



# Artificial Neural Networks and Its Applications 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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## ABSTRACT

Artificial neural networks, as an important part of artificial intelligence, have a wide scope of development to improve the traditional production technology of chemical processes with its inherent advantages of parallel structure and parallel processing, fault tolerance, full approximation of any complex nonlinear relationships, learnability and self-adaptability, etc. Thus, it has a wide scope of development to improve the problems of lagging diagnosis, difficult to optimize control, large errors in physical property estimation and inability to deal with nonlinear complex situations. This paper summarizes the theory of artificial neural network, including its structure and characteristics, and introduces its applications in different fields, especially in chemical industry.

**Keywords:** Artificial neural network; application; chemical industry.

## 1. INTRODUCTION

Artificial Neural Network (ANN), a mathematical model for information processing by applying a synaptic connection structure similar to that of

the brain, is simulated on the basis of human understanding of their own brain organization and thinking mechanism, which is rooted in the results of neuroscience research to achieve the processing of information, and is an emerging It

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is an emerging cross-discipline that not only promotes the application and development of intelligent computing, but also revolutionizes the research methods of information science and neurobiology, and is now successfully applied to brain science, cognitive science, pattern recognition, intelligent control, mathematics, statistics, physics, computer science, and engineering science 1. It is proposed based on the results of modern neuroscience research, which attempts to process information by simulating the neural network of the brain to process and remember information. ANN by imitating the structure and function of the human brain and draws on the research of biological neuroscience, computer science and many other fields 2. This paper will summarize the theory of artificial neural network, including its structure and characteristics, and introduces its applications in different fields, especially in chemical industry.

## 2. ARTIFICIAL NEURAL NETWORK

Psychologist Mcculloch, mathematician Pitts proposed a neural network model, since then the era of research in neuroscience theory was opened up, and half a century neural network technology has flourished. A neural network is a computational model that consists of a large number of individual neuron nodes and the weighted values of their interconnections, each node representing an operation called the activation function. The output of the network depends on the structure of the network, the way the network is connected, the weights and the incentive function. The network itself is usually an approximation of some algorithm or function in nature or human society, or it may be an expression of a logical strategy. The idea of constructing neural networks was inspired by the operation of neural networks in living beings. Artificial neural networks, on the other hand, combine the understanding of biological neural networks with mathematical statistical models toward the implementation with the help of mathematical statistical tools. On the other hand, in the field of artificial perception in artificial intelligence, we enable neural networks to have human-like decision making abilities and simple judgments by means of mathematical statistics, an approach that is a further extension of traditional logical algorithms 3.

An artificial neural network is composed of a large number of simple information processing units (neurons) called nodes, each node sends

inhibitory or excitation signals to other nodes in its vicinity, and the information processing of the whole network is accomplished through the interaction between these nodes. A node can be represented by an activation function  $f$  as follows: 4.

$$y = f(\sum_{i=1}^n w_i x_i - \theta_i) \quad (1)$$

where  $y$  is the output of the node,  $x_1, x_2, x_n$  are the input components of the node, which are the information received by the neuron;  $w_1, w_2, w_n$  are the weights, also known as connection strength, and  $\theta$  is the threshold.

The working process of artificial neural networks can be divided into two phases: training and testing. In the training phase, a set of input-one output pattern pairs is used as a training sample set to train the network. The process of network training is the process of adjusting the network parameters (including weights, thresholds, etc.). In the test run phase, given new inputs, the network is able to compute the corresponding outputs. Usually, the learning (or training) of ANN can be divided into two ways: one is supervised or tutored learning, which uses the given sample criteria for classification or imitation; the other is unsupervised or tutorless learning, which only specifies the learning method or certain rules, and the specific learning content varies with the environment (i.e., the input signal situation) in which the system is located, and the system can automatically discover the environmental characteristics and regularity, with a function more similar to that of the human brain 5.

### 2.1 Structure of Artificial Neural Networks

The current structure of artificial neural networks contains an input layer, a hidden layer, and an output layer. The input layer is responsible for receiving external information and data; the hidden layer is responsible for processing the information and continuously adjusting the connection properties between neurons, such as weights and feedback; and the output layer is responsible for outputting the results of the computation. Among them, the weights reflect the strength of the connections between units; the feedback reflects the positive and negative correlations between units, and the processing of information is reflected by this information in the connection relationship between units. Due to the unknown of the overall result, the weights and feedback in the hidden layer need to be adjusted continuously to finally achieve the best fit 6.

Once the structure of the neural network is determined, the next task is training and learning. The neural network mainly completes the training and learning process by changing the connection weight of each neuron node in the network rather than by changing the processing unit itself 4. Therefore, the only element that is used to change the performance of a processing unit is the connection weights if the unit is to learn to handle the given problem correctly.

## 2.2 Classification and Characteristics of Neural Networks

Neural networks are classified according to different structures, functions, and learning algorithms, and can be divided into: perceptron neural networks: the simplest type of neural networks, with only a single-layer neural network structure, using hard limits as the network transfer function, mainly for simple linear two-class division problems; linear neural networks: neural networks with a single-layer structure, using linear functions as the network transfer, mainly for solving linear approximation problems 9.

**Inherent parallel structure and parallel processing:** Artificial neural networks are similar to the human brain in that not only are they structurally parallel, but their processing order is also parallel and simultaneous 11. The processing units within the same layer are operated simultaneously, i.e., the computational functions of the neural network are distributed over multiple processing units, whereas a general computer usually has one processing unit whose processing order is serial.

**Distributed storage of knowledge:** In neural networks, knowledge is not stored in specific storage units, but distributed throughout the system, and many links are required to store multiple knowledge. In a computer, a data or a set of data is available at a given address. In a neural network, the stored knowledge is obtained by "association", similar to the associative memory of humans and animals. Humans are good at recognizing shapes correctly based on associations, and so are artificial neural networks.

**Fault tolerance:** Artificial neural networks are highly fault-tolerant. It can learn from imperfect data and graphs and make decisions 11. Since the knowledge exists in the whole system, not just in a single storage unit, booking a

percentage of nodes that are not involved in the computation does not have a significant impact on the performance of the whole system. Capable of handling data that is noisy or incomplete, with generalization and a high degree of fault tolerance.

**Adaptive:** Adaptivity finds out the intrinsic relationship between input and output based on the data provided, through learning and training, so as to find the solution to the problem, rather than based on empirical knowledge of the problem and rules, and thus has an adaptive function, which is very useful for weakening the weight determination human factor.

**Pattern recognition capability:** There are various neural network models available, and many of them are good at pattern recognition 16. Pattern recognition is one of the most important features of ANN. It not only recognizes static information, but also has great potential for processing complex dynamic information (varying over time and space) in real time 15. Pattern recognition is often very complex, with interactions between factors that present complex nonlinear relationships, and artificial neural networks provide a powerful tool for dealing with such nonlinear problems 16.

## 3. APPLICATIONS OF ARTIFICIAL NEURAL NETWORK

### 3.1 Aspects of Pattern Recognition

Pattern recognition includes text recognition, speech recognition, image recognition, speech synthesis, sonar or radar target recognition, seismic waveform recognition, time-varying signal recognition, and multidimensional pattern recognition 17. Neural networks have shown capabilities in this area that surpass traditional methods including statistical, static and artificial intelligence methods. Among them, text recognition involves storing in the computer a representative pattern of each text that contains the main features of that text, such as symmetry, position of the center of gravity, number and direction of strokes, etc. The main task of recognition is to extract the main features of this text from the input text pattern containing a large amount of noise, and to compare these features with those stored in the computer to obtain the correct response to the input text pattern. Speech recognition allows the computer to simulate human hearing and to recognize the sound signal coming in from a microphone or a

telephone. Speech signals are complex functions influenced by the physical characteristics of the speaker (e.g., source and channel structure), environmental characteristics (e.g., background noise and transmission channel), and other factors, so that speech data collected from different people and from the same person at different times are highly variable. The adaptive learning function of neural networks can adapt to such variations. Image recognition is to use the original image or the appropriately pre-processed imaged as the input signal of the network, and to classify or recognize the input image at the output of the network. It mainly includes two-image data compression, image edge detection, automatic image classification, automatic medical diagnosis, automatic target recognition, and image correction 4.

### 3.2 Aspects of Signal Processing

Neural networks are also widely used in signal processing, such as target detection, clutter denoising or recovery of distorted waveforms, multi-target classification of radar echoes, velocity estimation of moving targets, and multi-target tracking 19. Neural networks can also be used for multi-detector signal fusion, where the signals collected by multiple detectors are processed to obtain the maximum possible complete information about the detected target. Neural networks have been used to detect whether a space satellite flight maneuver is stable, tilted, rotating, or swaying in four states 20, with a correct rate of up to 95%. To summarize, neural networks are mainly used in signal processing (adaptive filtering, time series prediction, spectral estimation, array processing, noise removal, detection, etc.), nonlinear signal processing (nonlinear filtering, nonlinear prediction, nonlinear coding, modulation/demodulation, median processing, etc.).

### 3.3 Adaptive Human-machine Interface Aspects

According to the principle of human-machine symbiosis, the work of human-machine interaction will become more and more common. Obviously, a good human-machine interface will greatly improve the overall efficiency and quality of the system. However, different human users usually have many different habits. Therefore, a good human-machine interface should have the ability to automatically adapt to different human users. Neural networks are expected to be an ideal tool to solve such problems.

### 3.4 Computational Aspects of Optimization

The basic idea of optimization algorithms is to move in the direction of decreasing to the minimum of the objective function in the space of possible combinations, and finally find the optimal solution. For large-scale optimization problems, such as the traveling salesman problem (TSP), using the conventional exhaustive search method would be computationally staggering, and the computational effort increases exponentially with  $n$ . When Hopfield solves the TSP with a neural network (the same method is used to solve other optimization problems), the variables of the optimization problem to be solved are represented by the states of the neurons, and by making the problem function and the network The weights of the connections between the neurons are determined by aligning the problem function with the energy function of the network. When the network starts from a certain initial state, the energy of the network decreases as the state changes, and finally reaches an equilibrium state with minimal energy, the state of the neural network reflects the value of the variable that makes the objective function minimal. Using such a method, Hopfield finds one of the 107 better solutions in milliseconds from a large number of solutions of order 1030, and although this is a suboptimal solution, the optimal solution may be obtained if the smallest method is randomly selected from the resulting solutions starting from different initial states 21. Solving optimization problems is a very important application of neural networks. There are many such problems in the real world and a wide range of applications, so there are great hopes for the application of neural networks in this area, expecting a hardware implementation to exploit its highly parallel strengths 21.

## 4. ARTIFICIAL NEURAL NETWORK IN CHEMICAL INDUSTRY APPLICATIONS

### 4.1 Fault Diagnosis

The application of neural networks in fault diagnosis is currently the most valuable chemical process application of neural networks, where efficient fault prevention, fault detection and fault diagnosis of processes and devices are necessary for safe, stable and quality production 24. BP networks, radial basis (RBF) networks,

and adaptive networks are currently used more commonly for fault diagnosis 25.

The BP algorithm, the most popular feedforward network for fault diagnosis, requires corrections to the ownership and threshold values of the network during the training process, calling it a global approximation neural network. Back in 1993, Downs et al. 27 proposed a simulation system based on an actual chemical production process at Tennessee Eastman Chemical Company, which mainly applied BP neural network. The TE process mainly consists of five typical reaction units: reactor, condenser, gas-liquid separator, desorption tower, and circulation compressor. There are 4 reactions in the whole production process, and 2 kinds of products are produced, and there is also a by-product and an inert material. Through 4-dimensional vectors to represent 15 known fault sequences, and adding perturbation, 500 sets of data are taken out as the data for neural network training, and then 100 sets are taken out as the test data, which are trained by adaptive learning rate momentum gradient descent back propagation algorithm or Levenberg-Marquardt back propagation algorithm, both of which can get neural network with good generalization ability and fault recognition capability is higher.

Radial basis (RBF) network is a local approximation function that requires only a small number of corrections to the weights and thresholds for each training sample, so it is fast to train and has gradually become the preferred choice for fault diagnosis in recent years, but it does not guarantee that the optimal solution can always be obtained 28, and, deciding the optimal structure of the RBF network is not straightforward and requires experimentation and error approximation. Adaptive networks, on the other hand, can overcome the stability problem in the network learning process and are improved competitive learning 29.

There are many features of artificial neural networks applied to fault diagnosis, including the ability to form and store knowledge about the process and learn directly from quantitative historical fault information by training artificial neural networks; the ability of artificial neural networks to filter out noise and draw conclusions in the presence of noise, making artificial neural networks suitable for online fault diagnosis and detection; and the ability of artificial neural networks to discriminate between causes and types of faults 24.

## 4.2 Process Control and Optimization

With the continuous development of automation process in various industries, the requirements of chemical processes for automatic control and optimization are also increasing. The uncertainty, nonlinearity, time lag, and strong coupling of multiple variables in chemical control and optimization processes make conventional control systems sometimes difficult to work 31, and the emergence of artificial neural networks has led to further improvements in the control and optimization results of various processes 32. The principle of artificial neural network-assisted process control and optimization is that when a process receives a disturbance signal, it is fed back to the artificial neural network, which corrects its mathematical model and thus controls the process system 33. ANN were first used in the control community by James et al. 34 in 1986.

In 2016 K. Guo et al. 35 used a fuzzy neural network of BP network for PID control of a normal decompression device. The  $K_p$ ,  $K_i$  and  $K_d$  parameters of traditional PID control cannot be adjusted with the change of operating conditions during the regulation process, and for complex operating conditions, there is often a large amount of overshoot and a long time to restore the balance, which cannot adapt to the high-quality control requirements. And PID controller as a linear controller, for non-linear system control effect is relatively poor. In contrast, fuzzy control is a control method based on artificial intelligence, which has good nonlinear adaptability and can realize the control of the system model when it is not very accurate. Combining fuzzy neural network with PID control can solve the drawback that PID parameters cannot be adjusted at any time during the operation of the control system, which not only improves the system's adaptability to nonlinear high-order systems, but also enhances the robustness of the system, so that the anti-interference ability and stability of the control system can be further improved. Its control principle is shown in Fig. 1.

Matlab is used to implement the PID control of fuzzy network, and the temperature at the top of the decompression tower, which is the most complicated controlled object, is selected as the research object. Considering the hysteresis problem, the cascade control is used, with the return flow rate at the top of the tower as the

secondary object and the temperature at the top of the tower as the primary object. The final obtained system Simulink model is shown in Fig. 2.

The simulation uses step response as the main signal input and the step amount is 60. By analyzing its step and robustness, its final simulation results show that the use of fuzzy neural network control can improve the robustness of the decompression tower top temperature cascade control system in the normal decompression device.

### 4.3 Quality Control

The introduction of artificial neural networks into the field of quality control is of great significance for practical production, as it depends mainly on the quality of the product to maintain the best-selling trend in the market. In 1996, Tsen et al. 36 used a hybrid artificial neural network model in an intermittent polymerization reactor for vinyl acetate emulsion, and the results matched better with experimental data. In 2006, Zheng et al. 37 performed intelligent control of process quality based on Elman-type feedback neural networks

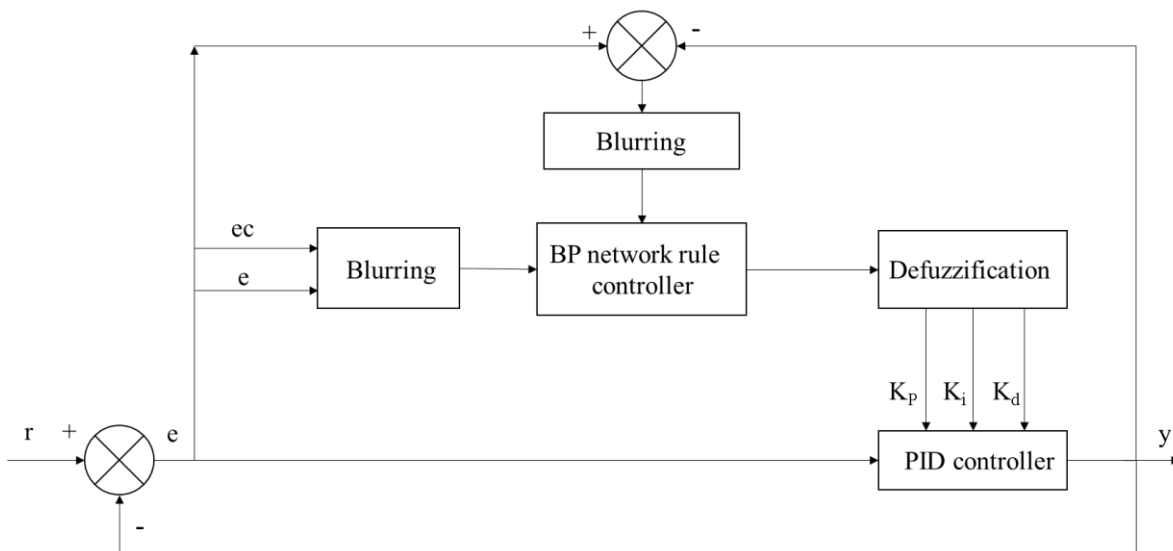


Fig. 1. BP network fuzzy controller control principle

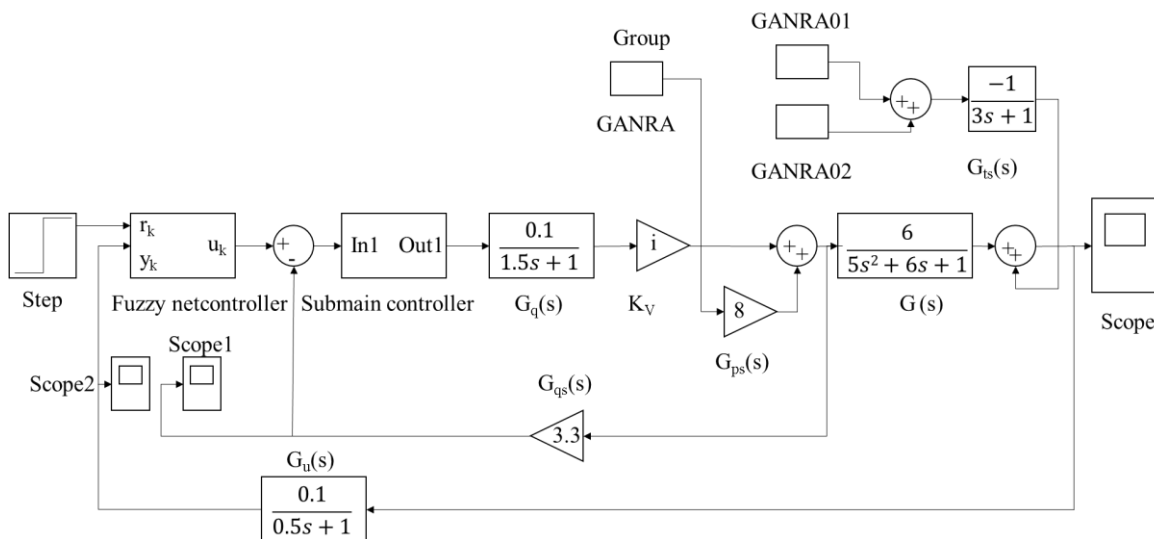


Fig. 2. Simulink model for fuzzy neural network control

and fuzzy neural networks, and the results showed limitations in quality control stability and convergence speed in small batch production lacking data. In 2015, Pengfei Zhu et al. 38 combined hybrid kernel function partial least squares and artificial neural network to construct a soft measurement model, which was applied to the quality index control of vinyl chloride polymerization process and achieved The quality index was smoothly controlled and the production consumption was reduced, which can guide the actual production.

#### 4.4 Property Estimation

There are three basic problems that must be solved when using neural networks to estimate the properties of substances: the first one is the characterization of substances; the second one is which neural network to use and its algorithm; the third one is the normalization of input and output data of neural networks 39; Hopfield neural networks have the potential to be applied to physical properties estimation if the problem to be solved (e.g., fitting bias minimization problem) can be transformed into the energy function of the network 40. As early as 1995, Zhang Xiangdong et al. 41 used neural networks to estimate the basic physical properties of organics and obtained an estimation accuracy that could meet the requirements of chemical calculations. In 2007, Pan Yong et al. 42 established a group contribution model based on BP neural networks to predict the flash point of organics, and the prediction of the flash point of organics and alkanes by this method was basically consistent with the experimental values 43, and the absolute average, absolute error and small absolute mean relative error. In 2015, Khazaiepoul et al. 44 used multilayer perceptual neural network with inputs of temperature, pressure, critical temperature, critical pressure, density, molecular weight and eccentricity factor to train the solubility of supercritical CO<sub>2</sub> dispersion fuel and by comparing with NSA and GE models, the results showed that the ANN model had the least error.

#### 4.5 Expert System

Artificial neural networks have good ability to approximate arbitrarily complex nonlinear systems and have been widely used in recent years for simulation and prediction of chemical processes 45. There are many theoretical and technical problems in the development of expert systems so far, such as knowledge

representation, knowledge acquisition, knowledge verification, etc., and the neural network model is essentially different from the traditional generative expert system, firstly, the knowledge representation is changed from explicit to implicit 46; secondly, the knowledge is not acquired automatically by human processing but by operators 47; finally, the inference mechanism is not the traditional inductive reasoning, but changes to competition for weights at the competitive level 48.

#### 4.6 Clustering Analysis

Cluster analysis is the analytical process of grouping a collection of physical or abstract objects into multiple classes consisting of similar objects, and the goal of cluster analysis is to collect data for classification on the basis of similarity. The statistical clustering method and the neural network method are the two main methods of cluster analysis, and the neural network method has been used more research and developed more rapidly in recent years.

### 5. CONCLUSION

At present, the application of artificial neural network in chemical industry is very extensive, and the technology gradually tends to mature, with the development of the times, artificial neural network has become an indispensable part of the chemical production process. The application of artificial neural network has greatly saved a lot of human and material resources, and made the production process more intelligent and large-scale. Of course, there is still a lot of room for the development of artificial neural networks, and people can develop new models based on the existing ones to better adapt to the development of the times. The future will definitely be the era of big data, which requires artificial neural network models to have a stronger ability to synthesize and analyze information to cope with more complex chemical production processes. The continuous improvement of artificial neural network technology and the development of application software based on artificial neural network technology are the important development directions of artificial neural network in chemical industry.

#### COMPETING INTERESTS

Authors have declared that no competing interests exist.

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