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Application of Artificial Neural Networks in Chemical Process Control

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Authors' contributions

This work was carried out in collaboration between both authors. Both authors read and approved the final manuscript.

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Review Article

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ABSTRACT

An important data-driven model is the artificial neural network. Artificial neural networks have been widely used in many domains of chemical processes due to its robustness, fault tolerance, self-adaptive capability, and self-learning ability. For the chemical process with nonlinearity and strong coupling, artificial neural networks can model and control the process well and make up for the lack of traditional PID control technology. As a result, ANN has emerged as a significant positive trend for chemical process control. In this paper, the principle, development history, and common structure of artificial neural networks are first outlined. Then the role of artificial neural networks in chemical process control is introduced in three aspects: improved PID control, improved model predictive control, and for hybrid models. The important effect of artificial neural networks in chemical process control is reflected by comparison. Finally, it is proposed that chemical process control can be more developed by applying more deep learning algorithms and developing multiple neural networks and hybrid models in chemical process control.

Keywords: Artificial neural network; process control; chemical process; model predictive control; hybrid model.

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1. INTRODUCTION

Since the concept of “deep learning” was introduced, the development of artificial neural networks (ANN) has been in full swing. ANNs are nonlinear, adaptive information processing system composed of a large number of interconnected processing units. As an effective empirical modeling tool, ANNs have functions such as associative memory, nonlinear mapping, classification recognition, and optimization computation [1-3]. ANNs are "black box" model that do not require in-depth knowledge of the intrinsic connections and patterns of input and output data. With a large amount of data, a neural network model can be trained and validated, and then the model can make effective predictions of the output from new inputs [4,5]. As the core technology of artificial intelligence, ANN has been widely used in intelligent control, pattern recognition, and nonlinear optimization.

The chemical industry is an important area for the application of ANNs. The data of chemical production processes is sea-quantized, high-dimensional, strongly coupled, nonlinear , and dynamic. The complex data brings great difficulties to the optimal control and fault diagnosis of chemical processes. ANN has the advantages of processing such high-dimensional nonlinear data. ANN was first applied to chemical process fault diagnosis in 1988. Since then, ANN has gradually played an important role in CE fields such as chemical fault diagnosis, process control and optimization, physical property estimation, quality control, and cluster analysis [6,7].

Process control occupies an important position in the chemical process and is essential to reduce costs and increase efficiency and production stability in production. In the chemical process, a large number of control processes use PID control technology, which is a combination of proportional, integral and differential control algorithms. PID control has the characteristics of simple structure, easy realization, good control effect, and high steady precision [8]. In conventional PID control, there is a linear mapping relationship between the change in system characteristics and the control variables. However, many chemical processes are multivariable dynamic nonlinear systems with highly nonlinear and time-varying characteristics. Therefore, traditional PID control techniques are not effective in solving control problems for nonlinear chemical processes with large time delays. To improve the control performance of chemical processes, it is necessary to develop more accurate process models. Due to the complexity of chemical processes, it is difficult to obtain an accurate mathematical model to describe the process. Therefore, artificial neural networks, the "black box" modeling approach with arbitrary nonlinear mapping capability, strong fault tolerance, associative memory, and strong robustness, have been increasingly applied to chemical process control [9]. In this paper, the characteristics and development of artificial neural networks are sorted out, and how artificial neural networks are applied in chemical process control is introduced by cases.

2. OVERVIEW OF ARTIFICIAL NEURAL NETWORKS

2.1 Basic Principle and Characteristics of Artificial Neural Networks

The artificial neural network is developed based on the research of the biological neural system. It is a distributed parallel information processing system built by abstracting and simplifying the structure of biological neural network and its information processing mechanism [10]. A routine neural network generally consists of four parts: nodes, connections between the nodes, the weights associated with each connection, and the recipe for obtaining outputs from the inputs of the nodes [11]. These components are also associated with the biological nervous system, such as weights corresponding to the synapses of neurons and output signals corresponding to the output pulses. A simple neural network structure is shown in Fig. 1. The basic network topology is formed by several connections between nodes, and the information is input and processed by several hidden layers according to certain rules, and then output by nodes [12].

Artificial neural networks work in the form of curve fitting, which is essentially an empirical modeling tool. Compared with other computing methods, ANN has the following features: (i) Massively parallel distributed processing. This enables it to process a large amount of high-dimensional information simultaneously and quickly. (ii) Distributed storage. The data is stored in a dispersed form in different but interconnected neurons. This storage feature also makes ANN highly robust and able to draw appropriate conclusions from noisy data. (iii) The associative access makes it self-adaptive, self-

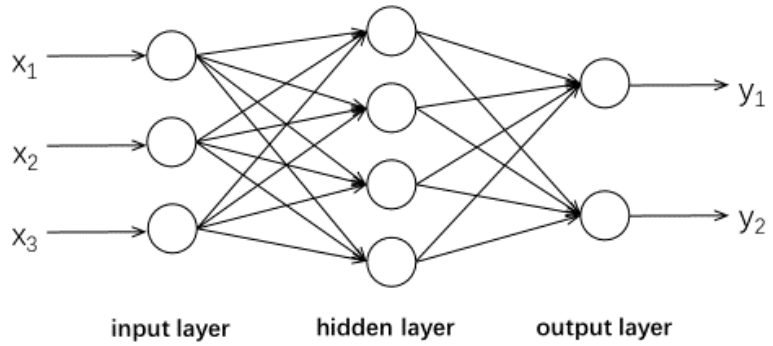

Fig. 1. Structure of artificial neural network

organizing, and self-learning. For example, ANN can adjust the strength of signals emitted by nodes by back propagation to correct for errors [13,14].

2.2 History of Artificial Neural Networks

In 1943, neurobiologist Warren McCulloch cooperated with young mathematician Walter Pitts to study the action of nerve cells by using mathematical models. The concept of the artificial neural network was put forward and an artificial neural network based on the simple logic operation was established, that is, the threshold component model of neurons referred to as MP model. This model proves that artificial neural networks can calculate any arithmetic and logic function in principle [15]. In 1949, Hebb proposed that information in neural networks is stored by connecting weights and established Hebb rules [16]. Since then, the study of the adjustment algorithm of the weights has been carried out. In 1958, Rosenblatt introduced the concept of "perceptron" based on the MP model with the addition of a learning mechanism. This neural network has self-organization and learning ability, which led to the first climax of neural network research [17]. In 1969, Minsky and Papert proved that neural networks can only deal with simple linear problems, and many complex functional relationships cannot be obtained through single-layer network training. At the same time, the actual effect of multi-layer networks is difficult to prove [18]. This conclusion brought the study of ANN to a low point for more than a decade.

In 1974, Werbos put forward the principle and algorithm of back propagation, which provides a feasible way for training multilayer neural networks [19]. In 1982, John Hopfield proposed the Hopfield neural network, which made it possible for neural networks to solve complex problems and triggered the second climax of neural network research [20]. Hinton et al. proposed the restricted Boltzmann machine (RBM), then developed the deep Boltzmann machine (DBM) and deep confidence network (DBN) [21]. In 1986, Rumelhart and McCelland rediscovered the backpropagation algorithm of multilayer forward neural networks [22]. In the same period, Werbos solved the problem of weight adjustment by the exhaustive analysis of multilayer backpropagation, and also solved the problem of the limitations of ANN proposed by Minsky [23]. The radial basis function (RBF) proposed by Broomhead and Lowe, which simulates the local response properties of neurons, allows the network to have a fast learning convergence rate [24]. In 1987, IEEE held the first international academic conference on neural networks, with more than 2000 scholars attending. In the 1990s, simpler methods such as support vector machines became more popular [25]. This method has no local optimal problem and can obtain ideal results in the case of fewer samples. Relatively, the computer performance and data size at that time could not support the training of large-scale neural networks. And the BP algorithm is prone to fall into local optimum solutions and overfitting when the number of hidden layers is too many. Neural networks have the disadvantages of vague theoretical basis, difficult optimization, and poor interpretability. These problems led neural network study to a low tide [26].

In 2006, Hinton and Salakhutdinov introduced the concept of "deep learning", which effectively solved the problem of difficult training of deep neural networks by "pre-training" and "fine-tuning" [27]. With the significant success of deep neural networks for tasks such as speech recognition and image classification [28,29], as

well as the rapid increase in computer computing power and the accumulation of large-scale data, ANN has ushered in another climax of development and has a wide range of applications. The main application areas are intelligent driving [30,31], automatic control of power systems [32,33], signal processing [28,34], health care and medical treatment [35,36], process control and optimization [37-39], image processing [40,41] etc. For example, artificial neural networks were used by Dalibor Petkovic et al. to optimize biodiesel emission parameters, estimate wind speed fluctuations, and predict calorific value of biomass [42-44].

2.3 Classification of Artificial Neural Networks

There are various ways to classify neural networks. They can be classified into continuous and discrete networks by variable type; feedforward and feedback networks by topology; and supervised and unsupervised learning networks by learning rules. Each type of ANN has its own characteristics. When applying, several factors such as the number of variables for the inputs and outputs of the process and the purpose of the application need to be considered in order to select the appropriate structure and method to increase the accuracy of the model [1].

With the development of ANN, there are hundreds of neural network models now [45], and some common forms of ANN will be introduced as follows.

2.3.1 Multilayer perceptron (MLP)

The multi-layer perceptron, i.e., feedforward neural network, has the structure shown in Fig. 2 [46]. Neurons in one layer are connected to all neurons in the next layer. Information is passed as indicated by the arrows in the directed diagram, so the data flows in one direction. The most important feature of this neural network is that it can learn and store a large number of highly nonlinear mappings without building a mathematical equation to describe the mapping relationships in advance, exhibiting excellent nonlinear matching and generalization capabilities [47,48]. The structure of MLP consists of input layers, hidden layers, and output layers. Among them, the number of neurons (nodes) in the input and output layers is determined by the actual situation of the problem under study, while the number of nodes in the hidden layer is determined by you. In an MLP, the weights of the connections start out as random values. Training is required to make the weights into suitable values. The common algorithms used for weight adjustment during training include back propagation algorithm (BP), gradient covariance descent (GCD), and Levenberg-Marquardt algorithm (LMA). The BP algorithm has become the most widely used algorithm for MLP due to its solid theoretical basis, rigorous derivation process, clear physical concepts, and high generality [6].

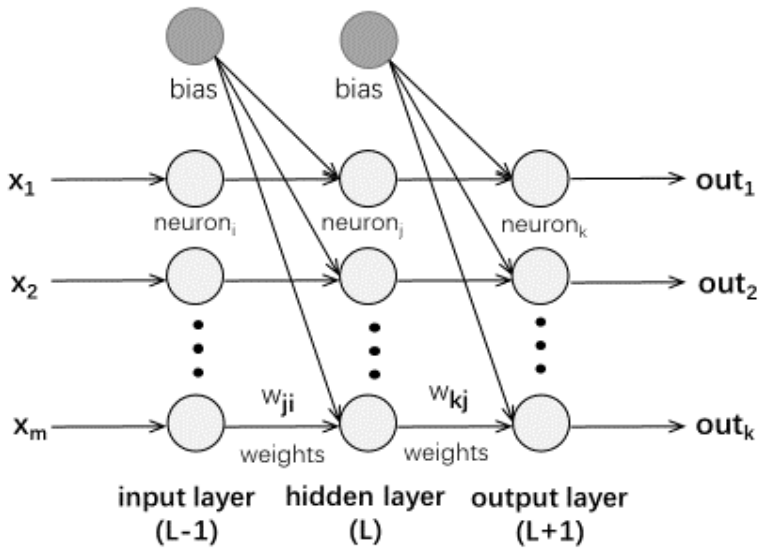

Fig. 2. The general structure of feed-forward neural networks

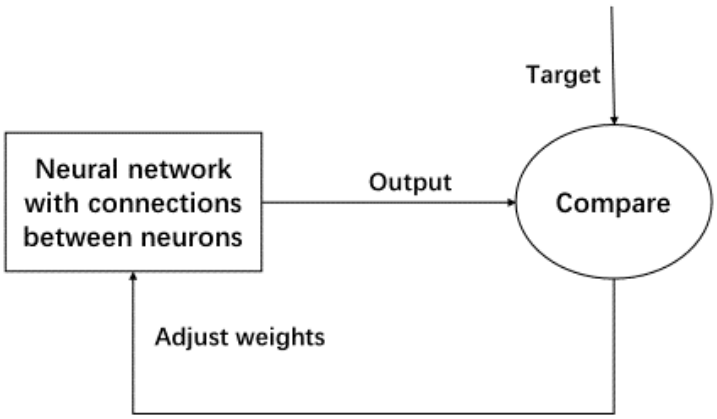

Fig. 3. Basic neural training method

The BP algorithm is based on the bias between the simulated value and the target value generated by forward propagation, and it continuously learns and corrects the weights and thresholds between the layers to minimize the error. It consists of a forward propagation process and an error backward propagation process. Forward propagation process: The control sample is introduced to the input layer and then transferred to the implicit layer for processing, and finally reaches the output layer. If the output of the output layer and the expected output do not meet the requirements, the whole network is transferred to the back propagation stage. Error back propagation process: After the output error is obtained, the error is transmitted from the output layer to the input layer and the weights and thresholds are adjusted according to the first-order derivatives of the error on the weights to reduce the error, which is the back propagation of the error. The whole transfer process is repeated until the target error is reached or the set number of learning times is reached, and the neural network ends the training [24,49]. Fig. 3 shows the basic training logic of ANN [50]. The BP algorithm is a supervised learning algorithm because it needs to constantly compare the output with the target value during the training process.

2.3.2 Radial Basis Function (RBF) networks

The RBF neural network is a three-layer feedforward neural network, and its structure is shown in Fig. 4. The transformation of the RBF neural network from the input layer to the hidden layer is nonlinear. The function used by the nodes in the hidden layer is the radial basis function, which is a non-negative nonlinear function with radially symmetric decay to the centroid of a local distribution. The commonly used radial basis functions are Gaussian function, thin-slab spline function, etc. Considering that the linear combination of signals from the hidden layer is sufficient to model any nonlinear function, the output nodes adopt linear activation functions [45,46,51].

When training an RBF neural network, the number of input and output units of the network is determined by the training samples, and the hidden layer has only one layer. The parameters to be determined include the number of cells in the hidden layer, the center vector and width

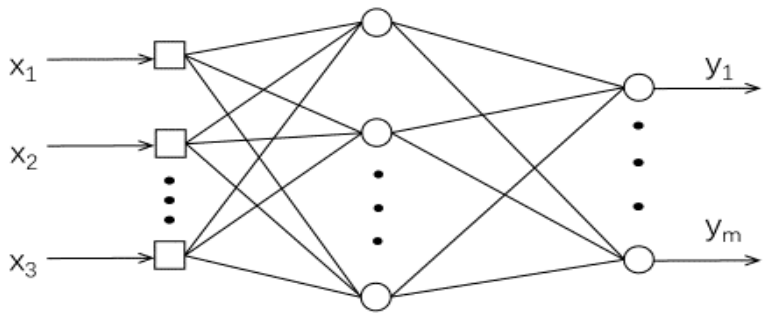

Fig. 4. Topological structure of RBF neural network

parameters needed for the Gaussian function, and the weights of the connections [52]. Compared with BP neural networks, RBF neural networks do not have the problem of local minima and have a faster learning speed [53].

2.3.3 Stacked neural networks

ANN is a data-driven model. Sometimes it is difficult to make suitable predictions due to the size limitation of the training set and overfitting, etc. [54]. Therefore, multiple neural networks with different structures can be combined into a whole, called ensemble neural network or stack neural network. In stacked neural networks, multiple neural networks have the same relation, but the structure and weights of neural networks are different. Learning methods and training sets may also be different [55]. Different neural networks give different results and these results are combined to get the output of the stack neural network. By this method, the final output is better than the outputs of each neural network, and therefore the stability of the neural network can be improved. An important part of stacked neural networks is the method of combining neural networks. There are various methods of combining neural networks, such as linear, nonlinear, super Bayesian, and stacked generalization [50].

Linear combinations of neural networks are more common. There are generally two types of linear combinations: simple averaging and weighted averaging. The common weighted averaging methods are principal component regression (PCR) and multiple linear regression (MLR). Non-linear combination methods are more complex, including majority voting, Tumer, and Ghosh method, etc. [56]. The structure of the stacked neural network is shown in Fig. 5 [57,58].

2.3.4 Artificial neural networks for hybrid modeling

The artificial neural network model is a data-driven model, which is obtained based on a large amount of data and certain algorithms. It does not require a lot of process mechanisms in the training phase and has the advantages of low computational effort, fast solution speed, and high accuracy in the range of data established by the model when applied. However, the complexity of the data affects the modeling and model performance, while the low interpretability and extrapolation of the neural network model become its disadvantages. Therefore, by combining the neural network model with the mechanistic model of the process, better model performance can be obtained by taking advantage of different sub-models [59,60]. Compared with the mechanism model, the hybrid model is easier to build and can accelerate the computation speed by replacing part of the mechanism model, which is beneficial to online assignments. Compared with the neural network model, the hybrid model brings certain physical meaning to the structure and parameters of the model, which is convenient for making decisions based on process knowledge, and also facilitates the downscaling and updating of the model to improve the applicability of the model.

The hybrid model has three structures: series, parallel, and hybrid. As shown in Fig. 6, FPM is the first-principles model, and DM is the data-driven model. When building hybrid models in general, a simplified dynamics model is built with FPM, while ANN is used to provide more accurate dynamics parameters for FPM [61].

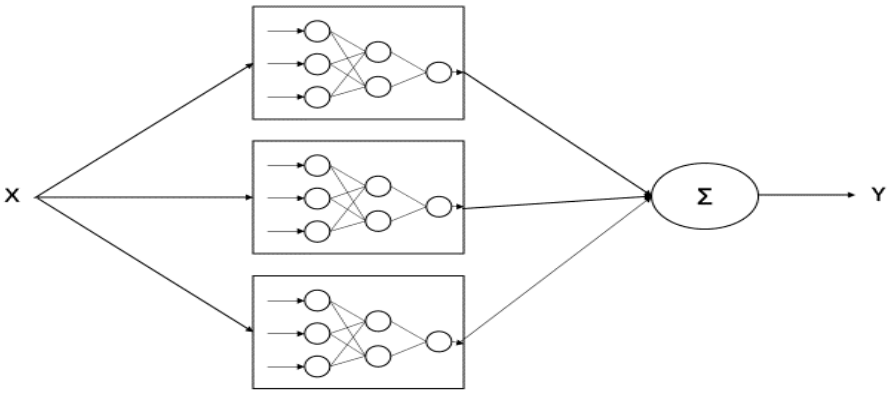

Fig. 5. Stacked neural networks

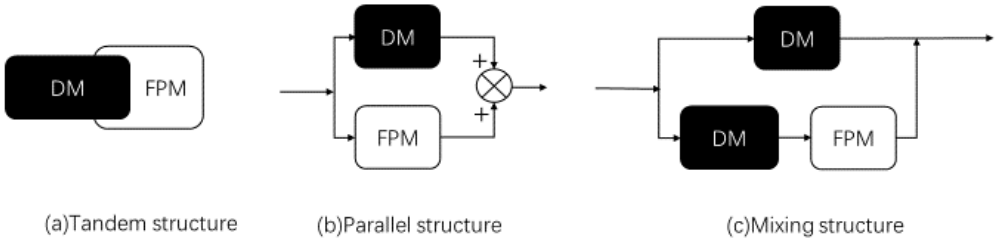

Fig. 6. Schematic of the structure of the hybrid model

3. APPLICATION OF ARTIFICIAL NEURAL NETWORK IN CHEMICAL PROCESS CONTROL

3.1 Neural Network-Based PID Control

Chemical processes are often complex time-varying nonlinear systems, and traditional PID control faces challenges in the face of such systems. Combining ANN with PID control, using the learning function of ANN to determine and adjust parameters of the PID control can effectively improve the performance of traditional PID control, and finally, make the control system with good self-adaptive or self-tuning ability [14]. At this point, the controller can be divided into two parts: one part is the structure of a traditional PID controller, which processes the deviation signals of the system by proportional, integral, and differential processing, and the results are weighted and summed by proportional, integral and differential coefficients respectively; the other part is a neural network model, which provides a part of the required parameters through iterative learning and adjustment based on the input and output information of the system [8].

Cheng et al. [62] optimized PID control using BP neural network to make the control system self-tuning. The control system comes from the FCC light gasoline etherification process. PID is utilized to control the concentration of light gasoline in this process. The control flow is shown in Fig. 7. θ and Φ represent the given and actual values of the flow rate of FCC gasoline, and the deviation between the two is denoted by e. In each sampling interval, PID controls the flow rate of gasoline by controlling the valve. To achieve a good control effect, the most important thing is to adjust the proportion of proportional, integral, and differential in the controller to find the optimal ratio of valve opening. Cheng et al. used a BP neural network to adjust the parameters Kp, Ki, and Kd of PID control.

Cheng et al. built a three-layer BP neural network, as shown in Fig. 8. The input layer depends on the state of the system, such as the inputs and outputs of the system at different moments, and the outputs are the three important parameters K_p, K_i, and K_d. The neural network continuously adjusts weights and biases through learning to achieve adaptive adjustment of PID control parameters. By building a simulation process with MATLAB, the researchers demonstrated that compared to traditional PID control, BP neural network-based PID control has smaller overshoot, shorter adjustment time, smaller steady-state error, and enhanced immunity to disturbances.

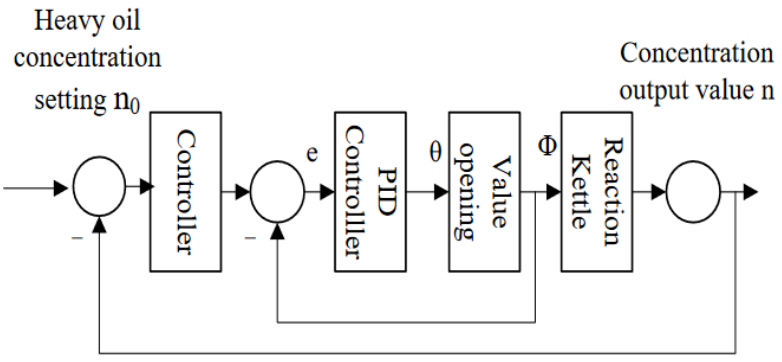

Fig. 7. Control principle of the gasoline concentration [62]

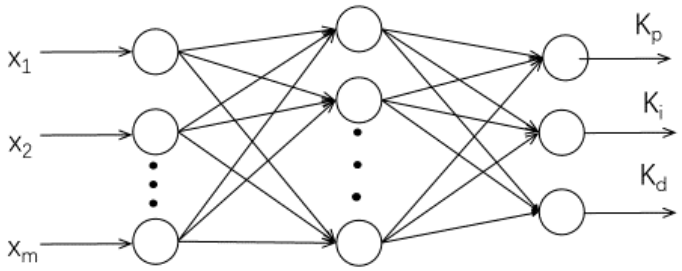

Fig. 8. Structure of BPNN

Similarly, Zhang et al. [63] used BP neural network to PID temperature control system of a beer fermentation tank, and established NNPID system as shown in Fig. 9. The BP neural network uses a sigmoid function as the activation function for the hidden layer and a non-negative sigmoid function as the activation function for the output layer. The momentum term is also added to prevent falling into a local minimum. The results of the simulation are shown in Fig. 10, where BPPID exhibits better static and dynamic performance. Zhu et al. [64] applied similar control systems to the main steam temperature system of boilers, and achieved good results. Ubaid et al. [65] used an inverse neural network in the temperature control system of a bioreactor for ethanol production and improved the steady-state performance of the system.

3.2 Neural Network-Based Model Predictive Control

In addition to combining traditional PID control techniques with ANN, more advanced control techniques have been gradually developed to achieve better control performance. Among them, model predictive control (MPC) has been widely used in plants since the late 1970s [66]. MPC is a class of computer control algorithms that directly use dynamic models to predict the future behavior of processes [67]. MPC manipulates controlled variables through predictions of the process model so that the future state of the process meets certain requirements, such as maximizing yield, minimizing cost, etc. The performance of MPC depends heavily on the quality of the process

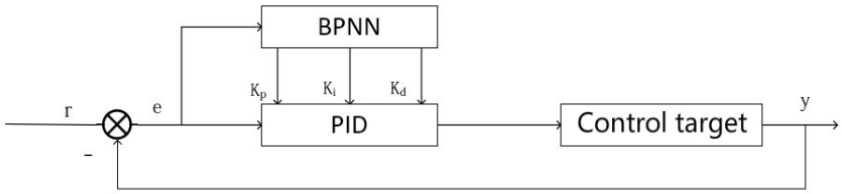

Fig. 9. The structure of NNPID

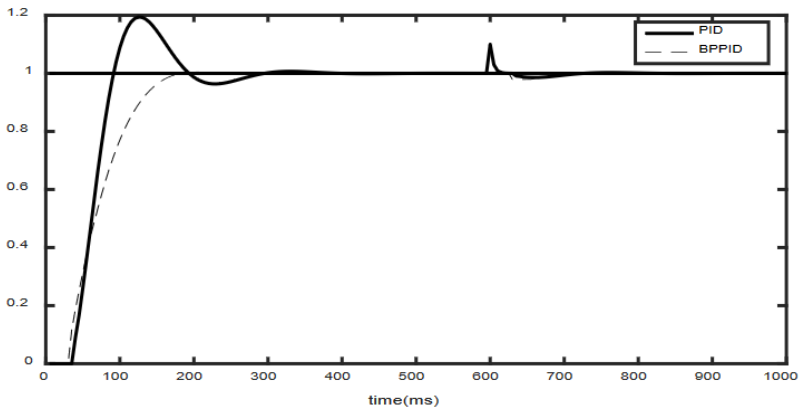

Fig. 10. The result of simulation

model, so the development of an effective process model is an important task required for MPC. In comparisons conducted by many researchers, MPC has better performance than PID control [68,69].

MPC can be divided into two categories: linear MPC and nonlinear MPC. Linear MPC is simpler to compute. However, for systems with nonlinear characteristics, nonlinear MPC has higher modeling accuracy. When MPC uses optimization functions, a large number of iterative operations need to be performed. The more complex the process model is, the more computation time is required to perform the optimization, which becomes a limiting factor in applying MPC [70]. For some chemical processes with many operating variables and a high degree of nonlinearity, real-time optimization by MPC is less effective [71]. Therefore, the MPC can play a better role in the chemical process with ANN's ability to predict future behavior with high accuracy.

Karol and Martin [72] applied ANN to a fixed univariate MPC system. The model predictive controller uses an algorithm called receding horizon policy proposed by Mayne et al. [73]. The repeated complex computation in the algorithm brings difficulties to industrial applications. Therefore, Karol et al. used a neural network model instead of a controller. The model takes the process variable *x*(*t*) as input and the manipulated variable u(t) as the training target. The initial training set is

$$\mathcal{X} = [x_{min}, \dots, x_{max}] \quad (1)$$

For each data point in the training set, the corresponding control action is calculated to form the set $\mathcal{U}$. $\mathcal{X}$ and $\mathcal{U}$ together form the learning data set for the hidden layer nodes of the neural network model. Eventually all nodes are aggregated. Karol et al. tested the performance of the experimental model with a multi-component chemical reactor. Reaction is $\mathrm{A} \rightleftarrows \mathrm{B} \rightarrow \mathrm{C}$. The process variable is the concentrations, and the feed concentration of component C is the manipulation variable. Thus, the input layer of the neural network includes three nodes and the output layer is one node. There are four hidden layers and each hidden layer has four nodes. 600 simulations were conducted after the model training, and the results are shown in Fig. 11. The controller performed with the optimality decrease below 1% in 94.5% of cases.

In 2020, Shin et al. [74] combined dynamic neural networks with MPC to develop a neural network model predictive control system (NNMPC). It was used in the control of a depropane tower to ensure that the variables would reach the set point smoothly in case of disturbances in the distillation system. The distillation process of the depropane tower is a typical multivariate nonlinear process. The operating variables in the process can be seen in Table 1. The ANN used is a three-layer feedforward neural network. The input layer consists of 14 nodes and the hidden layer consists of 15 nodes. The output layer includes 2 nodes, that is, the temperature of a specific tower plate and the propane molar fraction at the top of the tower. The model design process started with a mathematical model of the distillation column using Aspen HYSYS, and the neural network model was trained with the data generated from the dynamic simulation. After training was completed, the ANN model was integrated with the MPC system. The control flow of the system can be seen in Fig. 12.

Shin et al. compared the control performance of the NNMPC and PI controllers. As shown in Fig. 13, both control schemes were effective in ensuring the quality of the propane product ground when the disturbance occurred. However, the NNMPC was able to reach the set point faster, while the PI controller had a longer oscillation control time. Therefore, the NNMPC exhibits superior performance over the PI controller.

Table 1. Operational variables in the depropanizer

Manipulated variables (MVs)	Disturbance variables (DVs)	Controlled variables (CVs)
Condenser duty	Feed composition	Tower top pressure
Reboiler duty	Feed flow rate	Reflux drum liquid level
Reflux flow rate	Feed temperature	Reboiler liquid level
Overhead flow rate		Propane mole fraction in the overhead
Bottom flow rate		Tray temperature

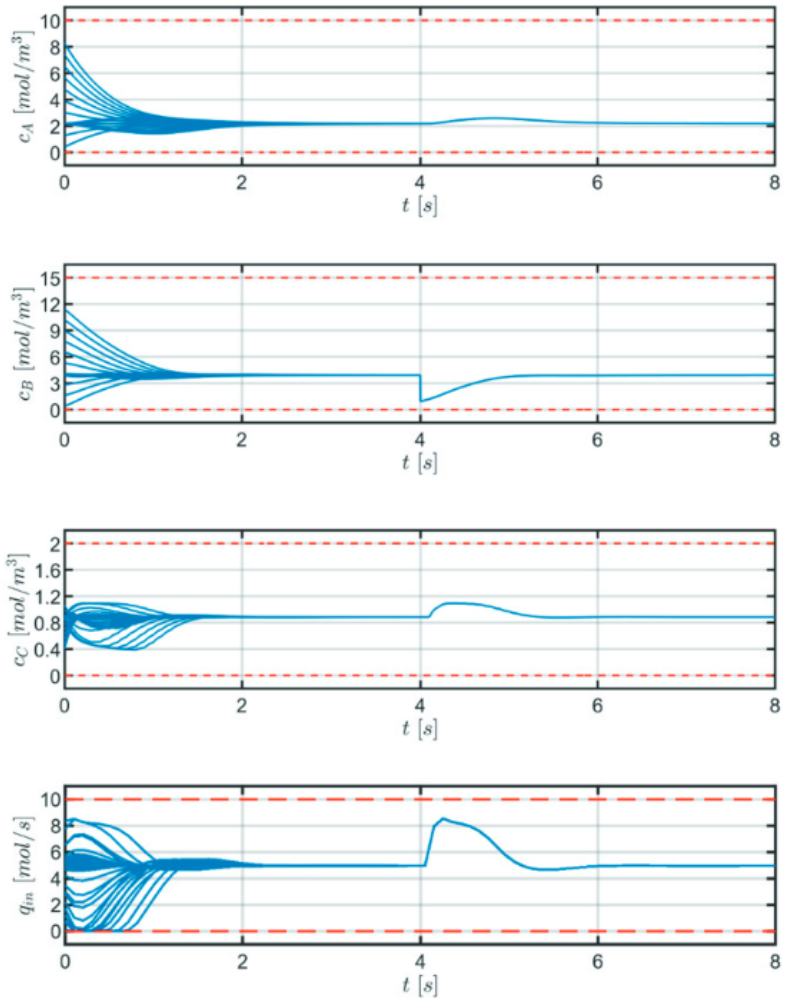

Fig. 11. Control performance of the NN-based controller with various initial conditions

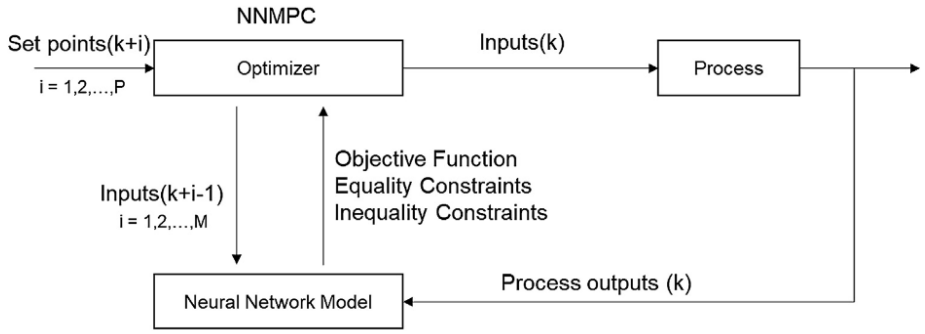

Fig. 12. Data flow diagram of NNMPC system

3.3 Neural Network-based Hybrid Model

As explained in Section 2.3.4, the combination of first-principles models (FPM) and data-driven models (DM) such as ANN can better model complex nonlinear, time-varying chemical processes [42]. These FPM-DM hybrid models with different structures are called "grey box" models. They avoid both the difficulties of building mechanistic models of chemical processes and the excessive desire for data by neural network models and can be better used in chemical process control [75].

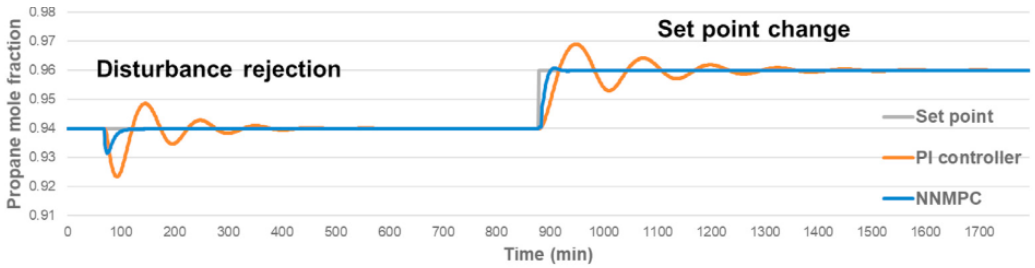

Fig. 13. Disturbance rejection and set-point tracking with NNMPC and PI controller

Xiong and Jutan [76] compared different control methods for temperature control of the continuous stirred tank (CST). First, there is the GMC controller using the mechanistic model. The approximate model of CST is expressed as a linear model:

$$y(t) = \frac{6.0067q^{-1}+1.9047q^{-2}}{1-0.6832q^{-1}}u(t-1) \qquad (2)$$

The control performance of the GMC controller using the linear model is shown in Fig. 14. The controller can perform well in the range of 40°C to 50°C, but as the set point gradually moves away from this range, the system gradually loses control. At 70°C, the controller completely failed. From this figure, we can also see that this linear model is only suitable to describe the variation of CST in the range of 40°C to 50°C.

Then a grey-box model GMC controller with the parallel structure combined with a neural network is used. Fig. 6 is a diagram of the structure. The control performance is shown in Fig. 15. The peak value that appears at the beginning of the experiment is due to the initial weights of the ANN being randomly given. Although the application range of the linear model is from 40°C to 50°C, this controller can still complete the task at 60°C to 70°C. This is because the self-learning capability of the ANN model compensates for the deficiency of the linear model.

From the comparison of the two controllers, the complementary advantages of the artificial neural network-based hybrid model (gray-box model) emerge. The combination of accuracy and model applicability has led to many applications of the hybrid model. For example, a tandem mixing kinetic model under the framework of a continuous stirred reactor (CSTR) was proposed by Chen et al. [77] The mechanistic model in the model was chosen as the easily determined linear CSTR mass balance equation, and then the more complex nonlinear part of the model was completed using an ANN model. The hybrid model effectively reduces the dimensionality of the input variables of the model, simplifies the model structure, and has good interpretability. The model was used in in-line internal model control (IMC) and used in an industrial distillation tower. The results show that under closed-loop IMC control, the spread of the error distribution around the setpoint is three times less.

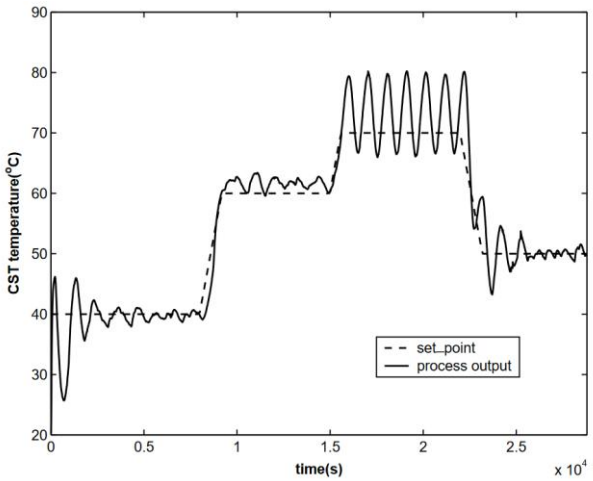

Fig. 14. CST temperature under GMC controller with linear model

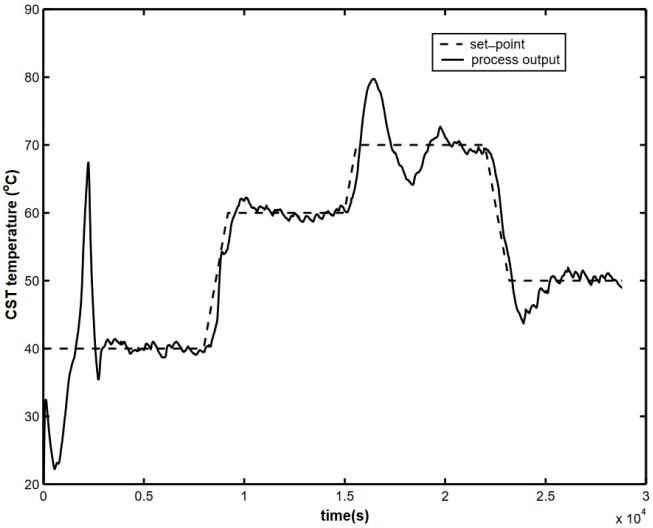

Fig. 15. Controlled CST temperature profile using grey-box model

4. CONCLUSION

This paper reviews the contribution of artificial neural networks to achieving control objectives for chemical nonlinear processes by assisting PID control for parameter self-tuning, providing process models for model predictive control, and participating in constituting hybrid models. It has been proved that artificial neural networks have played a significant role in the modeling and control of chemical processes, showing superior performance to the traditional control techniques for chemical processes. In particular, methods such as using stacked neural networks[33] and hybrid models to refine and complement neural networks may play a greater role in chemical processes. However, the structures of neural networks applied in chemical processes are relatively simple and still have great potential for development. The development and application of more complex and expressive models, along with enhanced database extraction for chemical processes, can take neural networks further in the field of chemical process modeling and process control.

COMPETING INTERESTS

Authors have declared that no competing interests exist.

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