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Application Progress of Artificial Neural Network in Chemical Industry

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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

The design and optimization of chemical equipment and devices and the control of chemical processes involve many factors and are very complex. The traditional methods and technologies cannot obtain satisfactory results. Artificial neural network technology has the ability to deal with complex objects and has been widely used in various engineering fields including chemical industry. In this paper, the research progress of artificial neural network in chemical industry is reviewed. The application progress of artificial neural network in signal peak recognition, catalyst optimization, industrial process, reaction process, physical data and other aspects is summarized. The advantages and limitations of artificial neural network in chemical industry are analyzed. Finally, the development trend of its application in chemical industry is prospected.

Keywords: Artificial neural network; reaction process; catalyst selection; physical properties data.

1. INTRODUCTION

Artificial Neural Network (ANN) is an operation model in the field of artificial intelligence, which has developed rapidly since the 1980 s. It simulates the structure of the brain nerve, which is composed of a large number of neuron connections, and has a strong ability to simulate nonlinear data. The self-learning and adaptive ability of neural network make it capable of dealing with unknown systems, and has the advantages of fast speed to find the optimal

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solution and good fault tolerance. Neural network used to be only used in the field of artificial intelligence, but its good nonlinear description ability makes it now has been used in many fields : health care, environmental protection, industrial production and market economy, etc [1-4]. For example, neural networks have been applied to information processing [5,6], language translation [7,8], image recognition [9,10], market analysis [11,12], complex process control [13,14] and other aspects, and have achieved excellent results.

In the first section of this paper, the structure and classification of artificial neural networks are given. Then, the application of artificial neural networks in chemical industry is divided into five parts: signal peak identification (2.1), catalyst (2.2), industrial process (2.3) and reaction process (2.4) optimization, physical property data (2.5). In these five parts, respectively, describes the artificial neural network in their fields commonly used model, and focus on its accuracy in use. Finally, in the third section, the advantages, limitations and development prospects of artificial neural networks in the chemical industry are discussed.

1.1 Structure and Classification of Artificial Neural Networks

The structure of artificial neural network is divided into input layer, hidden layer and output layer. The layers are connected by activation functions, and the neurons are connected by weights [15]. A typical neural network structure is shown in Fig. 1 [16]. The neural network is composed of minimum unit neurons. Neurons are a collection of many nonlinear functions, reflecting the complex mapping relationship between input variables and output variables. They have the characteristics of nonlinearity, unsteadiness, non-convexity and non-locality, etc. [17].

At present, there are more than 30 artificial neural network models, which can be divided into two categories by network topology or network information flow. According to the network topology, it can be divided into hierarchical structure and interconnected structure. Hierarchical neural network structure can be divided into input layer, hidden layer and output layer, respectively, responsible for data reception, processing and output; but any two nodes of the interconnected network are connected. According to the network information flow, it can be divided into feedforward network and feedback network. Feedforward network information processing direction is from the input layer to the hidden layer to the output layer, transfer layer by layer ;but all nodes of the feedback network have information processing capabilities and can interact with the outside world. Back propagation (BP) neural network widely used in various fields is a typical multilayered feed forward network.

In addition to BP neural network, the common ones are wavelet neural network (WNN) for image analysis, Radial Basis Function (RBF), Elman network for classification and pattern recognition, Counter Propagation Networks (CPN), Self-organizing Maps (SOM) network and other network models for statistical analysis [17]. Some new neural network designs and their performance are shown in Table 1 [18].

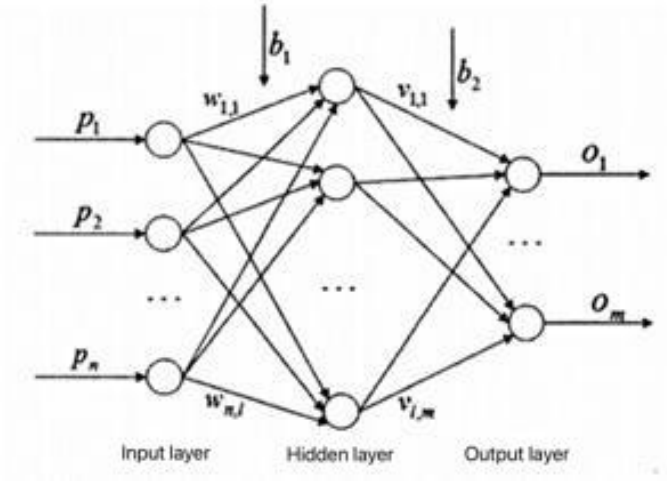

Fig. 1. Neural network structure

Table 1. New neural network design and its performance

ANN	Combination algorithm	Performance
MLP	Gray Wolf	Hidden layer connection weights more accurate
	Reduced Geometric Algebra	Processing multidimensional signals
BP	Adaboost	Higher accuracy, but lack of generalization
	Broyden-Fletcher-Goldfarb-Shanno (BFGS)	Convergence, accuracy improvement
	Particle Swarm Optimization	Closer to true than single BP, but accuracy decreases with step size
Region-CNN	Faster Region-Convolutional Neural Network(R-CNN)	Second-order network, more accurate, versatile, but slower.For image recognition
	Mask R-CNN	Better image segmentation, but huge computation

2. APPLICATION OF ARTIFICIAL NEURAL NETWORK IN CHEMICAL INDUSTRY

2.1 Identification of Signal Peaks

Neural network has superior performance in complex data recognition. In terms of spectral signals, the neural network uses the entire spectrum in the recognition process, not just a single peak. Hao et al. [19] used the symmetric point mode-deep convolution network to identify the infrared spectral data of alkanes and their mixed gases. The infrared spectra of single component and mixed gases of seven alkanes were transformed into images by semidefinite programming (SDP) and identified by Visual Geometry Group (VGG)19 convolutional neural network. The results showed that the network had better signal peak recognition performance.

Guo et al. [20] used Generalized Regression Neural Network (GRNN), support vector machine (SVM) and extreme learning machine (ELM) to analyze the dielectric spectrum to obtain the soluble solid content in apples. Principal Component Analysis (PCA), Uninformative Variable Elimination based on Partial Least Squares (UVE-PLS) and Successive Projections Algorithm (SPA) were used to extract feature variables from the full dielectric spectroscopy. PCA is a more powerful data compression method than UVE-PLS and SPA, but the performance of the development model based on PCA is not as good as that based on UVE-PLS and SPA. ELM model has less response time and better stability than GRNN and SVM models. Considering the calibration and prediction performance, stability and response speed, ELM-SPA model was considered to be the best model to predict the soluble solids content of three apple varieties.

2.2 Catalyst Selection

The performance of the catalyst is related to the geometry and the composition of the catalyst. Therefore, the artificial neural network can be used to predict the catalytic performance of a certain composition, which has a good effect. Lin et al. [21] developed selective catalytic reduction (SCR) de-stocking catalyst, using principal component analysis (PCA) to simplify the input parameters, including eight components with major contributions, covering geometry, physical and chemical values, chemical composition content, etc. The results show that Levenberg-Marquardt Backpropagation (LMBP) neural network has a better prediction effect on catalyst performance and can meet the research needs.

Huang et al. [22] used neural network to optimize the development of methane hydrogen production catalyst. The LMBP artificial neural network is selected, and the convergence speed is faster than the traditional BP algorithm. The improved hybrid genetic algorithm is used to optimize the model for 6 rounds. The error of the model is smaller than that before optimization, and the generalization ability is improved. Finally, the optimum formula was obtained.

2.3 Application in Industrial Process

A large number of studies have shown that artificial neural networks can be used to control large industrial processes. For example, chlorination process with certain risk has certain requirements for control accuracy, while traditional proportional、integral、derivative(PID)

control has great influence on the stability of the system due to long delay and long stabilization time. If the BP neural network is used to optimize the PID control in the chlorination process [23], the expected temperature, the actual temperature, the threshold value and the error are used as the input of the BP neural network, and the output is the basic parameters Kp, Ki and Kd of the PID control. The optimized controller structure is shown in Fig. 2. The neural network part is responsible for adjusting the parameters according to the input condition, and the PID control part is responsible for the control process according to the algorithm. The optimized algorithm is used for simulation test. It can be concluded that the neural network PID controller is superior to the traditional PID, with short stability time, short delay and less adjustment, which is helpful to maintain the stability of the system and reduce the influence of interference. Li et al. [24] also applied neural networks to the control of fluorine chemical processes, using a convolutional neural network (ACNN) with an input data attention mechanism to predict product quality with complex nonlinearity and strong time-varying. The results show that this method has better prediction results than other algorithms.

Neural networks can also be used in heat exchanger networks. Nida et al. [25] used artificial neural networks to predict the fluid dynamics of heat exchangers with transversely twisted and hot oil-based Single-Walled Carbon Nanotubes (SWCNT) nanofluids. The literature uses the Performance Evaluation Criterion (PEC) index to evaluate the performance. The results show that the neural network developed in the literature is very predictive of the PEC index. Carvalho et al. [26] proposed a Neural Network Model Predictive Control (NNMPC) to control the heat exchanger network. This technology investigated the output variable temperature and operating variable mass flow rate of set point tracking and interference suppression. The results show that NNMPC significantly reduces overshoot and the stabilization time is close to Model Predictive Control (MPC).

Neural networks can also be used to study a single device. Mona et al. [27] used artificial neural network to predict the solid retention in the axial and radial directions of gas-solid phase fluidized beds. The input variables are static bed height, axial height, surface gas velocity, radial position and particle size, and the retention rate is output through a hidden layer with 9 neurons. The experimental value and the predicted value can obtain a good consistency. It can also be applied to the study of solar collectors [28]. The artificial neural network is used to study the turbulence effect in the solar collector with corrugated pressurized reflector, so as to improve its heat transfer effect. The model uses Reynolds number and collector angle as input layer data and output layer output Nusselt number. The predicted value of the network after training is very close to the actual value, indicating that the network predicts the Nusselt number very accurately. Neural network can also be used to study refrigerator refrigeration [29]. Liquefied petroleum gas (LPG) refrigerant and nano-lubricant based on TiO2-mineral oil are used to replace R134a refrigerant to study refrigerator refrigeration capacity. The results are used to establish ANN model, and the prediction is more accurate, which can provide reference for the study of refrigerator system. Zhu et al. [30] used an improved convolutional network to identify flame images and solved the problem of low temperature measurement accuracy of

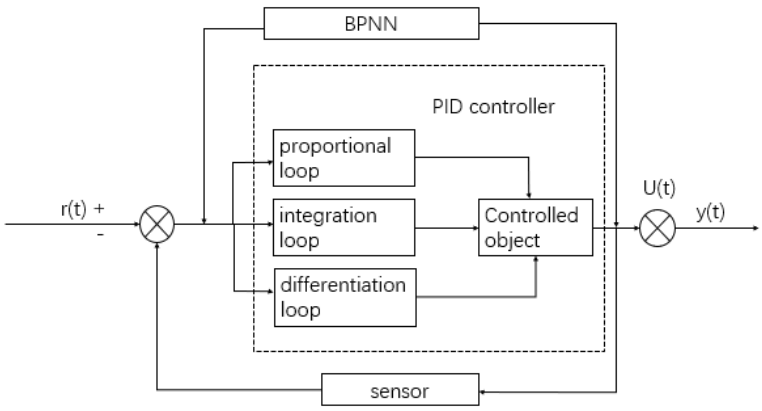

Fig. 2. BP neural network PID controller structure

thermocouples in ceramic shuttle kilns. The neural network embeds the Squeeze-and-Excitation (SE) module on the basis of the optimized Inception-Residual Network (ResNet)-V2 convolutional neural network module to effectively identify the processed flame image, and its positive prediction accuracy and anti-class prediction accuracy are higher than other algorithms.

Ashwani et al. [31] used artificial neural network for fault diagnosis of digital circuits. The response of different fault states is fitted by polynomial curve, and the coefficients obtained by least square method are used as neural network input. The input layer nodes of the LMBP neural network are 10, because there are 10 distinguishing features in the form of polynomial coefficients. The output layer node is 22, including 21 fault models and 1 non-fault state. It has good diagnostic ability for both circuit models, indicating that the neural network can be used for actual fault diagnosis.

2.4 Reaction Optimization

Artificial neural network is widely used in the establishment of reaction kinetics. Alonso et al. [32] designed a hybrid algorithm ANN-mathematical optimizations (MATOPT) for reaction kinetics to determine the parameters of different types of reactions. Four reaction types were studied in the literature: simple irreversible reaction (I), two irreversible reactions produce the same product (II), the same reactant produces two products through two irreversible reactions (III), continuous irreversible reaction (IV). The determination method is to determine the single rate constant and molar absorption coefficient by neural network, and then use it as the initial estimation of the mathematical optimization algorithm for the second stage to further improve the parameter accuracy. The designed hybrid algorithm is first tested by synthetic data, and then predicted by experimental data. The experimental design is shown in Figs. 3 and 4. The results show that for simple model (I), the parameters obtained by ANN are accurate, but for complex models (II, III, IV), mathematical optimization steps are necessary. There are also many studies that apply neural networks to specific reactions. Atiya et al. [33] established a kinetic model for the transesterification of castor oil with methanol, using the catalyst concentration, the molar ratio of methanol to oil, and temperature as input variables. The percentage content of the reaction fatty acid methyl ester is then output to estimate the rate constant of the kinetic model. Osen et al. [34] studied the kinetics and optimal conditions for the extraction of phenolic antioxidants from orange fish sweet potato varieties using water as a medium, and optimized the reaction time, temperature and solid-solution ratio. The linear interaction between the solid-to-solvent ratio was the most significant. Leo et al. [35] studied the optimization of reaction conditions of Homogeneous Charge Compression Ignition-Direct Injection (HCCI-DI) engine with waste edible oil biodiesel as direct injection fuel and diesel gasoline as premixed fuel. Neural network also has a good application in the removal reaction. For example, Berkan et al. [36] studied the biological photodegradation reaction of azo fuel in solar photoreactor. The initial dye concentration, pH value and flow rate were used as model input variables to simulate the decolorization removal rate and predict the best decolorization conditions. Leila et al. [37] optimized the removal of rhodamine B (RhB) by Ag, Mg co-doped ZnO nanoparticles. The results show that the amount of photocatalyst with the largest weight can be considered as the most effective parameter for RhB photocatalytic removal.

The neural network is also effective in simulating large reaction processes. Wu et al. [38] studied the process conditions of ethanol coupling to produce C4 olefins based on RBF neural network, and studied the effects of catalyst composition and dosage, ethanol intake and temperature on ethanol conversion and C4 selectivity. The influence weight of each factor is obtained by RBP network: temperature has a strong correlation with C4 olefin selectivity. The effects of Co / SiO2 and hydroxyapatite quality on C4 olefin selectivity are basically the same. The effect of Co loading on C4 olefin selectivity is slightly larger than that of ethanol conversion, while the correlation between the selectivity of C4 olefins and ethanol conversion is weak. Also, in the coal tar steam reforming process [39], artificial neural networks were used to simulate the steam reforming of naphthalene. The data set is developed by non-stoichiometric calculations of the Gibbs free energy minimization method. The effects of temperature and steam-to-oil ratio (STOR) on the selectivity of hydrogen, carbon dioxide, carbon monoxide and methane in the product stream were studied. The increase in temperature and STOR benefits H2 production during steam reforming. The conditions with the highest hydrogen selectivity

are obtained. Experiments show that it is feasible to apply artificial neural network to coal tar reforming.

Mats et al [40] applied artificial neural network to the microreactor data to study the conversion of automobile exhaust NOX under the oxygen-rich condition of silver / alumina catalyst. The temperature, NO, octane, oxygen concentration as input, need to predict the data is N2, CO, O_2, CO2 concentration. This research in microreactors focuses on the possibility of further optimizing the reactor by using more accurate process descriptions, monitoring the measurement results during the ongoing experimental program, discovering outliers in the data and improving and revealing the reaction structure, which facilitates the continuous improvement of the concept of bed structure and chemical properties for optimizing the interaction of gaseous and multiphase chemical reactions.

2.5 Physical Data

Behera et al. [41] studied fiber reinforced plastic drilling. In the current work, a multi-layer perception ANN architecture has been developed using the feedforward back propagation algorithm. The material thickness, drill diameter, spindle speed and feed rate are used as input parameters, and the stratification coefficient (Fd), average surface roughness (Ra) and root mean square surface roughness (Rq) of the

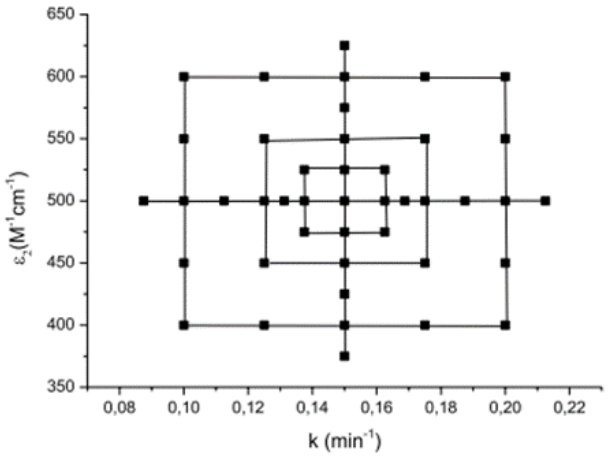

Fig. 3. Two-dimensional experimental design of system B1 → B2 (2 factors, k_1 and ε_2)

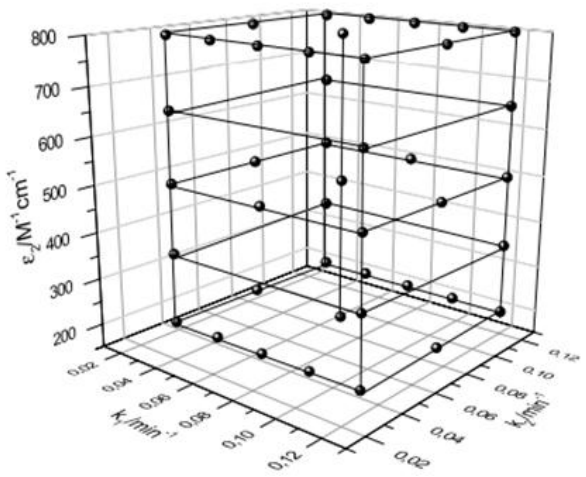

Fig. 4. Three-dimensional experimental design of system B1 → B2 → B3 (three factors k_1, k_2 and ε_2)

drilling inlet are used as output parameters. Then the artificial neural network model is used to check the influence of various input parameters on different response parameters. The developed model predicts that the surface roughness will increase as the feed rate increases, and a smaller diameter drill bit will help reduce the surface roughness. Lower feed rate will also reduce plastic delamination.

Nasiri et al. [42] developed a model for predicting Nusselt number in nanofluids by Reynolds number, Prandtl number, nanoparticle thermal conductivity, basic fluid thermal conductivity, and nanoparticle volume fraction. The predicted values of ANN model based on experimental data are in good agreement with the experimental values, which is helpful for the study of heat transfer coefficient of nanofluids.

Esfe et al. [43] studied the effect of temperature and volume fraction on the thermal conductivity of SWCNT-Al2O3 / ethylene glycol (EG) hybrid nanofluids. The neural network is established based on the experimental data. The output of the artificial neural network is compared with the experimental data. The maximum error is 1.94 %. This method has high accuracy in predicting thermal conductivity.

Belayadi et al. [44] studied the electrochemical impedance spectroscopy of potential-induced defects in self-assembled monolayer (SAM) CH3 (CH2) 3SH electrodeposited on the surface of single crystal gold rods, represented by Nyquist plots of impedance with real and imaginary parts (Z ', Z "). The predicted Nyquist plot calculated by ANN is close to the experimental value. The high performance of ANN in predicting and optimizing equivalent circuit is proved.

Deeb et al. [45] developed a linear and nonlinear quantitative structure-property relationship (QSPR) model for predicting the gas / particle partition coefficients of semi-volatile organic compounds based on partial least squares (PLS) and artificial neural networks to identify a set of structure-based numerical descriptors. The prediction results of PLS and ANN models give a very good determination coefficient (0.97). Consistent with experimental studies, it is shown that linear and nonlinear regression analysis is a useful tool for predicting the relationship between numerical descriptors and gas / particle partition coefficients.

Mozafari et al. [46] combined smoothed shear absolute deviation (SCAD) method and artificial neural network to study the Quantitative structure-retention relationship (QSRR), which is a new method (SCAD-ANN). The proposed SCAD method reduces the dimension of data before using ANN modeling method. A QSRR model was constructed between the most relevant molecular descriptors (MD) and retention index (RI) of two groups of volatile organic compounds to evaluate the accuracy of this method. After all ANN parameters are optimized, the statistical results show that more than 95 % of the data are in the confidence range, indicating that the prediction results of SCAD-ANN model are reliable.

Nagaraj et al. [47] studied the effects of sliding speed, load and sliding time on the Brinell hardness, tensile strength and wear loss due to friction of aluminum matrix composites. Artificial neural network is used to predict wear loss and friction coefficient. Experiments show that the artificial neural network model has a high wear prediction ability, and the model results are consistent with the experimental results.

Maddah et al. [48] studied the relative viscosity at different temperatures and different volume fractions and established an artificial neural network based on experimental data. Using SOM self-organizing map neural networks, temperature and concentration are considered as input variables, while relative viscosity is the output parameter of the neural network. Mean square error, correlation coefficient and standard deviation were used to evaluate the results. According to the results, the best model is a two-layer perceptron neural network with 25 neurons. Experiments show that the model can predict relative viscosity with appropriate accuracy.

Tatar et al. [49] measured the water absorption isotherms of fish oil microcapsules prepared from Gum Arabic (GA) and Gum Arabic-Hemicellulose (GA-HC). The Equilibrium Moisture Content (EMC) data are suitable for multiple empirical mathematical models. In the entire water activity range, the ANN model predicts the EMC of the sample more accurately than the empirical model. The adsorption heat of fish oil microcapsules was then predicted using the data obtained from the ANN model and fitted to the power model.

Kim et al. [50] used neural network to predict the wetting phenomenon of membrane distillation. Membrane wetting is unpredictable, and the effects of chemicals in the influent on it are

unpredictable. The response surface methodology(RSM) and ANN models were established using experimental data, and statistical verification was performed by variance analysis. The results show that the ANN model can accurately describe the wetting phenomenon after adjustment, and the ANN model is more accurate than the RSM model.

Adeniyi et al. [51] used artificial neural network to simulate the adsorption of herbicides and insecticides in aqueous media based on the sorbate-sorbent interface phase. Paired sample correlation showed that there was a strong positive correlation (0.980) and statistical significance ($p < 0.05$) between the model prediction and the experimental results. The study shows that the specific surface area of the adsorbent, the effective surface area of the adsorbent, the preferential adsorption of the adsorbate, the solubility of the adsorbate and the relative molecular mass of the adsorbate can be used to accurately predict the mass adsorption capacity of any herbicide and insecticide in aqueous media.

3. SITUATION AND PROSPECT

Artificial neural network has great advantages in the application of chemical industry. Artificial neural network has adaptive ability [52]. It is reflected in the algorithm that it adapts to different fitting contents or learning methods by changing the weight value in the learning process, which is one of the most different characteristics from other fitting methods. Artificial neural network has generalization ability. The lack of accurate prediction of samples without input has always been a common problem of many simulation methods, but artificial neural networks can make more accurate predictions, especially for noisy samples. Artificial neural network has nonlinear mapping ability. In the field of numerical calculation, such as the fitting of reaction kinetics in chemical industry, it is very accurate for the mapping of input and output of nonlinear model, and does not need to understand the system.

The application of artificial neural network in chemical industry still has some limitations. The neural network itself has problems such as over-fitting and slow convergence speed. If not solved, the error of fitting or prediction results will be too large. Therefore, when using the neural network, the over-fitting phenomenon will be improved by improving the model, such as dropout, reducing the number of neural network layers, etc. In addition, there is no accurate calculation method to determine the number of hidden layer nodes of neural network. Although the model can accurately predict the reaction results, it cannot give the relevant relationship, which is not conducive to the understanding of the reaction mechanism. Although the prediction results of the neural network are mostly better, as a data-driven model, it inherently has several percent inevitable errors. Like many fitting methods, the performance of artificial neural network is reduced when inference is made outside the known parameter space [53]. In addition, for complex and feature-rich models, neural networks are difficult to predict. In response to this shortcoming, new methods have been proposed to measure the reliability of solutions using artificial neural networks such as multiple independent training [54].

4. CONCLUSION

Artificial neural network has broad development prospects in chemical industry. Artificial neural network can be used in safety evaluation system. The safety evaluation system is one of the important contents of evaluating a long-term project. At present, it is widely used in the field of computer safety, and a small amount is used in the industrial field. For example, it is applied to carbon emission management [55]. Artificial neural network can ensure higher safety of the system. Artificial neural network expert system used to simulate the expert judgment can also be used in the chemical industry, the current application is mainly concentrated in the resin, plastic and silicate material properties of finished products, and for organic chemical synthesis field is less. With the development of science and technology, the application of neural network will become an indispensable part of the chemical industry, and promote the development of the chemical industry in standardization, scientification, systematization and greening.

COMPETING INTERESTS

Authors have declared that no competing interests exist.

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