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Catalyst Optimization Design Based on Artificial Neural Network

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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

Artificial neural network (ANN) has the characteristics of self-adaptation, self-learning, parallel processing and strong nonlinear mapping ability. Compared with traditional experimental analysis modeling, ANN has obvious advantages in dealing with multivariable nonlinear complex relationships in the process of industrial catalyst design. In the face of the complex structure of catalyst, the unclear reaction mechanism and conditions, the use of neural network for small-scale experimental data analysis can save the time and energy invested in large-scale experimental research and obtain more perfect results in catalyst formulation optimization and condition selection. This paper summarizes the development of artificial neural network. The application principle, construction method and research progress of BP artificial neural network model in catalyst optimization design are summarized and analyzed. The development and innovation of artificial neural network in the future, as well as its continuous application and accumulation, will provide a powerful tool for the research of catalyst design and optimization in the future.

Keywords: Catalyst optimization design; artificial neural network; industrial catalysis.

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1. INTRODUCTION

Catalyst is the heart of modern chemical industry, and the research and development of catalyst is one of its core problems. With the development of chemical industry, catalysts are widely used in petrochemical, coal chemical, chemical medicine, coating, grease and other industries. The output of chemical catalysts in China has been increasing year by year since 2010, and has reached about 41.5 tons in 2020. Due to the deteriorating ecological environment and the gradual strengthening of environmental protection, the requirements of downstream chemical industries for catalyst technology will continue to increase, and the R & D demand for new environment-friendly catalysts will also increase day by day [1,2]. Long-term studies show that there are many factors affecting the properties of catalysts. On the one hand, its own attributes such as formula metal, preparation methods, preparation conditions, activation conditions and other factors, on the other hand, the reaction conditions and operation will also affect its functional properties, which makes it difficult to study and predict the change trend of the properties of the catalyst under the parallel effect of various variables. The process of developing catalysts is long and complex [3].

Therefore, there is a certain contradiction between the increasing requirements for catalyst technology and the slow process of catalyst research and development. An efficient and convenient catalyst optimization design method is urgently needed to adapt to the current development trend of industrial catalysts.

Artificial Neural network (ANN) is a kind of network model which can be applied to deal with practical problems of multiple nodes and multiple output points. It abstracts human brain neurons, forms different network according to different connection modes, which has strong information processing ability. In the process of catalyst optimization design, reaction process is often complicated and affected by many factors, which makes traditional research usually has long experimental period and high cost. While, artificial neural network, with its intelligent characteristics of self-organization, self-learning and self-adaptation, has been more and more widely explored and applied in the catalyst design process, providing a convenient and feasible method for the problems that are difficult to solve in the traditional design process.

In this paper, the development of artificial neural network is summarized, and the research progress of BP artificial neural network model in catalyst optimization design is reviewed.

2. DEVELOPMENT OF ARTIFICIAL NEURAL NETWORK

2.1 Artificial Neural Network

At present, the definition of artificial neural network is not unified. According to Hecht Nielsen, an American neural network scientist, neural network is a computer system formed by multiply very simple processes units connected with each other in some way. The system processes information by making dynamic response to continuous or intermittent input states. Integrating the sources, characteristics and various explanation of artificial neural network, it can be simply expressed as an information processing system designed to imitate the structure and function of human brain [4].

Artificial neural network (ANN) has begun since 1940s. Pitts [5] proposed the first neuron model (M-P model) in 1943, taking the threshold function as the main characteristic of neuron calculation, which started the exploration of artificial neural network. In 1951, Hebb [6] proposed the Hebb rule of connection weight enhancement: in neural networks, the strength of synaptic connections between neurons is variable, and such changes controls the mutual excitation of neurons. Hebb rule lays a theoretical foundation for constructing neural network model with learning ability. At the end of 1960s, Rosenblatt [7] developed a perceptual model named Mark I based on the M-P model, which was the first artificial neural network with learning ability constructed physically. After experiencing the low tide of development, in 1982, Hopfield neural network (HNN) was proposed for the first time, which made a nonlinear mathematical generalization of the information storage and extraction function of artificial neural network, and proposed dynamic equation and learning equation, which provided theoretical guidance for the construction and learning of artificial neural network [8]. In 1986, Werbos et al. [9] made a detailed analysis of the error back propagation method of multi-level feedforward network with nonlinear continuous transfer function, namely BP algorithm, and proposed an effective algorithm for weight

adjustment for the first time. BP algorithm is one of the most widely used neural network algorithms.

Since the mid-1990s, the research of artificial neural network has attracted extensive exploration. While the existing theories have been deepened and popularized, new theories and models have been proposed and expanded, such as optical neural network (PNN), chaotic neural network, fuzzy neural network and so on. Neural network is an interdisciplinary science, the development of computer hardware, the accumulation of big data and the combination of other knowledge and technology have brought broad space for the development of neural network in the new era [10].

In 2006, Hinton et al. [11] proposed the landmark Deep Belief Network (DBN), and described a new method to convert high-dimensional data into low-dimensional code by training a multi-layer neural network. A network with a small central layer is used to reconstruct high-dimensional input vectors [12], which has led to a boom in the application of deep learning in various scenarios. So far, ANN has been successfully applied to intelligent driving [13-15], aerospace [16,17], signal processing [18-20], process control and optimization [21-23], safety protection [24-26], image processing [27-29], forest pest protection [30,31], time series forecasting [32-34] and so on.

2.2 BP Neural Network

At present, artificial neural network (ANN) has a variety of relatively perfect network models, such as MLP neural network, RBF neural network, BP neural network and so on. Among them, BP neural network is the most widely used in catalyst optimization design due to its excellent nonlinear mapping ability, good generalization ability and fault tolerance ability. The structure and operating principle of BP neural network will be introduced below.

The basic structural unit of neural network is node (perceptron), which simulates the neuron of human brain. Its function is to accumulate the input variables with weights and thresholds, which are transformed by the activation function and then obtain the output variables.

BP neural network is a kind of forward feedback artificial neural network, which is composed of multi-layer nodes. Its structure usually includes input layer, hidden layer and output layer. The output layer is the targets to be predicted. While, the input layer is the variables which affecting the output. However, the determination of hidden layer is complicated and may have one or multiple layers. The number of nodes is not only related to specific problems, but also closely related to the number of input and output nodes of the network. And the selection of hidden layer nodes affects the learning effect, convergence speed and generalization ability of the network. If the number of nodes in the hidden layer is too small, the input data cannot be fully learned by the network and the prediction accuracy is reduced; while if the number of nodes in the hidden layer is too large, the learning efficiency, the fault tolerance and generalization may become poor, and prone to over-fitting phenomenon [35]. Therefore, the correct selection of node number of hidden layer has a crucial influence on the performance of network model.

The selection of hidden layer nodes can be divided into two steps. Firstly, the empirical formula is used to infer the reasonable range of the number of hidden layer nodes. And then increase the nodes number from less to more, trial and error experiments are carried out to finally determine the optimal number of hidden layer nodes. At present, the common empirical formulas are [36,37]:

$$n = \sqrt{n_i + n_o} + a \tag{1}$$

$$n = log_2 n_i \tag{2}$$

$$n = \sqrt{0.43 n_i n_o + 0.12 n_o^2 + 2.54 n_i + 0.77 n_0 + 0.35} + 0.5 \tag{3}$$

n is the number of hidden layer nodes, n_i is the number of input nodes, n_o is the number of output nodes and a is constant.

After determining the number of nodes in the input layer, hidden layer and output layer, the basic structure of BP neural network model is constructed, which is as shown in the Fig. 1.

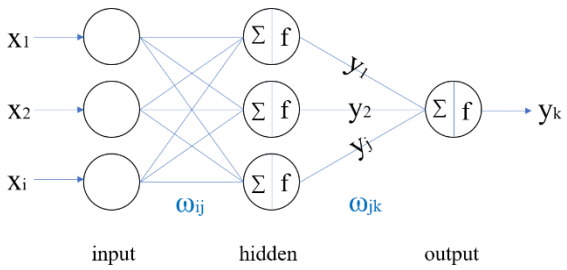

Fig. 1. BP neural network structure

x_i、y_i、y_k represent the input signal, the output signal of hidden layer and the final output signal, i、j、k represent the number of nodes of each layer, ω_{ij} and ω_{jk} represent the weight of each layer, and f is the activation function.

The operating principle of BP neural network: The operation of BP neural network is mainly composed of two parts: learning stage and testing stage. In the learning stage, the weights and thresholds of input data of each layer are initialized first, and the training data is propagated forward. Input data x_i of different nodes are given their respective weights $\omega_{ij}$and thresholds b_j , and the output data y_i of the hidden layer is obtained through the activation function f of the hidden layer. The formula is as follows:

$$y_i = f\left[\sum_{i=1}^{n}\left(\omega_{ij}x_i + b_j\right)\right], i = 1,2,3\cdots\cdots n \quad (4)$$

Similarly, the output data of each node of the hidden layer, as input values, enter the node of the output layer and are given different weights and thresholds. Finally, the output data y_k is obtained through the activation function f of the output layer, and the formula is as follows:

$$y_k = f\left[\sum_{j=1}^{n}\left(\omega_{jk}y_i + b_k\right)\right], i = 1,2,3\cdots\cdots n \quad (5)$$

The hidden layer and the output layer can adopt the same or different activation functions. In specific applications, different activation function combinations often have different influences on the global calculation efficiency and the convergence degree of the results. The standard BP neural network usually selects Sigmoid function as the activation function to simulate the characteristics of neurons, and the formula is as follows:

$$f(x) = \frac{1}{1+e^{-x}} \quad (6)$$

The output range is [0,1] and its derivative is $f^{'} = f(x)[1 - f(x)]$. It is very similar to the real response of biological neurons, and has a very simple derivative, which is very beneficial for the learning of BP neural network. However, when the net input of neurons is too large or too small, the output will enter the saturated region, prone to non-convergence phenomenon. Therefore, in the practical application process, in addition to the commonly used Sigmoid function, many other activation functions such as Tan-Sigmoid, linear function, trigonometric function, bipolar function and so on will also be selected.

The forward propagation of the input node data through the neural network generates the predicted value, which is compared with the output target value to calculate the error. The error between the predicted value and the target value is propagated back from the output layer, and the weights and thresholds between different layers are corrected according to the first derivative of the error to the weights and thresholds. The process above is repeated to make the errors meet the set requirements. The correction formula for weights and thresholds is as follows:

$$\omega_{ij}(n+1) = \eta\frac{\partial e(n)}{\partial \omega_{ij}(n)} + \omega_{ij}(n) = \Delta\omega_{ij}(n) + \omega_{ij}(n) \quad (7)$$

$$b_j(n+1) = \eta\frac{\partial e(n)}{\partial b_j(n)} + b_j(n) = \Delta b_j(n) + b_j(n) \quad (8)$$

$$\omega_{jk}(n+1) = \eta\frac{\partial e(n)}{\partial \omega_{jk}(n)} + \omega_{jk}(n) = \Delta\omega_{jk}(n) + \omega_{jk}(n) \quad (9)$$

$$b_k(n+1) = \eta\frac{\partial e(n)}{\partial b_k(n)} + b_k(n) = \Delta b_k(n) + b_k(n) \quad (10)$$

When the error between the predicted value of training data and the target value reaches the set requirement (or the maximum number of calculation times), the learning stage ends, and the neurons of the hidden layer and output layer of BP neural network get the optimal weight and threshold value.

The above traditional neural network algorithm is based on the error between the predicted value and the actual value, and repeatedly revises the weights and thresholds of the hidden layer and the output layer to realize the optimization of the network. This algorithm has clear physical concept and strong universality, but there may be problems in the application such as slow convergence speed, local optimal solution, poor generalization ability, etc. Therefore, many experts and scholars put forward a variety of methods to improve the algorithm performance. Currently, the commonly used optimization algorithms of BP neural network include BP neural network with additional momentum term combined with adaptive learning rate [38,39], GA-BP neural network combined BP neural network with genetic algorithm [40], PSO-BP neural network combined BP neural network with particle swarm optimization [41], BP learning

algorithm improved by Levenberg-Marquardt method [42,43]. Due to the different inherent characteristics of the problems to be simulated, the improvement effect of each optimization method is limited. At present, no universal optimization algorithm is found that is most suitable for solving all problems. Usually, the optimal learning algorithm is selected by comprehensive analysis and comparison of the convergence rate and prediction accuracy of each algorithm in the specific catalyst neural network.

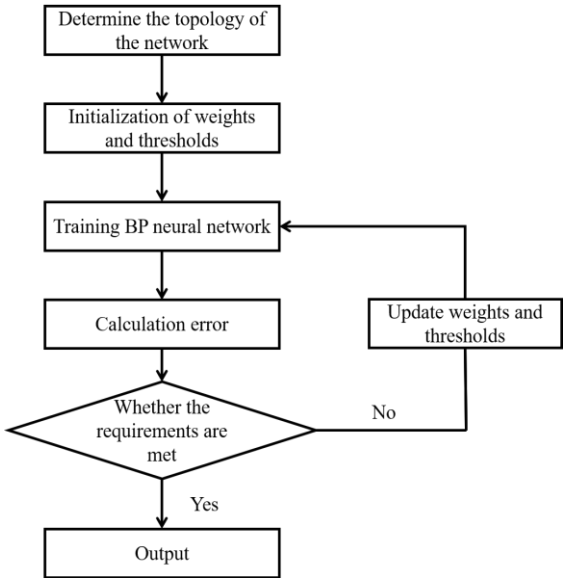

Fig. 2. Flow chart of BP neural network operation

In the testing stage, a group of experimental data different from the training data in the learning stage is input into the neural network for prediction, and the error between the predicted value of the test sample and the real value obtained from the experiment is compared to verify the prediction performance of the neural network. If the error is within the allowable range, the trained BP neural network model has met the practical application requirements.

3. RESEARCH STATUS OF CATALYST OPTIMIZATION DESIGN

The comprehensive evaluation indexes of industrial catalysts are activity, selectivity and service life. Catalysts may also be required to have good heat resistance, mechanical strength and resistance to carbon deposition for specific reactions under specific circumstances. Traditional catalyst design optimization mainly relies on the theoretical guidance of systematic catalyst design monographs, such as *Catalyst Manual* [44], as well as the specific experimental studies. Most of the catalyst design theories are summarized based on the accumulated research experience of predecessors, and provide limited guidance for the selection of catalyst components. However, when it comes to specific reactions, the determination of preparation methods and operating conditions of catalysts usually rely on a large number of synthesis and characterization experiments.

In recent years, the rapid development of artificial neural network (ANN) technology provides an efficient and convenient way for catalyst optimization design. Combined with artificial neural network technology, based on its nonlinear mapping ability and the characteristics of self-organization, self-adaptation and self-learning, parallel processing the effects of complex and diverse influencing factors on catalyst performance can obtain a more accurate relationship model, achieve a certain precision prediction with less date in a short time, which improves the efficiency of catalyst research and development.

4. THE OPTIMIZATION DESIGN OF CATALYST BASED ON BP NEURAL NETWORK

4.1 Construction and Application of Catalyst Network Model

In practical application, there are many factors that affect the operation efficiency and prediction accuracy of the artificial neural network catalytic model: the selection of training data, the number of the input layer, output layer and hidden layer nodes, the combination of activation function of the hidden layer and output layer, the learning algorithm adjust the weights and thresholds of the input data of each layer, as well as the initial weights and thresholds setting, in different application situation the highest fitness choice is usually different. Usually, the optimal BP neural network structure is determined by experimental analysis, i.e., to explore the optimal selection of various variable factors in the BP neural network structure in turn, build neural networks with multiple structures at this variable level, use the same data to train and test different neural networks, and compare the error between the predicted value and the real value obtained from the experiment. Considering the prediction accuracy and calculation efficiency of neural

network, select the optimal structure and apply it to the optimization design of specific catalyst.

After the neural network model of catalytic process is established, the influence weight of input factors on catalyst performance can be analyzed according to the model，according to which we can determine the main factors, eliminate irrelevant factors and clarify the optimization direction of catalyst. The commonly used methods include Pad method, weight method and Perturb method [45,46]. The established neural network model can also be used to simulate the catalytic process and find the optimal catalyst formula and process conditions. The values of various factors affecting the properties of catalyst can be collected by itemized intensive scanning technology as the prediction samples of the model. By comparing the predicted values of each group of data, the parameters of the optimal formula conditions can be selected. The other widely used method is that directly find the optimal catalyst formula and process conditions based on the global optimization ability of the combination of BP neural network and genetic algorithm or particle swarm optimization algorithm.

4.2 Application of ANN in the Optimization Design of Catalyst

Abbasi et al. [41] applied the artificial neural network (ANN) model linked with genetic algorithm (GA) to optimize of synthesis parameters in nanostructure $La_{1-x}Ba_xNi_{1-y}Cu_yO_3$ catalysts used in the reforming of methane with CO_2. The input layer contains 4 neurons, mole fraction of La, mole fraction of Ni, calcination temperature and reaction temperature and the output layer contains one neuron, conversion of methane as output variable. According to CCD, 20 sets of experiments designed, the date obtained from experiment will be used in the train and test of neural network.

To select the most appropriate topology, a small number of neurons in the hidden layer were used initially and then gradually added to reach the optimal number of the hidden layer neurons. Fig. 3 represents the average relative derivation (ARD) for different number of neurons in the hidden layer. The hidden layer with 11 neurons has the lowest amount of ARD, thus select topology 4:11:1 with a high performance as the most appropriate topology.

The activation function is selected by comparing six different combinations of activation functions of hidden layer and output layer of Tan-Sigmoid (Tan-S), Log-Sigmoid (Log-S) and linear function. Fig. 4 presents the results of this search. As shown in Fig. 4, the network composed of the hidden layer Log-S transfer function and the output layer Tan-S transfer function together predicted the results more accurately (exhibiting high R^2), which means that these transfer functions perform well.

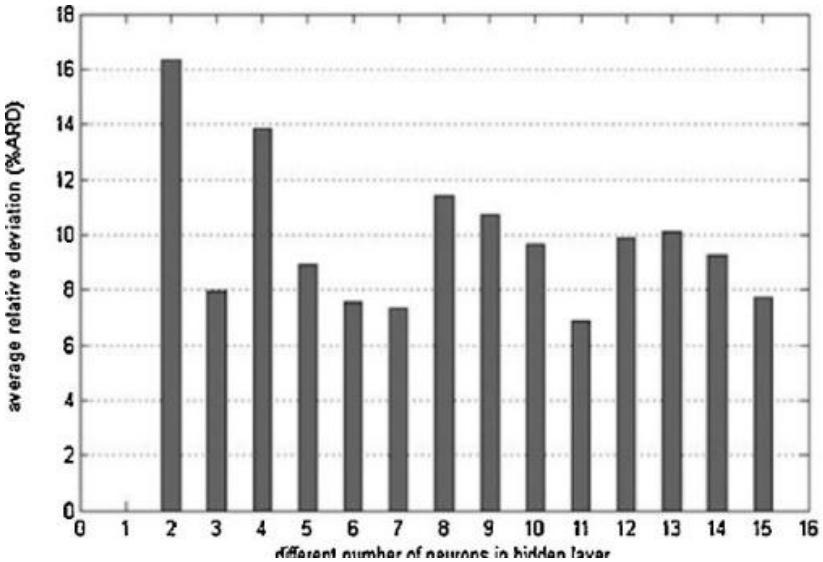

Fig. 3. Determination of optimum number of neurons for selected algorithms [41]

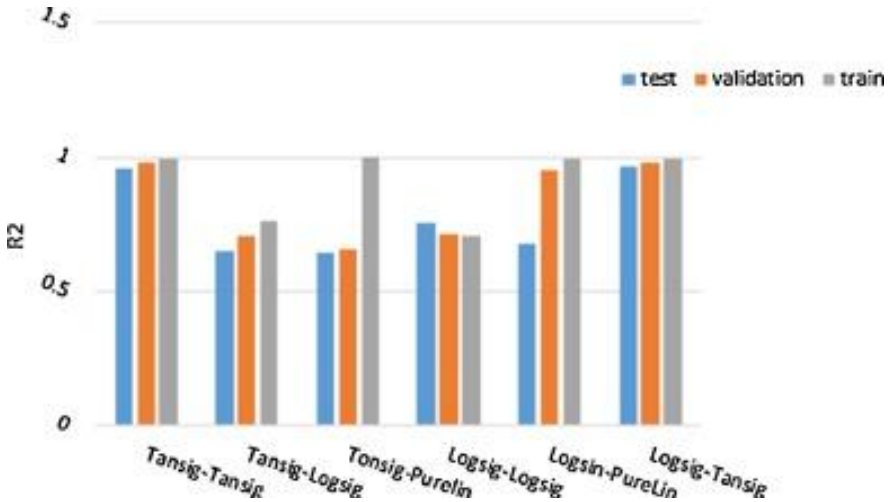

Fig. 4. Comparison of different transfer functions for hidden and output layer [41]

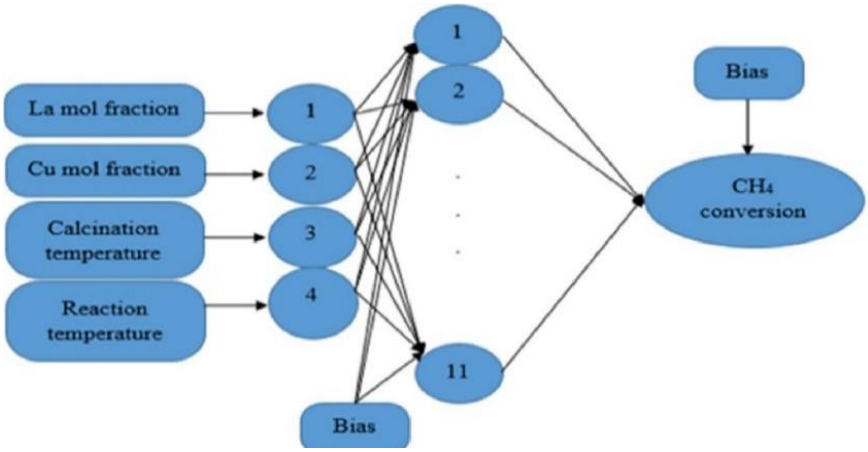

Fig. 5. Schematic of a multilayer perceptron with one layer of hidden neurons [41]

The Levenberg–Marquardt method was used for network training because of its convergence speed. The preliminary structure of artificial neural network is tested by multiple groups of data, and the prediction performance meets the requirements. And based on the weight calculation formula, it is concluded that the La mole fraction is demonstrated as the most significant factor, which is used for further optimization of the catalysts.

After obtaining a relatively perfect artificial neural network structure, combined with GA genetic algorithm, the La mole fraction, Ni mole fraction and calcination temperature were optimized in order to improve the methane conversion. According to the GA optimization, $La_{0.9965}Ba_{0.0035}Ni_{0.6028}Cu_{0.3972}O_3$ catalyst with calcination temperature of 734.45 °C was found to be the optimal catalyst. The predicted value of the neural network is consistent with the experimental results, and the catalyst obtained by optimizing the artificial neural network can significantly improve the methane conversion rate.

Huang et al. [46] optimized the formulation of Fe_3O_4 composite oxide catalyst based on BP neural network. According to the previous experience, the metal elements that can be used for Fe_3O_4 composite oxide are screened, select the first auxiliary elements (Cu, Ni, Zr, Pt, Co) and its ratio to Fe, the second auxiliary element (Cr, W, Al, V, Ti) and its ratio to Fe, drying temperature and roasting temperature as the input neurons of the artificial neural network, while the service life of catalyst and hydrogen generation rate are the output neurons. The orthogonal experimental table with six factors and five levels is obtained by CCD method, catalyst samples are prepared and analyzed according to this table. The obtained data are

used for the subsequent selection and optimization of neural network structure. The simple Sigmoid function is selected as the activation function, while the number of hidden layer nodes and learning algorithm are determined by comparing the training results.

In order to determine the number of hidden layer nodes, the catalyst data obtained from experiments were used as training samples of neural network to evaluate the generalization ability of four different hidden layer structure networks. The structural with too few nodes in the hidden layer is not accurate enough in simulation; the structure with too many hidden layer nodes reach over fitting and has poor generalization ability; for the structure of three hidden layers, the amount of calculation is too large, so they are excluded. Finally, the 6:12:4:2 structure was selected to model the formula of methane hydrogen production reaction system based on Fe_3O_4 composite oxide. For the selection of learning algorithm, the traditional BP algorithm, the BP algorithm improved by moment method and the BP algorithm improved by Levenberg Marquardt method are tested by the previously obtained catalyst sample data. According to the training results, the convergence effect of Levenberg-Marquardt method is far better than that of traditional BP algorithm and moment method, so the LM method was chosen for modeling. After the basic structure of the neural network was determined, the formula model of Fe_3O_4 composite oxide was optimized with genetic algorithm. The life of Fe_3O_4 composite oxide and hydrogen generation rate were combined to form a single objective optimization problem. All catalyst formulations and experimental evaluation results obtained in each round of optimization were added to the training set of the next round, and the initial weights were updated. The more learning rounds, the more accurate the network model. After six rounds of optimization, some of the optimized formula of Fe_3O_4 composite oxide is chosen as the satisfactory formula, which is shown in Table 1.

Hadi et al. [47] adopted ANN-GA model, to design and optimize of M-Mn/H-ZSM-5 (M: Ce, Cr, Fe, Ni) catalysts in conversion of methanol to propylene. The predicted and experimental values of propylene selectivity of the optimal catalyst were 54.3% and 54.8%, respectively, which shows that there exists a good agreement between model prediction and experimental data for the optimal catalyst which demonstrates the consistency of ANN-GA models and the catalyst performance was improved. Günay et al. [48] applied neural network to the design of Pt-Co-Ce/Al_2O_3 catalyst for selective CO oxidation in hydrogen-rich streams, using the artificial neural network model with 6:5:2:1 structure to determine the weight of Pt as the main influencing factor, and the catalyst was optimized accordingly. Fu et al. [49] used improved BP neural network to predict $Ni/A1_2O_3$ catalytic CH_4-CO_2 reforming reaction, and the results showed that reaction temperature and Ni loading had a great influence on reforming reaction, indicating the direction for catalyst optimization. Hossain et al. [50] used artificial neural network to model of hydrogen-rich syngas production from methane dry reforming over novel $Ni/CaFe_2O_4$ catalysts, demonstrated the viability of employing the ANN-based models for predicting hydrogen-rich syngas with excellent ability to represent the interrelationships between the input and the output parameters. Baroi et al. [51] used artificial neural network to assist the development of ozone catalyst $SrFe_xZr_{1-x}O_3$. Under the optimal formulation and process conditions, m-cresol conversion rate and TOC removal rate were significantly improved. Bahrami et al. [52] investigated the catalytic performance of CeO_2-$MO_{x\ (0.25)}$ (M = Mn, Fe and Cu) mixed oxide nano catalysts in NO + CO reduction. To model and optimize the NO and CO conversions, they used the approach established by combining an artificial neural network with a genetic algorithm. NO conversion predicted through ANN-GA system and obtained via experimental at 300°C were 91% and 90%, respectively, which implied that there is a good agreement between them for optimal catalyst. Yang et al. [53] applied a neuro-genetic machine learning system (ANN-GA) to optimize and predict the optimum preparation parameters for the precipitation synthesis of high-efficiency silver-doped manganese oxides (Ag/MnO_x) for toluene total oxidation. The resulting Ag/MnO_x-GA catalyst achieved the lowest T50 (CO_2) of 206℃ comparing with other methods.

It can be seen that artificial neural network has been widely used in catalyst design and optimization, and has played a significant role in finding the optimal catalyst formulation and process conditions.

Table 1. Some of the optimized Fe_3O_4 composite oxide formula [46]

Catalyst	Influencing factors					Experimental results	
	M_1-M_2-FeO_x	M_1/Fe	M_2/Fe	T_1/℃	T_2/℃	CL/h	FRH/mmol·min^{-1}·(g Fe)$^{-1}$
MHB-1	Zr-W-FeO_x	10.63	5.86	150	600	3.68	1.16
MHB-2	Ni-Cr-FeO_x	15.65	16.27	150	600	3.58	1.19
MHB-3	Pt-Cr-FeO_x	2.49	12.53	150	600	4.46	1.16
MHB-4	Pt-W-FeO_x	3.12	6.51	150	600	3.82	1.18
MHB-5	Zr-Al-FeO_x	16.53	10.94	150	600	4.19	1.15
MHB-6	Zr-Ti-FeO_x	10.85	13.05	150	600	3.96	1.15
MHB-7	Cu-W-FeO_x	14.59	8.42	150	600	4.00	1.14
MHB-8	Ni-V-FeO_x	9.37	5.67	150	600	4.10	1.16
MHB-9	Co-W-FeO_x	6.81	16.29	150	600	3.59	1.09
MHB-10	Zr-Ti-FeO_x	4.52	12.83	150	600	3.80	1.11

5. CONCLUSION AND OUTLOOK

This paper reviews the development of artificial neural network and its application in catalyst optimization design and emphatically introduces the principle of BP neural network and the process of catalyst model building based on the neural network. The application of BP and its improved neural network in the optimization design of catalyst has guiding role. In the face of the complex structure of catalyst, the unclear reaction mechanism and conditions, the use of neural network for small-scale experimental data analysis can save the time and energy invested in large-scale experimental research and obtain more perfect results in catalyst formulation optimization and condition selection. But the research level of artificial neural network still needs to be improved, on the one hand, the number of nodes in the hidden layer and the determination of the activation function are not yet under the guidance of universal theory and need to be further studied and improved, on the other hand, the topology structure and learning algorithm of the neural network need to be optimized at a higher level with faster convergence speed. More accurate neural networks also depend on developments in neuroanatomy and related mathematics. In conclusion, with the continuous improvement of the technical reliability of artificial neural network, the theory and practice of catalyst optimization design based on artificial neural network will provide a powerful tool for the research of industrial catalysts.

COMPETING INTERESTS

Authors have declared that no competing interests exist.

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