
Application of Artificial Neural Network in Optimal Design of Reactor

Abstract Reactor is widely used in biology, chemical industry, metallurgy, environmental protection and other fields, playing an irreplaceable role. With the development of science and technology and the concept of green development, the application of artificial neural network to optimize the reactor reaction conditions has become a trend. Artificial neural network plays an important role in reactor optimization because of its strong fault tolerance, the ability to express complex nonlinear relations and perform complex operations. This paper will briefly describe the basic principle and research progress of artificial neural network, and its application in reactor design.

Keywords : artificial neural network, chemical reactor, BP neural network, optimal design

1 Introduction

The reactor is a device that completes the reaction process and provides the necessary conditions and space for the reaction. For example, it can be used to complete the liquid uniphase reaction process, at the same time in liquid-liquid, liquid-solid, gas-liquid and other multiphase reaction process. A stirring device is usually installed in the reactor. The common stirring method is mechanical stirring, air stirring and so on. When the height of the reactor is relatively large, multilayer stirring blades are often used. Reactors can be classified into several types according to different grounds. Common reactors are: ① tubular reactor. Its main structure is filled tube or empty tube with large length, which can be used to complete liquid phase reaction and gas phase reaction process. ② Reactor with solid particle bed. The material can complete the multiphase reaction process by moving or stationary solid particle bed. It is further divided into fixed-bed reactor [1], moving bed reactor, fluidized bed reactor, trickle bed reactor, etc. ③ kettle reactor, also known as tank type, pot type reactor. Its main structure is a cylindrical container of small length. The reactor can be divided into batch reactor, semi-continuous reactor and continuous reactor according to the operation mode. Batch reactor operation is more flexible, more adaptable, high efficiency of mass transfer and heat transfer. It is often used in the production process of small batch size, large variety and long reaction time [2]. Its shortcomings are also very obvious, such as poor

product quality stability, the need for more auxiliary operations. Continuous reactors avoid the shortcomings of intermittent reactors and operate more stably [3]. The reaction process and reaction conditions determine the type of reactor to be selected. The role of reactor in industrial production is self-evident. Its performance, operation and reaction conditions are crucial to the quality and economic input of the product. The traditional reactor manufacturing process is cumbersome and not suitable for diversified production conditions [4]. Therefore, it is of great significance to study and optimize the reactor. Artificial neural networks have strong fault tolerance, can express complex nonlinear relations under maximum conditions, and can carry out complex operations [5], which plays an important role in chemical design, optimization operation, and production process regulation [6]. This paper will introduce the history, principle and research progress of artificial neural networks in reactors.

2、 Artificial neural network and its development

With the development of neurobiology, the field of artificial neural networks has gradually developed. Artificial Neural network (ANN) is also called neural network. It is an artificial skill technology that simulates the brain's information processing by connecting many artificial neurons [7]. It mainly expresses the complex functions of neurons with data by adjusting the intensity of each neuron [8]. It mainly includes three basic components: input layer, hidden layer and output layer [9], and has certain reasoning ability. The input layer is used to accept the external signal and input the external signal into the neural network. The hidden layer is between the input layer and the output layer, which is the part that transmits the received external signal to the output layer after processing. It may consist of one layer, or it may be made up of multiple layers. It processes the input information and transmits the processed information to the output layer. Then the processed information is output by the output layer [10]. According to the difference of their functions, artificial neural networks can be divided into feedback network and feedforward network [6]. Feedback neural network generally includes input layer, hidden layer, undertaking layer and output layer [11], which completes the transfer of the initial information state and makes the neural network reach a state of dynamic balance. The advantage of feedback neural network is that it can feedback the phenomenon in real time and then represent the complex content through data. Feedforward neural networks are simpler than feedback neural networks and are generally used to map nonlinear relationships. The advantage of feedforward neural network is strong recognition

ability. Even in the complex environment can also be relatively accurate recognition. In 1943, psychologist McCulloch and mathematician Pitts, inspired by biological neurons, first proposed the concept of artificial neural network and M-P model [9], which laid the foundation for the development of neural networks.

Hebb proposed Hebb's law and Hebb synapse in *The Organization of Behavior* in 1949. Rosenblatt pioneered the concept of perceptrons in the late 1960s. Perceptron is based on M-P model and has powerful learning function. This has aroused the interest of many scholars in artificial neural networks, and promoted the research of artificial neural networks to the upsurge. In 1985, Rumelhart et al. introduced BP neural network of multi-layer network into neural network for the first time. BP neural network has successfully reduced the computational amount of two-layer neural network [7], and has been widely used in various fields. It also triggered the second upsurge in the development of neural networks [12, 13]. In 1987, the first international conference on neural networks was held in Santiago, during which the International Federation of Neural Networks was established to provide space for the development of neural networks. Shuaijw proposed self-developing neural networks in 1996. Lecun proposed convolutional neural networks in the late 1960s. Convolutional neural network is based on BP neural network, which enriches the content of neural network. The development of neural networks can be roughly divided into four stages: the enlightenment stage from 1890 to 1969; The low tide from 1969 to 1982; The revival phase from 1982 to 1986; The new stage of neural network development since 1986 [14, 15]. After a long time of development, the existing neural networks mainly include feedback neural networks, forward neural networks and self-organizing neural networks. The BP neural network proposed by Rumelhart is the most widely used one. In recent years, the research of artificial neural gradually deepened, neural network has made great achievements in many fields, such as pattern recognition[16,17], automatic control[18,19], market analysis[20,21], chemical industry[22-24], game theory [25], medicine diagnosis [26-28], signal processing [29-31], troubleshooting [32,33], , machine Learning [34-36] and other fields. The construction of artificial neural networks is realized by the simulation of human brain function, rather than by complex mathematical models. Artificial neural network has solved many difficult problems and has a promising future. It can operate independently when working, which makes it possible to complete multiple controls without relying on the model[12,37]. Artificial neural networks are also a good choice for the control of complex nonlinear models.

3、 Application of ANN in Optimal Design of Reactor

The optimal design of the reactor plays an important role in the smooth operation of the chemical plant. The advent of artificial neural networks has greatly pushed reactors down a more economical and safer path. After 1988, the application of artificial neural networks in chemical engineering increased significantly [38]. Liu [39] compared the convergence and learning convergence speed of the improved fahlman correction algorithm and BP algorithm in the application of fault diagnosis of chemical reactors, and concluded that the improved fahlman correction algorithm was more applicable. The maintenance of good reaction condition is mainly predicted by reaction temperature, feed rate, inlet pressure and so on. Therefore, the reactor failure can be controlled in time. Through error analysis and echo comparison of the two algorithms, Liu concluded that the number of iterations of the Fahlman correction algorithm was smaller. The C procedure can be applied to different reactors and has strong versatility. This shows that neural network plays an important role in optimizing the reactor. Steyer JP et al. [40] combined fuzzy logic and artificial neural network to solve problems in anaerobic digestion fluidized bed reactor. Chen et al. [41] applied artificial neural networks to solve the problem of membrane contamination. Membrane contamination is a difficult problem in membrane bioreactors, which mainly affects the water yield of membranes [42]. Membrane bioreactor (MBR) is a kind of wastewater treatment system with high efficiency, which combines membrane technology and bioreactor to treat wastewater by biotechnology. It can remove organic pollutants in wastewater by decomposing organic matter in wastewater by aerobic microorganisms. In 2017, China became one of the countries with the highest utilization rate in the application of membrane bioreactor process [43]. To reduce the energy consumption of membrane bioreactors, advanced XDLVO method is commonly used to quantify the membrane fouling interface forces, but this method is complicated and time-consuming. Using the powerful data fitting ability of artificial neural networks to quantify the membrane fouling interface forces has become a feasible way. Chen et al. concluded that BP artificial neural network not only had lower quantization error than the advanced XDLVO method, but also needed only a few seconds through membrane surface morphology characterization, contact Angle measurement and Zeta potential test and analysis methods. This makes it possible to monitor membrane contamination on line, further make the membrane bioreactor run stably, and solve the problems in the reaction process. Shetty GR. Et al. [44] used neural networks to accurately predict membrane pollution in the nanofiltration

process of surface water and groundwater with less training.

The inner circulation reactor, which also plays an important role in sewage treatment system, has the advantages of small footprint, easy maintenance and stable operation [37]. Inner circulation reactor can use the energy of organic matter in wastewater for its own use, so it is more friendly to the environment. Due to the influence of various factors, accurate modeling of sewage treatment systems is almost impossible. However, artificial neural networks can be used to express the advantages of nonlinear relationships, which can be used to predict the results of the inner circulation reactor. Then improve the economic benefits and safety indicators. The genetic algorithm is used to solve the defect of BP neural network which is easy to appear local small, so that the average absolute error of the result prediction in the inner circulation reactor is only 0.0491. Before and after optimization, the proportion of samples in prediction errors within 5% is increased by 20%, and the proportion of samples in prediction errors within 10% is increased by 15%. Artificial neural network plays an important role in process optimization. Before the experiment, the simulation design and result verification are carried out to determine the experimental conditions and lay a good theoretical foundation. Hu et al. [45] optimized the operation conditions of expanded granular sludge bed reactor by using artificial neural network to model PH, hydraulic retention time, REDOX potential and other conditions. Based on the BP network model of EGSB system, response surface method is adopted to complete the optimization, which makes the expanded granular sludge bed reactor more flexible. As shown in Figure 1, the optimized BP neural network model is a three-layer network structure including 6 input layer, 12 hidden layer and 1 output layer, respectively. They obtained the correlation coefficient R of the linear relationship between the experimental value and the corresponding predicted value through regression analysis, which was about 0.8971, and the model was relatively accurate.

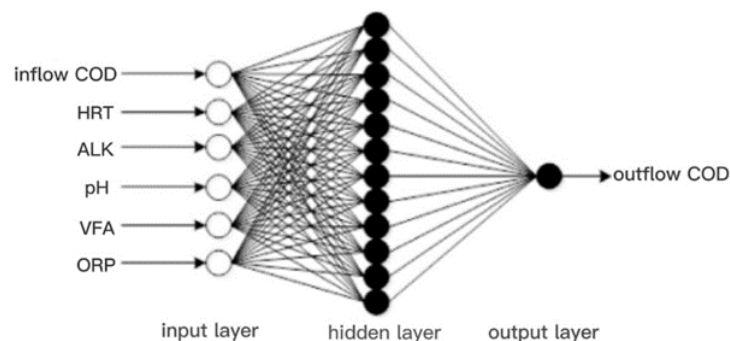


Figure 1 BPNN model topology [45]

Yin [46] simulated and optimized the design of stirred reactor through artificial neural network. The agitation in the stirred reactor is generally to speed up the reaction rate, fully mix the reactants, disperse bubbles, accelerate heat transfer and so on. The structure of the stirred reactor is relatively simple, but the design is often complicated because of the complex mixing process, reaction process and feeding process. Artificial neural network (ANN) plays an important role in the dynamic simulation of stirred reactor due to its high fault tolerance and accurate nonlinear description. Anna Witek-Krowiak et al. [47] applied artificial neural network based on response surface method to optimize biological absorption reactor. Yang et al. [48] established the model of batch reactor for direct coal liquefaction using BP neural network. The eight factors related to oil yield, coal conversion rate and comprehensive evaluation are predicted and analyzed, and the sensitivity order of these eight factors is obtained. Men and Que [49] used artificial neural networks to simulate the process parameters affecting the gas holdup of the slurry bed reactor, realized the optimization of the model, and obtained the predicted 3D stereogram of the samples. Wang and Xie [50] used the neural network toolbox of MATLAB to establish the BP network model, and introduced Levenberg-Marquardt algorithm to predict the kinetic model of the reaction mechanism. The BP neural network model needs to process the sample data through the maximum and minimum function first, and then use the training function in the MATLAB neural network toolbox to train the network. Figure 2 shows the training diagram of neural network. After training the network for 22 times, the network error reaches the requirement. Experimental results show that BP network prediction is more accurate than mechanism model prediction. The article concludes by pointing out that while automated testing is a significant time saver compared to manual testing, manual testing is not an alternative. Manual testing can be more efficient than automated testing for certain measurements.

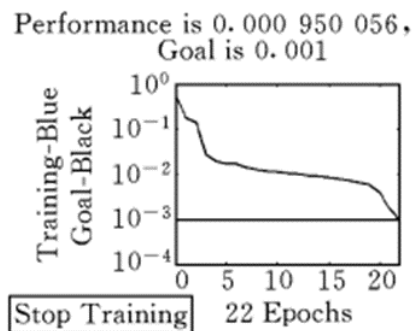


Figure 2 COD neural network training diagram

4 Conclusion

In recent years, artificial neural networks play an important role in reactors due to their simple operation, ability to simulate complex nonlinear relationships and accurate prediction. It not only optimizes the operating conditions of reactors, but also has a wide range of applications in product prediction, parameter setting and quality control. We should actively explore the problems in the practical application of artificial neural network, so that artificial neural network will be better applied in the chemical industry. The field of chemical industry will usher in a new vigor and vitality.

References

- [1] Zhao Z. Template preparation ceramic phase catalysis microchannel reactor and its application research [D]. Jinan university, 2021.
- [2] Huang Z, Li JH. Temperature and pressure prediction of runaway reaction in Tank reactor [J]. Journal of Safety and Environment, 2005(03):109-112.
- [3] Yang M, Wang PN, Zhao MY. Characteristics and design of continuous stirred tank reactor [J]. Petrochemical Industry, 1974 (05): 452-464.
- [4] Cao Y. Continuous micro series stirred tank reactor used for solid-liquid separation and reaction research [D]. East China university of science and technology, 2021.
- [5] Shi TF, Wu J. Artificial neural network application in the field of hydrology [J]. Journal of electronic testing, 2022, 4 (02) : 38-40.
- [6] Xi N. Application Progress of Artificial Neural Network in Chemical Industry [J]. Contemporary Chemical Research, 2017(03):41-42.

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- [7] Wang L, Zhang M, Zhu H, Liu Y. Artificial neural network and its application in earth science [J]. *World nuclear geology*,2021,38(01):15-26.
- [8] Jiang XD, Li WR. Application of artificial neural network theory to the study of potential source areas in the Yellow and Bohai Sea [J]. *Acta Oceanologica Sinica (Chinese version)*,1995(03):135-139.
- [9] Zhao CW. Review of Artificial Neural Network [J]. *Shanxi Electronic Technology*, 2020(03): 94-96.
- [10] Liu WH, Hong J, Li H, Sun Guixiang, Chen Yan. Application of artificial neural network in diagnosis informationization of traditional Chinese medicine [J]. *Journal of hunan university of traditional Chinese medicine*, 2017, 37(07): 809-812.
- [11] Zhang YX, Zhao J. Power generation power prediction of photovoltaic system based on feedback neural network [J]. *Protection and control of power systems*, 2011, 39(15): 96-101.
- [12] Li PZ, Yu J, Rong B. A review of the application of Artificial Neural networks in structural engineering [C]// *Proceedings of the 13th National Symposium on Modern Structural Engineering*, 2013: 1894-1898.
- [13] Miao JJ, Li DB, Li HJ. Based on artificial neural network of boiler heating surface dust prediction research present situation and prospects of [J]. *Journal of clean coal technology*, 2021, 27 (S2) : 212-220. The DOI: 10.13226 / j.i SSN. 1006-6772.21101101.
- [14] Yan YC. Application of artificial neural network in medical statistics and information processing [J]. *Journal of mathematical medicine and pharmacy*,2016,29(11):1676-1677.
- [15] Zhang C, Guo Y, Li M. Review on the development and application of artificial neural network model [J]. *Computer engineering and applications*,2021,57(11):57-69.
- [16] Gao J, Shi F. A Rotation and Scale Invariant Approach for Dense Wide Baseline Matching. *Intelligent Computing Theory - 10th International Conference, ICIC (1) 2014*: 345-356.
- [17] Mikolajczyk K, Schmid C. A performance evaluation of local descriptors. *IEEE T Pattern Anal* 2005; 27(10): 1615–1630.
- [18] Bloch G, Denoeux T. Neural networks for process control and optimization: Two industrial applications[J]. *ISA Transactions*, 2003, 42(1): 39-51.
- [19] Shi F, Gao J, Huang X. An affine invariant approach for dense wide baseline image matching. *International Journal of Distributed Sensor Networks (IJDSN)*, 2016, 12(12): 1-12.

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- [20] Zhu B, Lin J. Principal Component Analysis and Neural Network Ensemble Based Economic Forecasting, 2006 Chinese Control Conference, 2006, pp. 1769-1772.
- [21] Hansen JV, Nelson RD. Neural networks and traditional time series methods: A synergistic combination in state economic. *IEEE Transactions on Neural Networks*, 1997, 8(4): 863-873.
- [22] Sun L, Liang F, Cui W. Artificial Neural Network and Its Application Research Progress in Chemical Process, ***Asian Journal of Research in Computer Science***, 2021, 12(4): 177-185
- [23] Liang F, Zhang T. Prediction of Chemical Production Based on Neural Network, ***Asian Journal of Applied Chemistry Research***, 2021, 10(3-4): 51-65.
- [24] Zheng Z, Qi Y. Study on the Simulation Control of Neural Network Algorithm in Thermally Coupled Distillation. ***Asian Journal of Research in Computer Science***, 2021, 10(3): 53-64.
- [25] Bauso D, Gao J, Tembine H. Distributionally Robust Games: f-Divergence and Learning, 11th EAI International Conference on Performance Evaluation Methodologies and Tools (VALUETOOLS), Venice, Italy, Dec 2017.
- [26] Zhang J, Qian J, Yang T, et al. Analysis and recognition of characteristics of digitized tongue pictures and tongue coating texture based on fractal theory in traditional Chinese medicine[J]. *Comput Assist Surg (Abingdon)*, 2019, 24(sup1): 62-71.
- [27] Ozyilmaz L, Yildirim T. Artificial neural networks for diagnosis of hepatitis disease," *Proceedings of the International Joint Conference on Neural Networks*, 2003., 2003, pp. 586-589 vol.1, doi: 10.1109/IJCNN.2003.1223422.
- [28] Chen MZ, Cen YG, Cui LT, et al. Study on Observation Diagnosis Automatic Complexion Recognition Based on Image Processing. *Chinese Journal of Information on Traditional Chinese Medicine*, 2018,25(12): 97-101.
- [29] Gao J, Chakraborty D, Tembine H and Olaleye O. Nonparallel Emotional Speech Conversion. *INTERSPEECH 2019*, Graz, Austria, September 2019.
- [30] Pelenis D, Barauskas D, Vanagas G, et al.. CMUT-based biosensor with convolutional neural network signal processing[J]. *Ultrasonics*, 2019, 99:105956.
- [31] Hinton GE, Deng L, Yu D, et al.. Deep neural networks for acoustic modeling in speech recognition, *Signal Process. Mag.*, 2012, 29 (6) : 82-97
- [32] Alkaya A , Eker I . A new threshold algorithm based PCA method for fault detection in

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- transient state processes[C]// International Conference on Electrical & Electronics Engineering. IEEE, 2012.
- [33] Wold S . Method and device for monitoring and fault detection in industrial processes[J]. 2005.
- [34] Gao J, Chongfuangprinya P, Ye Y, Yang B. "A Three-Layer Hybrid Model for Wind Power Prediction," 2020 IEEE Power & Energy Society General Meeting (PESGM), Montreal, QC, 2020, pp. 1-5, doi: 10.1109/PESGM41954.2020.9281489.
- [35] Rohman B P A , Ahbb C H , Tridianto E , et al. Power Generation Forecasting of Dual-Axis Solar Tracked PV System Based on Averaging and Simple Weighting Ensemble Neural Networks[J]. EMITTER International Journal of Engineering Technology, 2018, 6(2):275..
- [36] Sperati S , Alessandrini S , Monache L D . An application of the ECMWF Ensemble Prediction System for short-term solar power forecasting[J]. Solar Energy, 2016, 133(aug.):437-450.
- [37] Tang J. Study on prediction of IC reactor wastewater treatment system based on BP neural network [D]. Southwest Jiaotong University,2018.
- [38] Wang ZK. Artificial neural network application in the chemical engineering [J]. Journal of modern chemical industry, 1996 (9) : 17-21. DOI: 10.16606 / j.carol carroll nki issn0253-4320.1996.09.004.
- [39] Liu M. Application of Artificial neural network in fault diagnosis of chemical reactor [J]. Liaocheng teachers college journal (natural science edition), 2000 (01) : 51-54 + 65. DOI: 10.19728 / j.i ssn1672-6634.2000.01.014.
- [40] STEYER JP, ROLLAND D, BOUVIER JC, et al. Hybrid fuzzy neural network for diagnosis - Application to the anaerobic treatment of wine distillery wastewater in a fluidized bed reactor[J]. Water Science and Technology,1997,36(6/7):209-217.
- [41] Chen YF, Shen LG, Lin HG. Artificial neural network in the application of quantitative membrane fouling interface reaction [J]. Journal of membrane science and technology, 2020, 40 (3) : 47-54. DOI: 10.16159 / j.carol carroll nki issn1007-8924.2020.03.007.
- [42] Shi BQ, Zhang HM, Yang FL, Meng FG, Zhang XW. Application prospect of artificial neural network in membrane fouling prediction of membrane bioreactor [C]// Proceedings of the Second Annual Conference of Water Treatment Chemicals Industry of China Fine Chemical

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- Association.[Publisher unknown],2006:207-214.
- [43] Fan JL, Liu HB, Xue ZY, Wang JX, Wang CN, Zhang RS. Based on artificial neural network [J]. Journal of MBR membrane fouling research status of membrane science and technology, 2021, 9 (4) : 154-159. The DOI: 10.16159 / j.carol carroll nki issn1007-8924.2021.04.020.
- [44] SHETTY GR., CHELLAM S.. Predicting membrane fouling during municipal drinking water nanofiltration using artificial neural networks[J]. Journal of Membrane Science,2003,217(1/2):69-86.
- [45] Hu YF, Yang CZ, Dan JF, Pu WH, Yang JK. Application of artificial neural network in expanded granular sludge bed reactor [C]// Environmental Engineering 2017 Supplement 1.,2017:187-191+34.
- [46] Yin JZ, Cheng SJ, Jia LY, Yin JW. Stirring reactor simulation and optimization design [J]. Chemical equipment technology, 2009, 30 (4) : 1-5. DOI: 10.16759 / j.carol carroll nki. Issn 1007-7251.2009.04.003.
- [47] Anna Witek-Krowiak, Katarzyna Chojnacka, Daria Podstawczyk, Anna Dawiec, Karol Pokomeda. Application of response surface methodology and artificial neural network methods in modelling and optimization of biosorption process[J] . Bioresource Technology. 2014
- [48] Yang ZK, Liu H, Li JW, Li CY. Artificial Neural network simulation of the performance of coal direct liquefaction batch reactor [J]. Coal Chemical Industry, 2007(02): 27-30.
- [49] Men ZW, Que GH. Prediction of gas holdup and volumetric gas-liquid mass transfer coefficient in slurry bed reactor using neural networks [J]. Petroleum planning and design,2009,20(06):17-20+50.
- [50] Wang JH, Xie HW. Research on prediction model of anaerobic sequential batch reactor based on BP network [J]. Computer development and application, 2008, 21(12): 13-15.