on top of the data that can be managed and stored. When there is a labeled dataset to train on, they classify data and help to group the unlabeled data based on the similarities between the example inputs. DNNs are stacked neural networks: the networks consisting of several layers made of nodes.

According to the prior layer's output, every nodes' layer trains on a definite set of features. The further you advance into the NNs, your nodes can recognize the more complex features as they collect and recombine features from the prior layer. [23]

A polymer structure factor, as a quantifiable physical feature, which indicates the density–density relationship can be studied both theoretically and experimentally. The main properties of polymers, including chirality, polymerization degree, and rigidity are analyzable when the structure factor fits with the scattering data through experiment. For Gaussian chains, this value can be calculated analytically, while numerical techniques, including Monte Carlo simulations (which can modify diffusion equations) are usually applied for wormlike chains. Wormlike chains can be taken into account as one of the most excellent semi-flexible chain models.

This is so because there are dissimilar regions of the chain rigidity and wave vector for these polymers. Thus, the structure factor has to be solved differently for them, and some computation processes are resource consuming. However, researchers do not require to detect structure factors by guessing the analytical formula if they apply a neural network to substitute it. Huang et al. [24] calculated the structure factor of a wormlike chain polymer via training a deep neural network. In this study, they did not consider the various regions of the chain rigidity and wavenumber. Using the experimental data of scattering and based on the trained neural network, they also predicted the Kuhn and contour lengths of some polymer chains. Their model is extremely compatible with the prior calculations in analytical and numerical approaches. Hence, this model can be a great tool for experimental researchers to explore the features of polymer chains.

The importance of polymer solubility, as another polymer feature, has been proven for different researchers and industrial applications, including drug delivery, plastics recycling, and membrane science. However, finding a suitable solvent for the dissolution of novel polymers is still challenging. One solution is polymer parameters examination to identify the suitable solvent for the polymer. However, this remains a solution and is not an applicable case. To develop a new data-driven model for polymer-solvent selection. Chandrasekaran et al. [25] used a deep learning approach to design a network. As depicted in Figure 7, this network takes a pair of polymers and solvent / non-solvent as the input and output of

predicting whether the proposed solvent is suitable for the polymer at the room temperature or is a non-solvent. For this purpose, the network was trained on a dataset containing 4,500 data pairs. Then, in the test phase, some hidden data pairs are given to this trained network to test its suitability. Following this, they see if the network can correctly determine the compatibility of each solvent with its corresponding polymer in that data pair or not. Based on their results, the proposed network can correctly predict the suitability of solvents in 93% of data pairs during the testing step (Table 1)

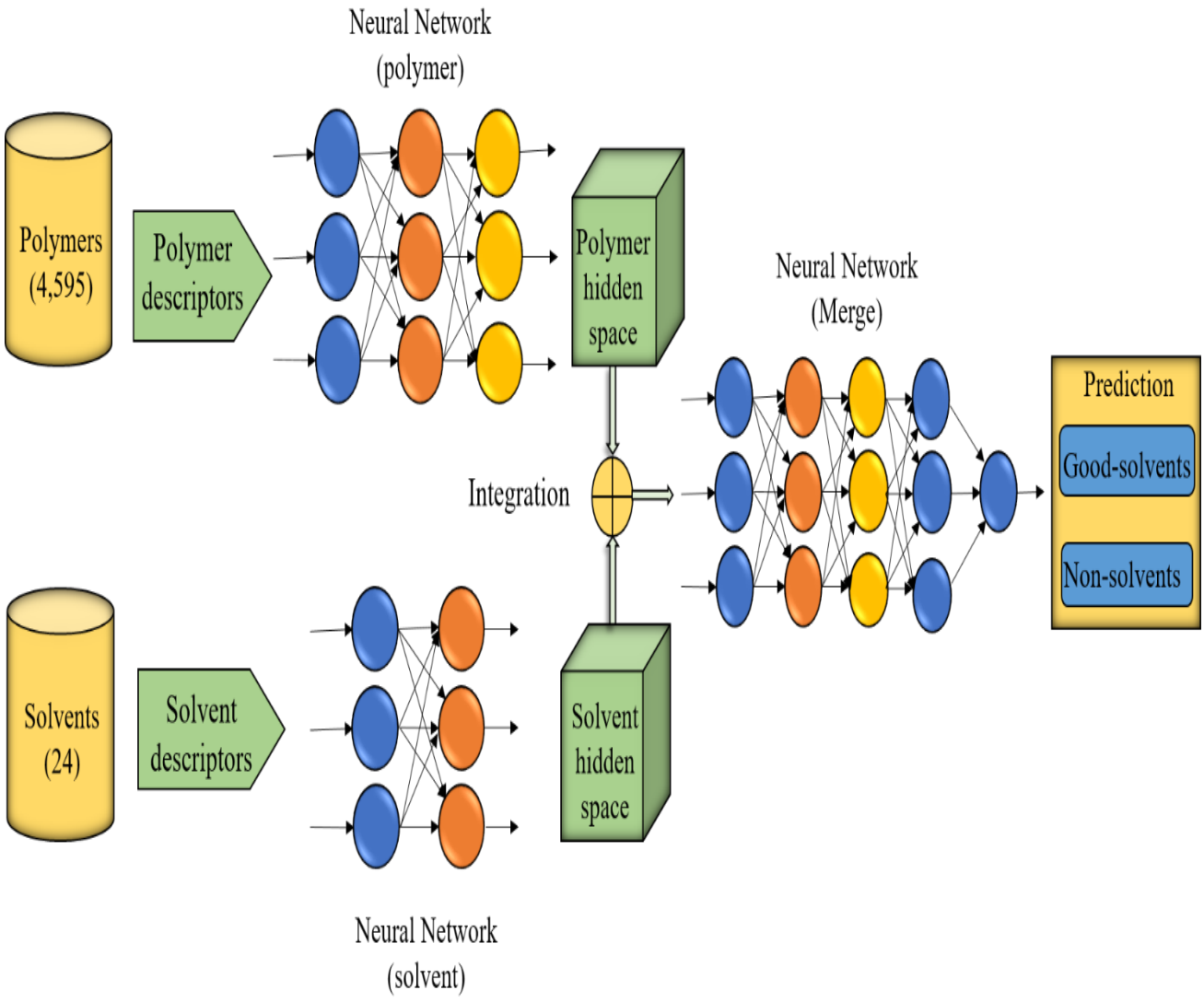



**Figure 7.** The architecture of the NN to predict the non-solvents and good solvents [25]

Recently, Frontal Polymerization (FP), has been introduced as an efficient technique to save energy and time for the production of Fiber-Reinforced Polymer-matrix Composites (FRPCs).

These polymer composites are significant polymers for automotive, aerospace, energy industries, and marine. However, the cure kinetics parameters of a thermoset polymer, as the matrix phase, can bring challenges to the process design and control. In a study conducted by Goli et al. [26],

one of the most efficient deep learning networks for Advanced Composites Manufacturing, ChemNet, in combination with FP was used to build these composites. ChemNet, consisting of nine fully connected layers of feed-forward type, is used to predict and optimize the parameters related to cure kinetics.

These parameters include enthalpy and reaction activation energy for a favorable fabrication approach. They trained the model by preparing input data via normal distribution and output data derived from the steady-state solver. This solver helps them prepare an immense data set serving to train their suggested ChemNet. Using this model, in the end, an inverse method was applied for the prediction of the cure kinetic parameters for a given front feature.

The fiber volume fraction and the resin chemistry have been chosen by them to focus on their critical role to adjust the product application as well as the fabrication time.

To customize and optimize the resin chemistry, particularly, they tailored its cure Kinetics parameters in a manner to achieve the followed results: Guarantee the favorable fabrication time and satisfy the application demand in terms of the needed fiber volume fraction.

High-throughput computational screening can be considered an important step in material development because it can examine the large areas of chemical space for special functionalities [27]. Although chemical accuracy has been sacrificed for numerical efficiency in density functional theory (DFT), it is not fast enough fast to represent the broad combinatorial landscape of possible chemical structures [28].

Recently, ML, a faster alternative to comprehensive calculations of quantum chemistry, has been introduced as an effective method for the reproduction of DFT results with enough training data. Hence, much larger compound libraries can be screened without a further decline in chemical accuracy via this technique [29]. Graph-based neural network architectures have been introduced as the most promising technique for prediction according to the molecular structure. However, these systems need optimal three-dimensional (3D) structural data of the molecules to obtain the greatest level of accuracy.

In a study carried out by John et al. [30], they developed a new database of selected molecules for organic photovoltaic (OPV) polymers and applied a message-passing neural network (MPNN). MPNN is an end-to-end learning technique, in which input charts with edge and node features make the predictions.

Comparable to the current datasets, the provided data set not only possesses completely larger molecules (more than 200 atoms) but also includes extrapolated features for polymers with a long chain. They displayed the fact that for the types of the intended molecules, trained MPNNs with 3D structural data could present the same performance and accuracy compared with the trained models without 3D structural data. These results indicated that for larger molecules, almost optimum prediction results are achievable without applying optimized 3D geometry as the input. In fact, they concluded that a pre-trained DNN on one DFT functional can improve the prediction ability on a relevant DFT functional, particularly in the case of restricted data.

*2.2. Bayesian deep learning*

The Bayesian technology, which presents a way to update our previous information about the model parameters, applies Bayes' theorem. This theory is according to the idea that there may be previous information (belief or knowledge) about the distribution of a parameter value prior to taking a sample of observations [31]. During the recent decades, researchers have broadly developed safety assessment techniques based on Bayesian analysis and applied them in the chemical process field. To overcome the shortages of traditional approaches such as fault tree in the absence of the application of dynamic safety analysis, Bayesian network and hierarchical Bayesian analysis would be efficient [32].

Process systems can be the complicated socio-technical systems liable to disastrous events due to the instrumentation, mechanical and human dangers that exist in these systems. The management of uncertainty can play an important role in the prediction of any process disorders. This can lead to a reduced emergency response time to decrease the harshness of the result. Researchers introduced Grid of Resilience Analysis to introduce a well-known system characterization managing the systems and improve its capability for strong performance. Resilience engineers examined the Columbia disaster and, based on their conclusion, the perspective of resilience will provide anticipation regarding the variable risk patterns prior to the occurrence of harm or failure, unexpected or expected disturbance. Using Bayesian deep learning via the virtue of the Markov Chain Monte Carlo (MCMC) simulation in a recent study, Jain et al. [33] developed a framework of process resilience analysis. Their technique possesses the following features: non-expensiveness, dynamism, being data-driven, integration, quantitative state, system-based nature, and uncertainty management. Avoidance (initiating events), survival (propagation events), and recovery events are the three phases of this new framework that can cover the general anatomy of a process disturbance (Figure 8a). They developed three statistical models for three uncertainties, namely reactant mischarging, cooling average temperature, and agitator failure. The bath process of Ploy vinyl chloride (PVC) suspension polymerization has been selected because the polymerization process is the main process that contributes to the reactions of the thermal runway. The flow diagram which displays the steps taken to calculate the parameters posterior distribution by the Bayes theorem is presented in Figure 8b. Using the failure numbers from historical data, the majority of existing risk evaluation techniques for the rates of failure cannot present the real image of the processing system. The resultant technique not only is easy to understand and perform in the real process system, but also allows risk assessors to make risky decisions. This decision-making according to their process plant data can lead to an effective, profitable, reliable, and secure system of process.

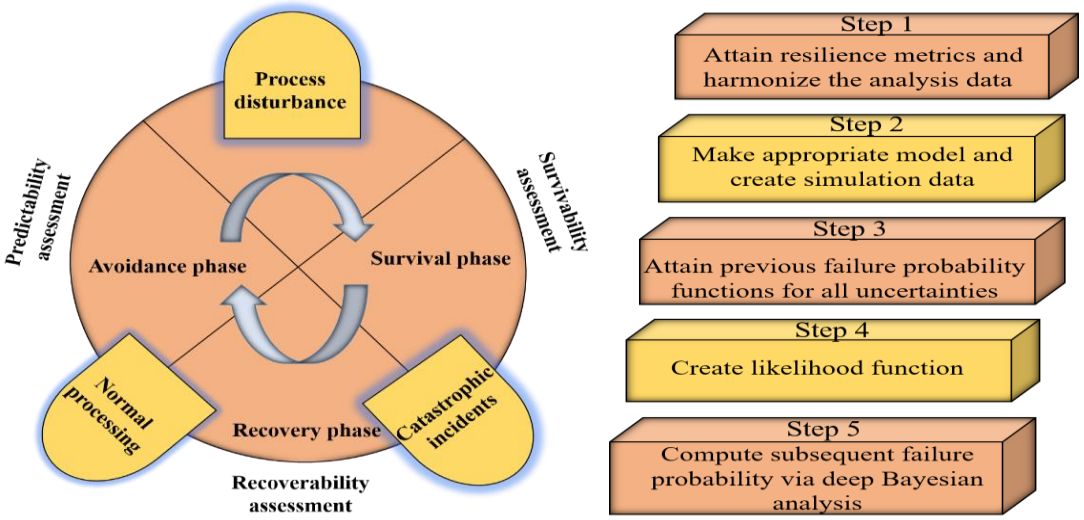



**Figure 8a.** Process Resilience Analysis Framework**.** There are three principal system states in the system of PVC process, including normal operation, catastrophic state and process-upset event. Predictability assessment: error-tolerant design, early detection and plasticity/ survivability assessment: plasticity, error-tolerant design/ recoverability assessment: plasticity, recoverability). **Figure 8b.** The steps taken to calculate the parameters posterior distribution by the Bayes theorem in a diagram [33].

*2.3. Deep reinforcement learning*

In Reinforcement Learning (RL), an agent can learn the interaction with a specific environment through trial and error. A robot or an agent (software or hardware) should receive a great representation of its environment before selecting an optimal action. The environment representation may be obtained or may be given. Although, in RL tasks, a human expert often presents the environment features according to his/her knowledge of the task, this work must be done automatically in some applications of the real world. To deal with this challenge, there are different solutions, including function approximation, Carlo Tree search, and hierarchical reinforcement learning.

The RL agent acquires a reward via acting in the environment. Hence, the goal would be learning how to choose the actions maximizing the expected reward over time. An RL agent could be modeled as a Markov decision process (MDP) which can be as a discrete-time stochastic control process, providing a mathematical framework to model decision making in conditions where outcomes are partially under the decision-maker control and partially random [34].

To enhance sustainability and profitability, scientists are making many efforts to apply DL tools to improve smart manufacturing, especially in the field of chemical processes. In this type of manufacturing, advanced computer intelligence can learn the data to make smart decisions. Deep reinforcement learning (DRL), as a strong option to develop future controllers in production industries, is recognized for its supernatural ability in control tasks when AlphaGo wins the chess in competition with human champions [35], [36]. Machines can learn control behaviors through the self-exploration of the environment in RL.

For instance, for a reaction system, the learned approach can be achieved from numerical data, which it does not need real-time optimization or tuning parameter. This adapts the RL to the various control tasks effortlessly when the framework is determined. In the polymerization reactor control, the trajectory-based scheme of control can be considered as a generally applied technique, while Automatic Continuous Online Monitoring of Polymerization processes (ACOMP), is a strong platform for the monitoring of the polymerization reaction. This platform provides a real-time evaluation of the significant characteristics of polymerization system, markedly weight-average molecular mass ($M_W$). Hence, after an optimum $M_W$ trajectory in real-time, the target Molecular Mass Distribution (MMD) can be obtained. MMD can dictate different polymeric architectures and the quality of the polymeric product, which is merely detected at the end of the semi-bath process. Thus, this makes the control of the polymerization process hard for people [37]. Online monitoring methods with soft sensors such as Raman, optical, and UV/Vis spectroscopy are utilized for polymerization reactions as control solutions [38]. This has been shown in a study undertaken by Ghadipasha et al. [39] in which they applied soft sensors to provide an evaluation of MMD and $M_W$ in a free-radical polymerization of the acrylamide–water–potassium persulfate system. They obtained this aim by tracking the MW path in real-time and regulating manipulative variables like feed flow rate. A polymerization system controller including optimized instructions to regulate the initial flow rate and a

proportional-integral (PI) controller to control the flow rate of monomer have been built by them.

An alternative solution studied by Ma et al [37] is the use of DRL for controlling the polymerization system via modifying both initial and monomer flow rates at the same time to follow the optimum trajectory of goal MW in a simulative environment. Their results proved the fact that the DRL controller successfully learned a great control approach in the reaction process and displayed excellent potency to handle complex tasks in the chemical systems of manufacturing industries. The whole methodology of this research has been displayed in Figure 9.

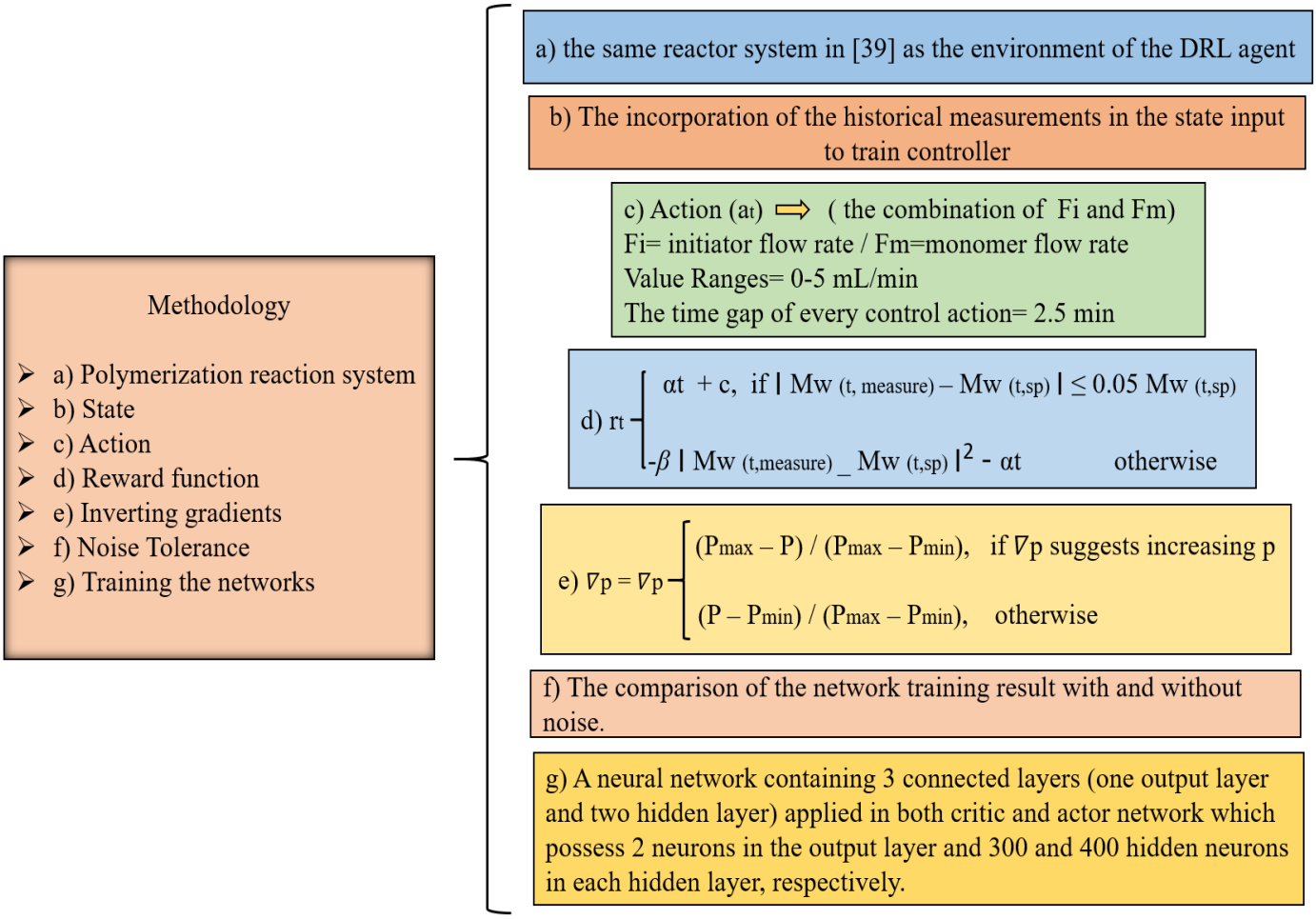



**Figure 9.** A reward ($r_t$) is received from the environment (E) at every time step. In the reward function, $c$, $\alpha$, $\beta$ are constants. By inverting the gradient approach, the gradients are inverted when the parameter surpasses the limit of the range and down-scaled if they approximate the boundary values. In the equation of the inverting gradients, P indicates the adjusted parameters and $P_{min}$ and $P_{max}$ are the lower and upper boundaries of the parameters. Based on the noise tolerance results, even in the noisy environment, the DRL controller can learn the control policy [37].

Recently, reinforcement learning advancement has paved the way for a computing system to lead vehicles via a complicated simulation environment. Again, to regulate the shape of polymer molecular weight distributions (MWDs) in a study by Li et al. [40], atom transfer radical polymerization (ATRP) was used as the simulated reaction system. It allows the polymer preparation with flexible polydispersity, narrow MWDs, and preplanned molecular weights. They normally perform via preparing a primary chemical mixture at a constant temperature and under other reaction conditions. A higher MWDs diversity would be achievable by taking such actions as the addition of chemical reagents during the process. According to the common reaction state, Li and their colleagues applied the DRL technique to decide which actions could be taken. This is like a human who continually takes actions to guide the reaction towards the target MWD, including Gaussian distributions with more complex shapes and different widths. The primary untrained controller results in ending MWDs with wide flexibility, which enables DRL algorithms to examine a wide search space. After training by the actor-critic algorithm, the RL controller can detect and optimize the control approach leading to various target MWDs. The trained controller can be transferred from the simulation environment to the actual laboratory in a future application. A RL problem can usually be expressed as an agent, which interacts with an environment. In this work, as Figure 10 displays, an ATRP reactor simulator and an RL controller are considered as the environment

and the agent, respectively. At separated times via constant gaps ($t_{step}$), the agent interacts with the simulation. This interaction consists of three factors, each of which is indexed by subscript t. ⅰ) State ($S_t$), at every timestep ⅱ) Action ($A_t$) ⅲ) Reward ($R_t$), at every timestep. To choose the actions, the state vector is applied by the agent. St can be ⅰ) the solution volume ⅱ) the non-trace species concentrations: Cu-based ATRP catalysts, dormant chains (P1Br,⋯,PNBr) and monomer ⅲ) double indicators of whether each of the adding reagents has reached its budget. The set of actions which is fixed throughout the simulation includes the enhancement of an unchangeable amount of a chemical reagent, a no-operation (no-op), meaning that no action is taken on the environment of the reaction simulation. The agent may still choose a similar action even when a reagent reaches its budget. However, this is a no-op and does not change the environment of the reaction simulation. The agents acquire a reward merely when the reaction is completed, meaning that the reward is based on the final MWD. Until all the added reagents have reached their budget, the agent is allowed to interact with the simulation.

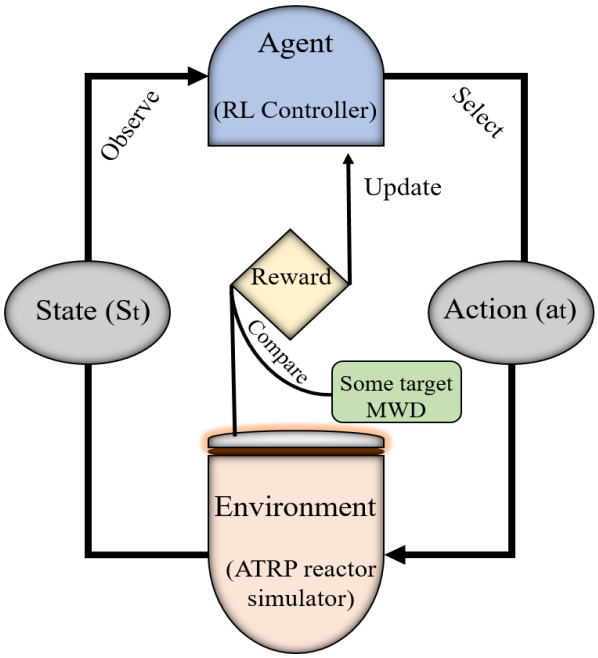



**Figure 10.** A schematic shape of using deep RL in the reactor control setting of the ATRP. The simulation proceeds for a $T_{terminal}$ of a 105 seconds, after the all added regents have reached their budget. Then, a reward is provided to the agent by simulation environment, which is based on the difference between the target MWD and the final dormant chain MWD. A structure of the two-level reward is determined empirically. The maximum absolute difference between the target MWD and normalized ending MWD is less than $1 \times 10^{-2}$ and the reward is 10, the maximum absolute difference between the target MWD and normalized ending MWD is less than $3 \times 10^{-3}$ with the $_{reward}$=1.0. [40]

### *2.4. Autoencoders*

Recently, autoencoders, as an unsupervised learning ANN algorithm, is involved inside the DNNs, which has made the autoencoder concept more broadly applied for learning. An autoencoder, which commonly contained a hidden layer between the decoder and encoder, learns a representation for a set of data, typically decreasing the data dimensionality [41]. As it is obvious in Figure 9, in this technique, the number of neurons in the output and input layers is the same and the number of neurons in the hidden layer is less than that in the output and input layers. This is useful for data compressing and learning efficient features from data. To get a new representation, the encoder decreases the original data dimension. Next, the input data can be restored through a new representation by the decoder. [22]

The high-dimensional conformation is converted into a low-dimensional code via the encoder network. Then, the decoder network recovers the configuration from the code that is considered as the feature to represent the polymer structure (Figure 11). In an autoencoder system, therefore, the average square error can be employed among the input and decoded output. The representation of the polymer configuration via the code is provided by the minimized loss between the original and reconstructed data as much as possible [37].

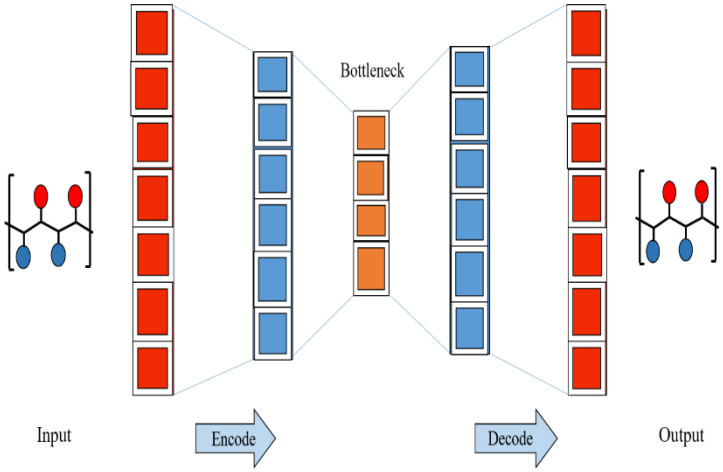



**Figure 11.** Schematic diagram of autoencoder network with 5 layers

It has been found that brain neural networks are structured in 3D space evolving through learning and development whereas current 2D crossbar devices have been fundamentally optimized for a fully-connected neural network leading to an enhancement in unused memristors. Considering the fact that the process of polymer wire growth can be directly connected to the learning action of artificial synapses, Akai-Kasaya et al. [41] presented the concrete application of conductive polymeric wires to an ANN. Similarly, because the presence or absence of synapses between neurons is learned by AI techniques, the presence or absence of conductive polymer wires between the electrodes in the monomeric solution can be learned according to the ANN network. To do this, they first trained a simple ANN, the

perceptron, with a linearly separable dataset (Boolean functions), which included synaptic media and their corresponding electrical controller.

Then, they used an autoencoder to extract features, in which 3 × 3 (9 pixels) binary letters are well-compressed into 3-pixel data by 54-polymer synapse on an electrode collection tip. A poly (3, 4-ethylenedioxy-thiophene) doped with poly (styrene sulfonate) anions (PEDOT: PSS) has been used as the selected polymer since their 2D array, as well as their applications to rudimentary nonvolatile synapses, are recently proven. They resulted in the great ability of the resistance array of polymer wires when the number of wires linking between electrodes increased.

Surely, their results would be beneficial to extend the development concept of space-free synapse, which means the extension of 2D synaptic media to 3D.

The application of the autoencoder system is also reported for the polymer configuration identification due to the fact that DL is used for the recognition of phase transitions. To classify various states of configuration, the critical behavior has to be studied. A DL technique that is based on a supervised approach can be applied for the categorization of matter phases both in symmetry breaking and topological modes.

In this approach, the prior labeling of the states in renowned regimes such as a state belonging to a globule or coil phase is necessary. This fact, however, has to be taken into account that supervised learning label confines the feasibility of using this method to identify undetected states. Without prior labeling, unsupervised techniques can achieve properties from the unprocessed data while the supervised ones do not have this capability. Hence, when the taxonomy is unknown to us, unsupervised learning can be considered particularly worthwhile. In a study conducted by Sun et al. [42],

tool was introduced for the identification of polymer configuration. They used an unsupervised method based on the autoencoder system as well as a self-organizing map (SOM) to detect critical transitions of phase from a raw conformation. Presenting this unconventional tool to recognize polymer configuration, researchers do not need to engineer hand-operated features.

They trained the network from the encoder layer to code layer via two modes. First, they applied a Restrictive Boltzmann Machine (RBM) to initially train the network parameters. Second, the trained parameters are copied to the decoder and encoder network. To make the decoding data near to the input data, they finally used the Back Propagation (BP) algorithm to further train the intermediate code of the NN. They compared the labeled supervised, unsupervised learning, and traditional computing results. The labeled supervised learning resulted in lower accuracy, while the result of the unsupervised learning prediction was closer to the simulation results.

### *2.5. Convolutional neural networks*

The CNNs apply the approach of local connection and weight sharing. This decreases the network complexity and enables the network to employ the image directly as an input. These networks possess two significant characteristics. First, the learned features from the image are non-deformable and translational. Second, the higher convolutional layer is the sign of the more complex and abstract extracted features.

The CNN consists of the convolution layer composed of filters, the pooling layer, and the fully connected layer. In the convolution layer, every filter is equivalent to a small window moving on the image in order to learn features from the image. To draw the features that are more representative and improve the accuracy and robustness of the model, the learned features can be subsampled via pooling. Eventually, the prediction result can be outputted by the fully connected layer. [22]

It has been discovered that the cells of the animal visual cortex are responsible for light detection in receptive fields. CNN, as a known DL architecture, is inspired by the explained visual perception mechanism of the alive creatures. Although there are a large number of CNN architecture variants in the literature, their main components are not dissimilar. [43]. CNNs, which are largely for the popularity of Neural Networks, have been recently introduced as a significant aspect of deep learning [44].

They are efficient for computer vision problems because they can manage translation invariances in pictures, which can be done just by relying on shared weights. Moreover, they can manipulate spatial locality by imposing a local connectivity design between adjacent layer neurons. Considering this and based on the fact that they needed a model to identify various kinds of scaffolds and differentiate them from each other, Akogo et al. [45] used CNN to recognize three classes of 3D polymer-based scaffolds.

These scaffolds are useful for tissue regeneration containing one from an airbrushed set and two others produced from steel wires and an electrospun fiber set. They aimed to develop a network model to identify and categorize these sets to introduce a tool that is beneficial in the biomedical industry. Their proposed method, named ScaffoldNet, takes the scaffold images related to the scanning electron microscope. Then, they classify them accurately by a six- layer CNN. This model was done on a dataset with 3043 images where 2376 images were used for training, 368 images for validating, and 301 images for testing the model. An imaged scaffold is taken

in as the input and then the probability of belonging the input image to all three classes can be calculated. Finally, they chose the class with the highest probability and marked this class as the output, which was Electrospun with the probability of 0.98. Their model, which obtained the up-to-date results amongst other methods with an accuracy of 99.44%, can present a great potential in the complicated problems related to the screening of fibrous and biological structures of fibrous shells and the cortical bone (Table 1).

The majority of polymers display low Thermal Conductivity (TC) that cannot be considered adequate for many applications requiring great heat conduction. Based on the experimental studies and Molecular Dynamics (MD) simulation, scientists have proven that the polymer chains as materials with low-dimension can possess great TC [46].

Therefore, there is an expectation to develop new polymer materials possessing high TC [47]. Polymers orientation [48], crystallinity, crystal form [49] and chain structure [50], [51] are the factors that affect the TC of polymers. Among the mentioned characterizations, the chain structure that includes molecular conformation and composition and determines different polymers of TC is the first level of the structure. Based on the equation of Debye (i.e.k = $Cpvl/3$), TC is related to $v$ (the phonon velocity), $Cp$ (the specific heat capacity per unit volume), and $l$ (the phonon mean free path). Generally, $v$ and $Cp$ of polymers are principally determined by the backbone bonding strength and the features of the monomer repeat the unit in the individual chain [52].

However, expensive and long experiments prevented the possibility to design advanced and novel polymers having functional thermal features. Combining big data methods and material science, researchers have used machine learning techniques to increase the speed of material development. To predict the TC of different single-chain polymers, Zhu et al. [53]

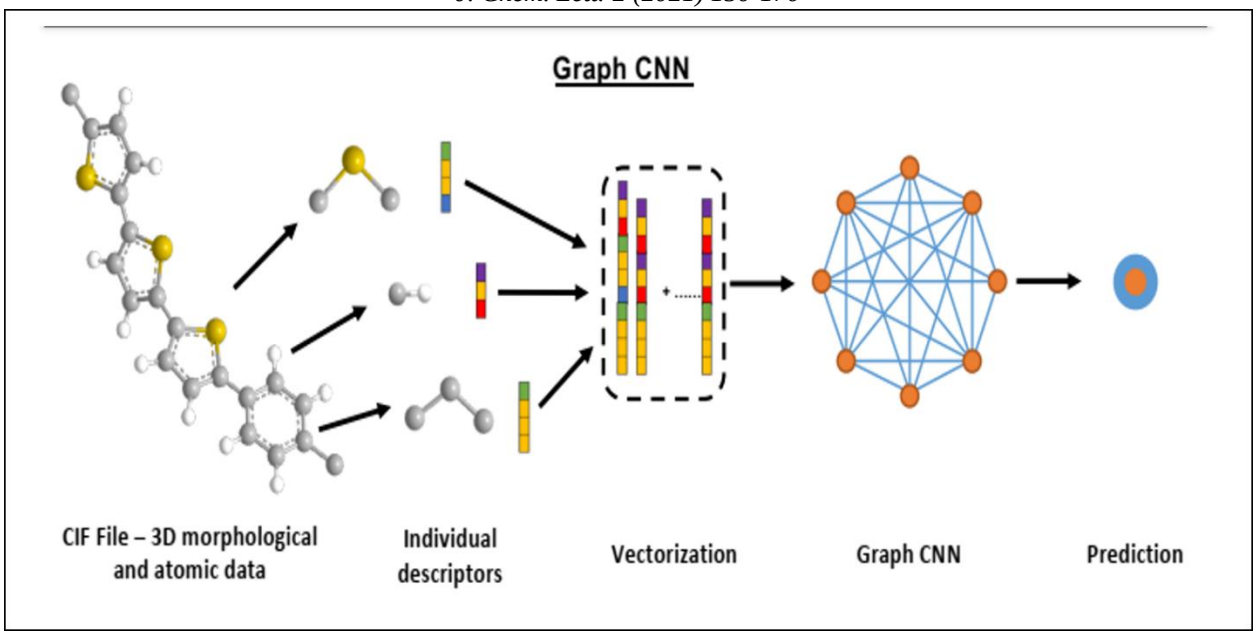
applied CNN and, then, investigated the link between the TC and molecular structure of polymers. Finally, they identified the assumed polymers possessing great TC. Their investigation showed this fact that polymers with functional groups like -(C= O) which possess strong bond strength present high TC due to the constrained rotation of segments. This is worthwhile to state that polymer chains with well-arranged spatial structures often have higher TC. Their general technique can be a promising method to present the systematic and screening identification of high thermal conductivity.

Researchers have applied a high-priced DFT on the small materials, but it can be used to predict the features of bulk polymers. As a section of the Harvard Clean Energy Project, a dataset with the size of 20,000 is made by scientists [54]. The excellent estimation ability of drug efficiency, photovoltaic efficacy, and solubility is provided by using a neural fingerprinting technique developed on a SMILES. This is the result of representing molecules on graphs with bonds as edges and atoms as vertices via a subset of Harvard Clean Energy Project data [55]. The use of direct morphological data instead of DFT for fingerprinting which reduces the material innovation time is an important improvement in the exploration of novel materials. However, a deep understanding of the related and most beneficial descriptors which affects the polymer features is needed. It has been found that the symmetry of inorganic crystals in which a long-range order is required can be reflected by the lattice, whereas the basis is the repeating unit. Nevertheless, polymers, as amorphous materials, do not display a long-range order because they do not conform to any lattice.

Nevertheless, this fact has to be considered that the ground state property, including the polymer bandgap and dielectric constant determined by the monomer unit can be well translated to actual applications. The dielectric constant which is the bonding nature result between the component atoms is the reflection of the polymer electronic polarizability and the bandgap is contingent on the bonding strength.

Considering these facts, everyone assumes that knowing the bonding type between atoms as well as the atoms constituting the monomer, as a fingerprint morphological character is enough to predict these features. Scientists can transform these data into a two-dimensional (2D) graph and then apply them as input into a CNN to estimate the mentioned characterizations [56].
In a comprehensive study carried out by Zeng et al. [57], the prediction of the bandgap and the dielectric constant of polymer compounds has been made by Elegant Graph Convolutional Neural Network (GCNN). Applying the different machine learning algorithms such as gradient boosting, random forest, graph convolution neural network, kernel regression, and conventional neural network, they predicted the energy band gap and dielectric constant of polymers. Their results proved that GCNN with the minimum average error for both features could make a quick and correct development in the field of polymer properties prediction. A schematic difference between the GCNN and traditional methods has been shown in Figure 12. Therefore, this method can provide the route for inverse design, in which polymers can be structured in mind with an ultimate property.

This study proved the fact that it is merely required to take into account the morphological features of polymers in order to obtain the accuracy and speed in predictions.




Traditional Methodology

| Polymer Lable | Descriptors | | | Properties | |
|---|---|---|---|---|---|
| | SMILES | QSPR | Morphology | Dielectric Constant | Bandgap |
| Polyurea | $D_{11}$ | $D_{12}$ | $D_{13}$ | $\varepsilon^1$ | $\varepsilon_g{}^1$ |
| Poly(vinyl chloride) | $D_{21}$ | $D_{22}$ | $D_{23}$ | $\varepsilon^2$ | $\varepsilon_g{}^2$ |
| Poly(2-cyanoheptyl acrylate) | $D_{31}$ | $D_{32}$ | $D_{33}$ | $\varepsilon^3$ | $\varepsilon_g{}^3$ |
| ... | ... | ... | ... | ... | ... |
| C6H4-C4H2S-C4H2S-C4H2S- | $D_{n1}$ | $D_{n2}$ | $D_{n3}$ | $\varepsilon^n$ | $\varepsilon_g{}^n$ |

**Figure 12.** Comparison between GCNN and other machine learning algorithms. The conventional techniques depends on hand engineered characterizations crafted from quantitative structure-property relationship, SMILE string polymers morphology. One considerable benefit of graph CNN is its capability to automatically learn the map polymer structure and the chemical environment of polymers to abundant feature vectors for a quick and correct prediction on polymer features [57].

Researchers have developed the models of Quantitative Structure-Property Relationship (QSPR) recently. To save resources and time in industrial development, this would be very important for the material designers to predict the new material's behavior before synthesizing them. This would also accelerate the scientific knowledge of structure-property linkage in polymer science. Especially, these predictions are more interesting when only the chemical structure of monomers is used since no information from complicated calculations or experimental evaluations is required. To establish the structure-property linkage among various QSPR modeling techniques, ANN has been introduced as an appropriate and helpful approach, particularly along with the fast improvement of graphical processing units (GPU) and computers [58]–[60].

In a work conducted by Joyce et al. [61], a fully connected network-based technique has been introduced with the hidden layers of more than three. In this work, the monomer chemical structure was partly presented by a numerical version of SMILES. Unfortunately, this method requires the addition of many numbers to every monomer code to consider other data like a position in the structure or element period, which can be expensive and difficult to automate and encode. In another study, Miccio et al. [8] used an ANN model with the ability to encode all of the structures and composition data that are contained in the SMILES code into a readable binary image. They focused on the Thermogravity (TG) prediction merely with the chemical structure of their repeating units (monomer) via a combination of CNN coupled with fully connected (FC) layers. It is worth mentioning that their method which does not need any

calculations or experimental measurements can be applied for the prediction of other polymer features, including fragility or polarizability.

The products of corrosion can cause environmental pollution. The degradation of alloys or metals due to corrosion can decrease their lifetime. Based on the studies, protecting layers can postpone these destructive consequences, among which the most efficient and easiest one is the corrosion inhibitor adsorption on the metallic surface [62]–[65]. On the numerical data such as the curves of electrochemical impedance spectroscopy and quantum chemical calculations, researchers used DL for the steel corrosion analysis under various inhibitors. The expectation that images need to keep further information on the already made coatings and their feature complication as well as the necessity for their automated representation cause DL to be the best option for this task [66]–[68]. In a study conducted by Samide et al. [44], the deep learning technology has been used to investigate the formed Polyvinyl alcohol (PVA) and Ag nanoparticles/PVA coatings on the surface of copper in 0.1 molL hydrochloric solution. To extract the dissimilarities/similarities between protected/unprotected surfaces and demonstrate the ability of PVA and nAg/PVA to slow copper corrosion, they organized the morphology of material surface via convolutional neural networks without any human influence. The electrochemical assessment proved the polarization resistance (Rp) enhancement and the corrosion current density (icorr) reduction with either nAg/polyvinyl alcohol or polyvinyl alcohol. Hence, they can be introduced as efficient inhibitors of copper corrosion in an acidic environment which can make the protective coatings of polymer-metal surface adsorption.

Studies have shown that the filler addition to the matrix can enhance the mechanical, optical and dielectrical features of polymer nanocomposites in comparison with the unfilled matrix system [69]. A variety of micromechanical models, including Halpin-Tsai, Mori-Tanaka, and self-consistent schemes have been used by researchers in order to predict the thermomechanical characterization of nanocomposites [70]–[72]. To completely capture the morphology information or dispersion state of the applied fillers, these analytical techniques are insufficient while the models usually include structural features. To investigate the nanocomposites behavior, Finite element (FE) simulations, as the best option for this goal, can thoroughly capture the structural information and also adjust the systems of non-homogenous material with a clear configuration of all material phases [73]–[75]. The data-driven methods founded on the process-structure-property (PSP) linkage, as a significant area in material science, have received considerable attention combining statistics, computer, and material science [75], [76].

In the field of nanocomposite, scientists have developed NanoMine which is a data-driven web-based program to computational archives as well as experimental data on nanocomposites. This platform includes measured features, processing techniques, composition, and microstructural images of nanocomposites to provide visualization and quick data queries [77], [78]. In another work, researchers applied NanoMine data to develop a data-driven technique for modeling the relationship between structures and processing [75].To design and model the new structures and systems, including the design of computational models, experiments, and machine learning techniques, a simulation-based data-driven system was developed by researchers in another study [76]. DL can be used in material science, especially when the structural images are studied. For example, a deep convolutional network was used by Yang et al. [79] to design structure-property linkage for the microstructures of a high-contrast elastic 3-D composite. To investigate this linkage for polymer nanocomposites, Wang et al. [70] applied a database of simulated data. The exploration of a broad range of structures and the capability to produce and analyze a considerable amount of data can be presented by the flexibility provided by simulations. The first study to create a structure-property relationship to predict the mechanical characteristics of polymer nanocomposites has been conducted by them via experimental data from NanoMine. In this research, there are three property interests among the mechanical features of the bulk composites, including rubbery modulus, glassy modulus, and tan $\delta$ peak. First, they examined the effect of the microstructure descriptors (filler dispersion and composition, interphase) and the mechanical features by using both the finite element simulations and microstructure reconstruction techniques. Then, a combination of multi-task learning and convolutional neural networks was presented by them to quantitatively estimate the relationship between the property values and microstructure. The presented deep learning method can enhance the prediction accuracy of rubbery modulus, glass modulus, and tan $\delta$ peak as much as 34.2%, 45.2%, and 19.7%, respectively. It has also the potential to be generalized to realize other features and material mechanisms along with the guidance for the design of the material with given performance.

The great stiffness-to-weight and strength-to-weight ratios of polymer composites made them the main component for spacecraft and aircraft construction. Generally, the fabrication process of highly performed composite parts can be performed done by autoclaves in which a circulating flow of air is applied to heat them [80]. Microwave processing technology as compared with conductive heating has low energy consumption and short processing time. There is, however, one problem regarding the use of this technology, which is the unbalanced distribution of electromagnetic field, resulting in the uneven temperature on the surface of the composite. So far, various methods have been introduced

for the temperature uniformity improvement on the composite material surface. Focusing on the device configuration optimization, some scientists improved the evenness of the static electromagnetic field via the enhancement of the number of electromagnetic modes or altering them within the cavity of microwaves. Hence, the temperature uniformity can be improved by possible incidental compensation impact existing between different modes of electromagnetics. In another effort, other researchers have attempted to create a relative motion between the electromagnetic field and processed material during microwave heating [81]. For example, in the food industry, a turntable was introduced by Cuccurullo et al. [82] to lead the food moving via alternative low and high power areas. However, these approaches are not successful to guarantee the high need for accurate temperature control on the surface of polymer composites during the curing process. Considering these shortages, an online smart temperature control based on deep CNN to realize a microwave curing process for high-quality composite materials has been developed in 2019, as displayed in Figure 13. In this study, Zhou et al. [80] applied CNN to learn the composite temperature performance during curing under different strategies of microwave control. They introduced the provision of proper solutions to the various distributions of temperature with considerable improvement in comparison with current representative approaches.

In another attempt, Li et al. [81] reported a study in which a new data-driven technique has been suggested to model the complicated linkage between heating pattern (HP) and microwave control strategy (MCS). They employed many historical HP-MCS data to train and test an optimized CNN as their selected numerical tool. Then, they applied this well-trained CNN in order to give the result: MCS of the monitored uneven temperature distribution during the process of microwave curing. Based on their results, a 13.7%~43.9% of temperature reduction in temperature change has been obtained during the curing process of polymer composite microwave. This is along with the reduction of about 53% in temperature difference in comparison with the current techniques that can prove the efficiency of this approach. Despite the unique advantages of composite structures, including the corrosion resistance feature particularly under the freeze-thaw cycle effects and great strength to the weight ratio in engineering application, they have some disadvantages. These disadvantages are normally hidden and may cause disastrous structural failures. They are not only easy to delaminate but also liable to fiber crack and matrix breakage. The external as well as internal damage can be the result of the production process, design techniques, and quality control. Because of the increasing demand for high strength and lightweight materials in the market in special applications, fiber-reinforced composites (FRC) composed of natural or synthetic materials have gained more attraction. The introduction of either natural or synthetic fibers in composite material fabrication has

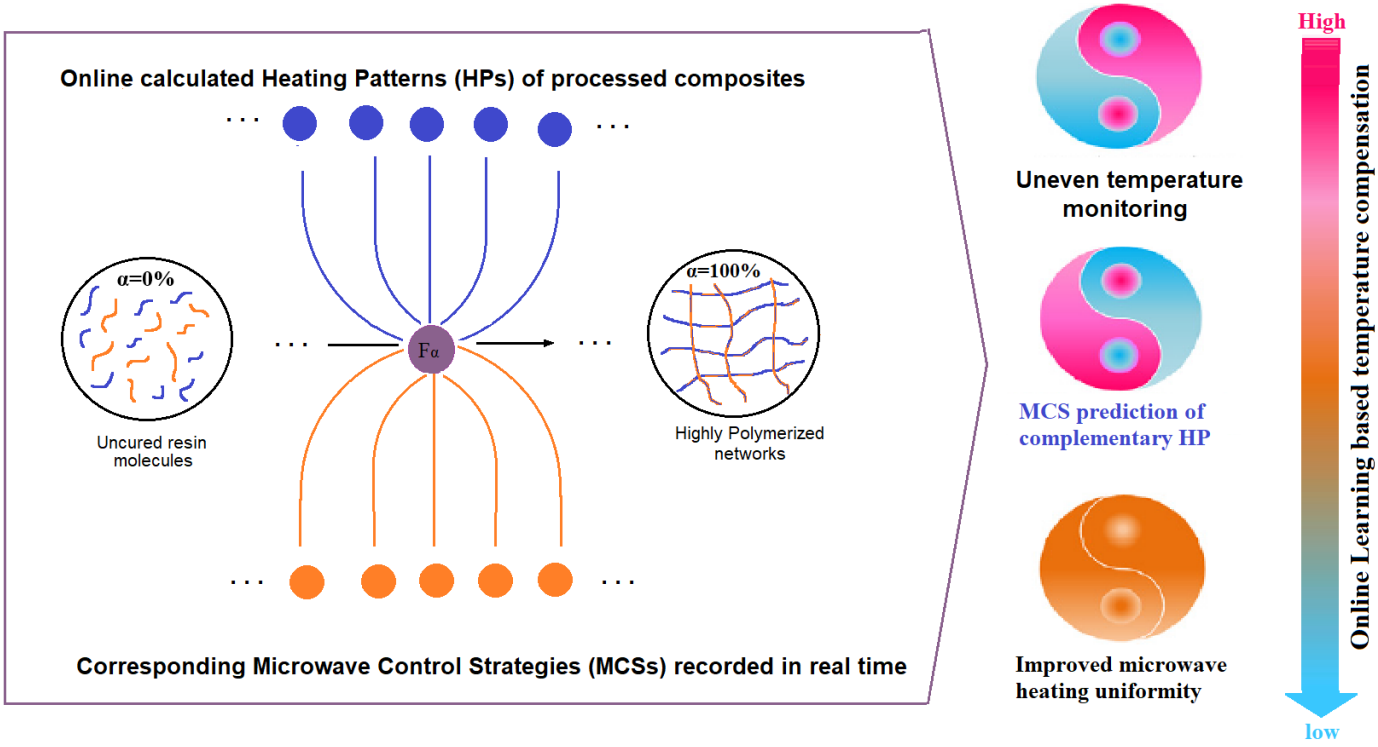



**Figure 13.** Online learning according to the smart temperature control during polymer composites microwave curing process [80]

disclosed important applications in several fields like automobile, aerospace, biomedical, mechanical, construction, and marine areas. The failures induced by bend, tensile, temperature, corrosion, strain, unsuitable

installation, and attachment join, as the principal failure modes of FRP, are complicated and their identification, localization, and quantification are difficult, particularly during the shared impact of several factors. Infrastructure systems are degradable with time and can be damaged under natural dangers as well as other unpredictable disturbances. Hence, the construction of endurable, ecological, and resilient infrastructure systems is of importance.

One of the most significant civil infrastructure components, utility and gas pipeline networks, and systems, should be appropriately designed to withstand failure and damage during their lifespan. Different analytical and monitoring techniques have been developed for damage detection like a conjugated beam method (ICBM), the theory of long gauge stress influence line coefficient for damage identification. In addition to them, the bearing capability evaluation of a bridge and electrical capacitance sensors for the fatigue damage detection of composite pipeline systems have been introduced. To collect the vibration signal reaction of soil surrounding the pipeline and categorize several types of activities by an artificial neural network, Wang et al. [83]

applied a long-distance fiber which was based on the sensing and monitoring system. Another promising approach reported by scientists is modal macro strain-based damage detection as it is more effective and sensitive compared with other related techniques. Proposing a modal macro-strain (MMS) vector, researchers have verified an effective damage detection algorithm for the damage localization of flexural structures using the extraction of modal parameters from the dynamic macro-strain responses. It is not easy to assess the structural health condition in real time when we are involved with complicated industrial and civil structures and there is the corruption possibility of measured structure signals because of the environmental noise. The necessity of a non-modal-based technique for the damage identification of these structures can be addressed by DL because it possesses adaptive and superior dataset learning. In a study conducted by Zhao et al. [84],

the analysis of a pipeline system of basalt fiber-reinforced polymer (BFRP) is reported which was done by long-gauge distributed fiber Bragg grating (FBG) sensors. The reflection of internal damage to images when they are taken from the outside of the structures would make it difficult to go for the damage identification application based on the image. Thus, the deep learning usage for image-based damage identification can only be effective in detecting external structural damages. Besides, these images may include various amounts of shadow and light and noise disturbance. To create a category of 1.2 million high-quality images in this work, they utilized a large deep CNN and prepared a 3D beam-based damage identification to reflect the exact structure status instead of a 1D model. In comparison with direct image extraction techniques for damage diagnose in this method, which is markedly appropriate for the variable and complicated environment, firstly the plot distribution map of structural modal macro strains which is sensitive to structural hurt is studied. Then, the convolutional neural network is applied to train and test these "feature maps" to recognize the support and external excitation location as well as the damage extension inherently. The processing of structural fiber-reinforced polymer composites to produce the materials that have with the desired fatigue, stiffness, strength, and resistance to environmental impacts can be in the form of a thermoplastic and thermoset resin into a fabric system via the polymer matrix penetration.

Improved structural composites have provided their widespread use in military aircraft and civil applications due to the high level of maturity in terms of design and manufacturing process. To optimize materials and cost reduction in the future, the automation of process steps, the increase of part integration level along with constant demand for zero-defect manufacturing, guided by The Fourth Industrial Revolution (or Industry 4.0) can be a significant step. A dry cloth covered and put into a mould to saturate with a liquid resin by imposing a pressure gradient is the beginning of the Liquid moulding of composites (LCM).

Today, LCM approaches can deliver composite articles with complex shapes and high-quality industries. This fact, however, has to be considered that the main challenge with them would be the natural uncertainty about the flow patterns created when resin saturation is severely influenced via various processing disorders. To make the first examination of machine learning techniques to identify automatically flow disorder resulting from the presence of unlike regions of the permeability in LCM, González et al. [85] used a supervised regression machine learning system according to the CNN. Using this method, they estimated the size, position, and relative permeability of a dissimilar material region during the manufacturing of composites by LM (liquid moulding). The presence of a region of dissimilar material causes the deformity of the pressure field. This is followed by the flow patterns detected via by analyzing the pressure alternations registered by a distributed network of sensors. They found that the effectiveness of CNN techniques in overcoming the physical and engineering challenges relating to various datasets was closely allied to the Industry 4.0 concepts.

Recently, the realistic models of woven composite materials have been developed significantly. The current production technique for the material finite element model is classified into three categories: (1) Ideal geometry creation based on the statistical data such as tow level analysis (2) Geometry extraction from the numerical simulation results like the simulation of fabric

density, and (3) a A model development based on actual microtomography (μ-CT) images. The first method is the most evident way to get the model; however, creating an ideal geometry that is close to the real shape seems difficult and the resulting volume of the ideal tows can be lower than the real one. To create a real shaped model, in the second method, the geometry of the fabric is produced from a simulation.

Again, of this method is the regulation of the model parameters required to get the favorable shape. The third method is modeling textile geometry based on μ-CT information, which includes image-based meshing and μ-CT image processing. Again, the usual complexity of μ-CT image processing results in a low resolution and contrast among various material constituents such as resin and carbon is the major challenge. Manual segmentation, an alternative to automatized segmentation, can be time-consuming because of the size of these datasets's size.

To find an efficient image segmentation technique for μ-CT data of carbon fiber reinforced polymers (CFRP), comprising of a simple woven tows structure at the meso-scale with a low contrast to noise ratio, Sinchuk et al. [86] used two methods, including a variational approach and convolutional neural network. The X-ray imaging data of carbon composites may be of low quality, which makes them difficult to segment. These reasons include the low resolution of μ-CT data depending on the diameter of the fiber, and low μ-CT data resolution between the material constituents. In this study, they made limited modifications to the network structure and evaluated the various criteria and concluded that the best results are obtained with a deep learning approach with U-Net neural network. Generally, this proposed solution can considerably expand the image range, which is applied on the automatic preparation of the realistic textile geometry. In comparison with manual dataset segmentation, their methods displayed reasonable results, even for noisy μ-CT data.

*2.6. Deep belief networks*

The greater performance of DBN (Deep belief networks) in language processing and image recognition has been confirmed recently. DBN consisting of four or more layers is the kind of deep neural network with a deep structure trained in two training stages, including supervised and unsupervised training phases [87]. The principal DBN theory is that it takes Restricted Boltzmann Machines (RBMs) into account as the hidden layers in which one RBM can be as an individual single layer. DBN is constructed via stacking various RBMs. There are merely two layers in the RBMs: the hidden layer and the visible layer consisting of hidden units and the visible units, respectively. The hidden layers are applied as a feature vector, while the visible layer is used for the training data input. Every layer is represented as a vector, while every dimension can be represented via every independent neuron. The advantage of this is providing the values of all the explicit elements that are independent of each other. The features of the explicit layer can be extracted more precisely by the trained TRB machine. This trained machine can also restore the explicit layer based on the represented features by the implicit layer. As displayed in Figure 14, different RBMs can be connected to create a DBN. In these networks, the hidden layer of the prior RBM is the visible layer of the following RBM machine, meaning that the output of the previous RBM machine would be the input of the later RBMs. Before training the RBM in the current layer, the full training of the RBM in the higher layer is required in the training process. This technique continues to the last layer. [22]

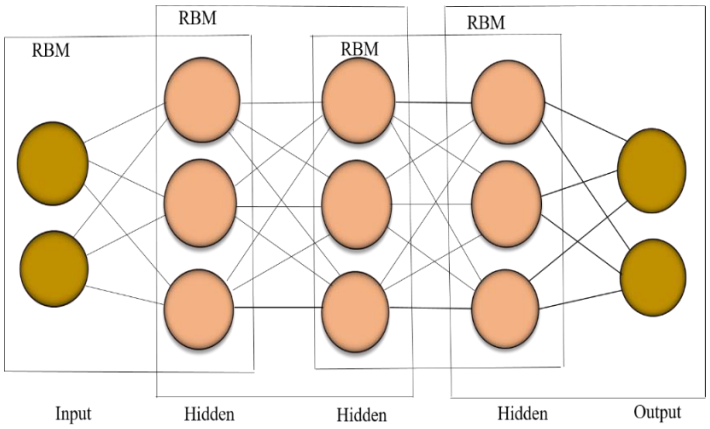



**Figure 14.** Different RBMs are connected to create a DBN.

Modern monitoring approaches require to be introduced for the production system in the industry because hardware measurement instruments to assess the variables of product quality online are not cost-effective and they are not easy to be developed. Based on the connection modeling between hard-to-measure quality variables and easy-to-measure process variables, many important variables of product quality can be easily measured. To do this, soft sensors are introduced, among which the data-driven ones have attracted much popularity in the chemical process in the last two decades. Because of the great generalization ability of DBN, Zhu et al. [88]
used it to estimate the melt index of produced polypropylene via continuously stirred tank reactors (CSTR) during an industrial polymerization system. Melt index as the main variable for the representation of polymer quality and a difficult value to be evaluated online is related to some easy-measured process variables although the relationship is commonly nonlinear. In this study, the development of nonlinear empirical models is required as the propylene polymerization process is nonlinear. To determine a DBN model structure, no common rules have been defined. The number of 25 various DBN models with different neuron numbers was constructed to compare the performance of different DBN models where the testing error is the principal

element for the determination of the DBN structures in this work. The presented DBN models possess a visible layer, two hidden layers as well as an extra top layer for training. Weights, as the most significant parameters of the model, can be regulated in suitable regions via RBMs, and then DBN will be well-tuned via back-propagation. Once the model is trained from primary weights, neural networks give weak results. Hence, the unsupervised training process can be efficient and crucial for the DBN model. As mentioned before, a DBN model development includes supervised and unsupervised training processes. The input layer units are chosen as Gaussian units since the process variables are continual and the hidden layer units are usually selected as binary units. After the unsupervised training of the DBN, an extra top layer is added to the developed RBMs whose weights can be initialized incidentally and the whole DNN can be trained through the gradient descent and backpropagation method. The weights can be adjusted in great regions by DBN which uses plenty of information behind the process data. The learning rates of 0.0015 and 0.001 have been selected for the supervised and unsupervised training techniques, respectively. The most suitable model structure is the model with the smallest testing error. They divided the 383 pairs of quality and process data into three sections (i.e., training, testing, and validation dataset). According to the cross-validation method, to train DBN and test its model performance, the training data and testing data have been applied respectively. After the determination of the model structure by testing the data, the final chosen DBN model, was validated by validation data.

Using a modern semi-supervised learning method, the deep belief network model showed better performance with the precise prediction of MI compared with the conventional neural networks. This is so due to the fact that the prediction of polypropylene MI by DBN can be improved by the 'unlabeled' process data, which cannot be applied by conventional process models. Therefore, it has been found that the DBN models are the best options when we have more samples of process variables accessible. Finally, they concluded that a deep belief network could be applied as an appropriate method for nonlinear chemical operations for hopeful applications in an industrial chemical process.

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**Table 1.** Some information about the architecture, datasets and parameters applied in some referenced studies

| dataset | Input layers nodes | Hidden layer numbers | Output layer nodes | Activation function | Loss function[1] | Dataset size (training test, validation test) | Accuracy | Ref. |
|---|---|---|---|---|---|---|---|---|
| two sets of scattering intensity datasets for the phenyl ring deuterated and fully deuterated PS | 2 | 4 layers each with 25 nodes | 1 | Sigmoid | MSE | Dataset size: 10'000 | MSE: 6.9*e-7 | [19] |
| TC dataset of polymers | A list of integer identifiers of 250 | 1-3 Conv[2] ., 1 pooling layer, 3FC[3]. Layers | molecular structure | NR.[4] | RMSE[5] and MAE[6] | Training: 90% | 94.79 | [48] |
| polymers and their solvents/nonsolvents | Two branches: Polymers and Solvents | Solvent branch:2 Hidden Layers, Polymer branch: 3 | 1(Binary classification: Good Solvent/NonSolvent | PReLU[7] | NR. | 4595 Training: 90% Test: 10% | 93.8 | [20] |
| Generated by normal distribution | 5 | 9 | 2 | ReLU | MSE & MAE | 1million Train:80% Validation:10% Test: 10% | Best loss: 5.577E-6 | [21] |
| polymers & their corresponding Tg | Binary Images of SMILES information | 2Conv layers, 1 Max Pooling, 1 FC | 1 neuron | ReLU | Median relative error | Train/test: 75/25 80/20 90/10 | 94% | [8] |
| scaffold images | 128*128 scaffold images | 6 | 3 | ReLU | Cross-entropy | 3043 train: 2376 Validation: 368 Test: 301 | 99.44 | [40] |
| available dataset at the Polymerge nome Project | two-dimensional graph | 2Conv, 1 Pooling Layer, 2 FC | physical property of polymers | A non-linear convolution function | MAE | 1073 Polymers Train:60% Validation:20% test:20% | MAE: 0.24 | [52] |

| | | | | | | | | |
|---|---|---|---|---|---|---|---|---|
| A dataset is created using generated microstructures and FEA model | 256*256 | 5Conv, 5Max Pooling, 2FC | 3outputs each with 1 Neuron | ReLU, sigmoid, tanh. | MAPE[8] | 11000 Data, Train:70% Validation:15% test:15% | mean of MAPE across trials: of: glass modulus/rubbery modulus/tan $\delta$ peak: 0.68%/ 3.12%, 3.58% | [70] |
| 3-D microstructures ( MVEs) | elastic 3-D composites (51*51*51 data) | 2Conv/ 2 Pooling Layer/ 1 FC | Effective property of given microstructure. | ReLU | MASE & MAE | 8550 data | MASE/MAE: 3.1% | [79] |
| HP-MCS data pairs | HP or Heating Pattern(4*3 data) | 3Conv / 2 FC | MCS or Microwave Control Strategy (21 nodes) | ReLU | MSE | NR. | 92.5 % | [80] |
| HP-MCS data pairs | HP data(4*5 matrix) | 3Conv / 2 FC | MCS | ReLU | MSE | 3000 Pairs Train:90%, Test:10% | 92% | [81] |
| NR. | PSD of MMS 256*256 Image | 2Conv/ 2Pooling /1 FC | damage types of pipeline systems | Sigmoid | NR. | 6800 Train/test: 6000/800 | 98.42% | [84] |
| pressure probes footprint images obtained with the mould filling simulations | 100*9 Images | 2Conv/2Max Pooling/3 FC | 5 nodes (correspond to 5 position) | ReLU | MSE | 3000 Images Train/test: 80%/20% | 99% | [85] |
| CFRP dataset | 3D gray-scale µ-CT Images | 32 Layers | NR. | NR. | NR. | NR. | Raw Imgs: 95.27, gradient images: 92.5 | [86] |

Loss: the error prediction of NN/ 1) Loss function: the approach of the loss calculation / Optimizer: to decrease the loss value, optimization techniques or algorithms (optimizers) including learning rate and weights is efficient. Optimizer for [24], [25], [26], [8], [45], [57], [79] is Adam. For [53], [81] and [85] is Adaptive moment estimation optimization method, Mini-Batch Gradient Descent and Adadelta, respectively. For other references is NR. Libraries / Platforms: Tensor Flow: [24]; Keras: [26], [85]; Keras and Tensor Flow: [79]; Keras with Tensor Flow backend: [70]; other references: NR

2) Convolution layer
3) Fully connected
4) Not reported
5) Root mean square error
6) Mean absolute errors
7) Parametrized rectified linear unit
8) Mean absolute percentage error.

## 3. Conclusion

There has recently been a huge increase in the usage of polymer and polymer composites in different areas. Based on this tremendous demand, researchers need to update the production system of these materials based on a smart manufacturing approach to optimize and accelerate their process system. Additionally, there is an urgent need to improve the polymer and polymer composites systems to increase the efficiency and decrease the environmental problems as well as the costs of failure, defect, and danger. Significant polymer features, including polymer structure factor, thermal conductivity, crystallinity, solubility, etc., as controlling factors, can play a crucial role in various industries like pharmaceutical ones. Besides, the linkage between structure and property can help researchers and industries improve their production landscape. Therefore, data-driven methods in the architecture of ML, especially DL can pave the way for researchers and manufacturers. In this review article, we tried to present a comprehensive classification based on the most applicable DL techniques in the field of polymer and polymer composites. This paper reviewed the use of DL method for the design, synthesis, and process system of polymer and polymer composites. We also discussed the advantages of DL usage in the polymer and polymer composite applications, which could make a huge difference in their safety and quality control. Based on our overview, CNN is the most popular technique with polymer technology researchers because it covered the vast scopes of applications ranging from the structure-property relationship to smart manufacturing. While for the

applications associated with the monitoring polymerization process, like tuning the MWD from a reaction system, DRL is the best option for researchers.

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