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Research Article

Design and Deconstruction of Chemical Process Flow Based on Deep Learning

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Chemical process design is something that researchers must do before conducting chemical reaction experiments, and this step is crucial for the entire chemical production. Because even if the relevant basic information of the institute is obtained, most of the above data have not been verified by experiments, and researchers need to confirm through experiments. In addition, because the market demand for chemical process products is very large, the types of chemical substances are increasing, chemical equipment and instruments are becoming more and more complex, and these require researchers to design and study in advance. This ensures the smooth production of products and the safety of researchers. However, the expansion of the equipment scale and the complexity of the equipment make it more and more difficult to design the chemical process flow. There are many influencing factors and levels to be considered when designing the process, and the data is also very difficult to predict and classify. In order to solve these problems, this study discussed the countermeasures to deal with chemical process flow design in depth. Using the method of deep learning, the problem of chemical process design was analyzed, and the performance of the method was experimentally studied. The results show that the chemical process flow based on deep learning is better than other process designs, and its accuracy rate is higher than 94% in 10 experiments, which is higher than the other three methods. It can be seen that this chemical process method can meet the needs of the current chemical process, and the product quality and work efficiency are greatly improved.

1. Introduction

The most important thing in modern technology is chemical technology, which plays a very important role in China's economic development and has a relatively high status. Due to modern technological innovation, China's chemical processes, both in terms of enterprise scale and production capacity, have been rapidly improved. People's demand for chemical processes is also increasing, and various chemical process products have brought very considerable benefits to people's lives. Modern society is inseparable from chemical production. The chemical process refers to the whole process of turning raw materials into products after the chemical reaction. There are many dangers of extreme conditions in the chemical process flow, which requires very strict design, in order to better control the smooth progress of the chemical process flow and fundamentally improve its level. At present, many scholars study chemical technology, but there are relatively few studies from the perspective of deep learning. Deep learning is a new form of machine learning, which can imitate the human brain to interpret data, and its performance on data is better than many methods. Therefore, this study based on deep learning to study the design and analysis of chemical process flow has certain practical significance, and may be able to obtain good results.

The wealth brought by chemical technology to China's economy is very large, and it has brought many conveniences to people's lives. Chemical process technology is also constantly improving, and many scholars study chemical processes. Al R studied the water quality testing problems of ordinary people, developed related chemical process methods, and optimized water-related parameters [1]. However, the algorithm he used to detect the concentration of water pollution in the article could not actually get an

accurate value. Bal'Chugov and Enhbat studied the chemical process experiments of the Ark model and introduced complex chemical process problems [2]. However, the data he uses in the article are not up-to-date, which will cause the results to be unrealistic. Frolkova analyzed the chemical process technology work of the past few years and elaborated the hierarchical structure of the chemical technology system [3]. But he did not have a comprehensive description of the technological innovations required by the comprehensive experts. Horvat et al. established a program to assess the cognitive complexity of chemical-technical problem tasks, and used experiments to verify the feasibility of this program [4]. But he did not take into account the possible influence factors during the experiment.

After analyzing the research results of other scholars, Makarov et al. studied the possibility of plasma chemistry technology in converting machine wastewater and confirmed the use of organic dispersion medium [5]. But his description of the water-coal composite fuel in the text is not very detailed. Song et al. studied the chemical process stability in calcium-peptide solar cells and carried out related experiments for analysis [6]. But he did not point out the specific process of calcium-peptide solar cells in the text. Mi et al. studied the formation process of the basic discipline of chemical technology and analyzed the most important links in the chemical process [7]. But the model he uses in the study is not the most appropriate.

The application field of deep learning is very wide, and it has many advantages. It can use more data or better algorithms to improve the results of learning algorithms. The innovation of this study is the use of a novel method, deep learning, to study chemical process flow. During the research process, a lot of relevant data were called for analysis in a convenient way to help the future chemical process.

2. Methods of Chemical Process Flow

2.1. Chemical Process. Chemical processing is the method of converting raw materials into products through chemical processing [8]. The scope of this technology is actually very wide, and the operation process is also more. The early chemical production was mainly based on experience, but after the progress of the times, the production of this handicraft can no longer meet the needs of society. Today's production is mainly based on modern technology based on scientific theory. The content of chemical substances is very complex and there are many types, and sometimes it is necessary to use empirical techniques. In fact, this subject is also set up in the curriculum of colleges and universities, usually industrial chemistry or chemical technology, and the content of these two subjects is basically the same. In general, the main development trend of this technology is to control automation, large-scale production, low consumption and low pollution, and optimize production parameters [9]. The process study of this technology can be seen in Figure 1 for details.

As shown in Figure 1, chemical production has to be carried out in specialized laboratories, and instruments and equipment also affect the entire chemical operation [10]. There are also many types of chemical substances, and the complexity is very large. Some chemical substances will produce toxic gases, which are quite harmful to the human body. Generally, when chemical reactions are carried out, laboratory personnel need to bring protective measures. In order to ensure the quality of the final output product, safety precautions must be taken when conducting experiments.

The chemical production process can generally be represented by three steps [11]. Specifically as shown in Figure 2.

As shown in Figure 2, the process of chemical production generally has three steps. The first step is the treatment of the raw material. In order to carry out the chemical reaction, the raw material needs to be pre-treated to make it reach the required state and specification as a chemical reaction material before proceeding to the next step [12]. Otherwise, the effect will be out of the experimental purpose. Different raw materials require different processing methods. Generally, different pretreatment operations such as purification, concentration, mixing, emulsification, or pulverization (pulverization is generally aimed at solid materials) are required. Just like the first step shown in the figure, industrial wastewater as a raw material needs to be pre-treated first. The second step is a chemical reaction. This is the most critical step in the production process. When the raw material is pre-treated to meet the requirements of the experiment, it is allowed to react under certain fixed conditions such as temperature and pressure. Of course, these conditions are generally extreme conditions for humans, so researchers need to pay special attention to safety issues, take protective measures, and consider safety issues first in the design of the entire experiment. When the raw materials reach the reaction conversion rate and yield required by the experiment, it means that the experiment is progressing smoothly. There are many types of chemical reactions, including oxidation, reduction, and polymerization. Through chemical reactions, people can obtain the desired product or a mixture. The third step is product refining [13]. This step is a finishing touch, and its purpose is to separate the mixture obtained in the previous step, remove magazines and other unwanted products, and obtain a product that meets the final rule. This step can be said to be better. In short, the entire chemical production process must be carried out in specific equipment and instruments, and the chemical and physical transformations need to be accurately completed after meeting the operating conditions.

2.2. Chemical Process Design. The chemical process design is also mainly divided into two stages [14]. The first stage is preliminary preparation. Because researchers need to understand the properties of the raw materials before proceeding to the next step. The second stage is equipment. This stage is the external conditions required in the chemical reaction and the equipment to carry out the chemical reaction. Together, these two phases are chemical process designs. Researchers need to understand the characteristics of the raw materials very carefully, as well as the properties of

Figure 1: Chemical process studies.

Figure 2: Chemical production process.

the instruments and equipment, relevant security measures should be fully implemented, in order to ensure the smooth progress of the experiment. And the researcher must work according to the research regulations and operate according to the operation drawings, and the final product can meet the target demand. The process design also has several basic features [15], as shown in Figure 3.

As can be seen from Figure 3, there are three basic features of this process design [16]. The first is the professionalism of the researchers. Because when conducting chemical reaction experiments, it is necessary to have very rich theoretical knowledge and practical experience of chemistry, that is to say, a very strong professional quality is required. And the professionalism of researchers is the guarantee for the safe conduct and successful output of experiments. And it also requires researchers to have very flexible on-the-spot responses. The researchers play the leading role in the whole design. They organize and analyze the materials to make the design of the whole experiment more scientific and accurate. The second characteristic is danger. As far as it is known, many raw materials will be used in the process design process, and some raw materials have great hidden safety problems, and the risk factor is relatively high, so the experimental process will also become dangerous. At this time, researchers need to have a very high degree of professionalism and take perfect protection and inspection measures, to ensure the safety of the experiment. The third feature is the complexity of the process [17]. The process involves a lot of raw materials and a lot of types of chemical substances. It not only requires researchers to be deeply familiar with the basic knowledge of chemistry, but also requires them to operate complex instruments and equipment. Therefore, the entire chemical production workload is very large, and the requirements for researchers are very high.

When designing this process, the following points should be paid attention to, as shown in Figure 4.

From Figure 4, we get information that three points should be paid attention to when designing [18]. The first point is the validity and completeness of the underlying data. Because most of the basic materials used by researchers are provided by scientific research units, which are basically theoretical knowledge, lack of experimental proof and actual production content, and the difference between chemical production equipment required for chemical reactions is still quite big. Therefore, these basic materials cannot meet the design requirements. These data are not up to standard in terms of completeness and availability. Therefore, researchers must carry out experimental verification of these data and test the correctness of the data to ensure the smooth progress of the design work. The second point is the selection and design of chemical equipment. Because the work of chemical production is very complex and the conditions are very extreme and harsh. When carrying out process design, some special equipment problems of pressure vessels or high-temperature resistant equipment will be encountered. At the same time, science and technology are constantly improving, the types of chemical materials are becoming

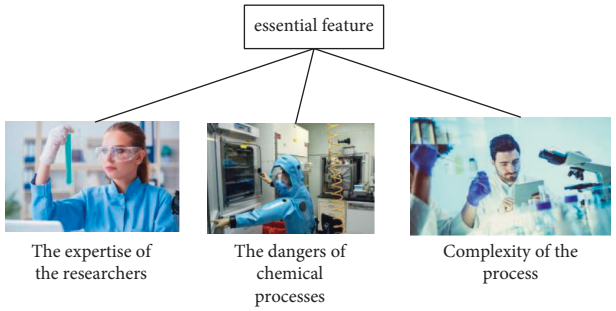

Figure 3: Basic features.

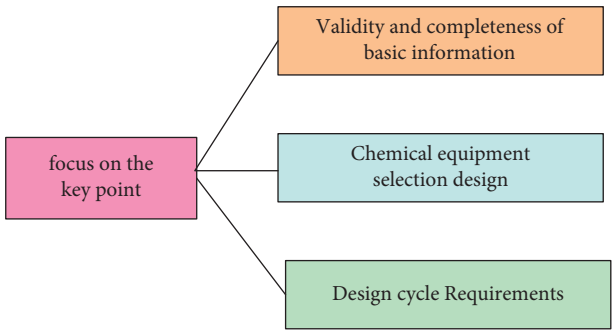

Figure 4: Points to note.

more and more, and the types of equipment are gradually becoming more abundant. Even the same production equipment may have different materials and equipment specifications. Therefore, when designing the equipment, researchers need to pay attention to the selection of the model of the equipment that must meet the process requirements. If there are special requirements, the equipment should also meet them. Even if the production scale is relatively large, the overall harmony and rationality should be considered when selecting equipment, and the equipment should be optimized. And the safety of the entire process progress needs to be guaranteed. The third point is the design cycle requirements. Because of the increasing demand for such products, the competition in the market is also very fierce. In order to increase competitiveness, some companies choose to shorten the design time of the process, resulting in a decline in product quality. Sometimes product performance cannot be guaranteed. Therefore, enterprises should correctly understand the importance of design, and ensure product quality in accordance with the prescribed design cycle.

2.3. Deep Learning. A deep learning algorithm that learns from historical data and then extracts useful information hidden in the data [19, 20]. The more common network structures in deep learning are as follows.

The first is a fully connected multi-layer neural network. Its structure is shown in Figure 5.

The propagation process of the network is divided into two types. The first is forward propagation. If the network

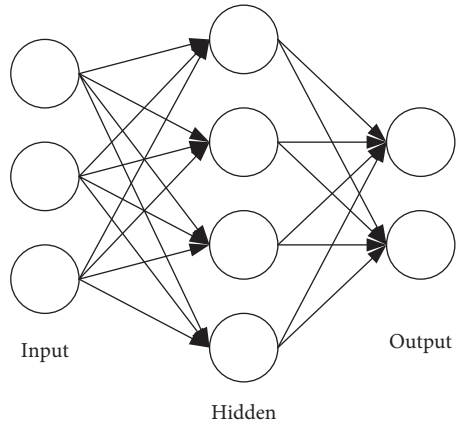

Figure 5: Network structure.

depth is A, the regular term coefficient is, the expression is as follows:

$$K = A(\widehat{U}, U) + \beta \varnothing(\vartheta). \tag{1}$$

The second is the backpropagation process. First, calculate the gradient of the last layer of the loss function K:

$$\begin{aligned} &H \leftarrow \nabla_{\widehat{U}} K, \\ &\text{FOR} L = A, A-1, \ldots, 1 \text{ DO}. \end{aligned} \tag{2}$$

Get the gradient of the output of each layer, it can be got a gradient of X_L:

$$H \leftarrow \nabla_{\widehat{XL}} K = H \bullet G'(X_L). \tag{3}$$

Finally, use the loss function K to calculate each layer:

$$\begin{aligned} \nabla_{EL} K &= H S_{L-1}^{Y} + \beta \nabla_{EL} \varnothing(\vartheta), \\ \nabla_{NL} K &= H + \beta \nabla_{NL} \varnothing(\vartheta). \end{aligned} \tag{4}$$

The second network structure is a convolutional neural network. It has representational learning ability. Each unit of its neural network can be represented by Figure 6.

If J_O represents the Oth layer feature of the convolutional neural network, the formula can be obtained:

$$J_O = G(J_{O-1} \times E_O + N_O). \tag{5}$$

If layer O is a pooling layer, it can be got:

$$J_O = \text{subsampling}(J_{O-1}). \tag{6}$$

Each layer of forward propagation mentioned above is actually activated by a nonlinear function. The general nonlinear activation function is as follows:

$$\begin{aligned} H(C) &= \frac{1}{1 + R^{-C}}, \\ H(C) &= \frac{1 - R^{-2C}}{1 + R^{-2C}}, \\ H(C) &= \text{MAX}(0, C). \end{aligned} \tag{7}$$

It can be seen from the above introduction that people measure whether the deep learning model meets people's requirements by the size of the loss function value. If the

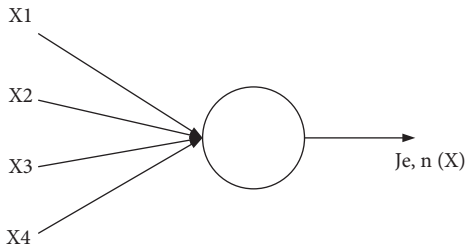

Figure 6: Neural network unit.

value of the loss function is less than the accuracy given by people in advance, it means that the deep learning model meets the requirements of people. Otherwise, the correction of the parameters in the model is achieved by the back-propagation algorithm until the loss function value is less than the given accuracy. In this part, people will briefly introduce the common loss functions in deep learning. In order to improve the generalization ability of the model, several common regularization terms are added to the loss function, such as:

$$K(\vartheta) = K(\theta) + \beta\varnothing(\vartheta). \tag{8}$$

The regular term generally has the following forms. For example, the regular term formula of A^2 parameters can be:

$$\varnothing(E) = \frac{1}{2}\|E\|_2^2. \tag{9}$$

The regular term formula for the A^1 parameter can be:

$$\varnothing(E) = \|E\|_1 = \sum_O |E_O|. \tag{10}$$

If U is the true value and $\widehat{U}(C)$ is the actual output value, the mean squared loss function can be obtained:

$$K = \frac{1}{2}\|U - \widehat{U}(C)\|_2^2, \tag{11}$$

M is the number of samples, then the cross entropy loss function formula is:

$$K = -\sum_{O=1}^{M}\left(U_O \mathrm{LOG}\left(\widehat{U_O}(C)\right) + (1 - U_O)\mathrm{LOG}\left(1 - \widehat{U_O}(C)\right)\right). \tag{12}$$

The exponential loss function and absolute value loss function can also be obtained as:

$$K = \frac{1}{2}\sum_{O=1}^{M}\mathrm{EXP}\left[-U_O\widehat{U_O}(C)\right],$$
$$K = |U - \widehat{U}(C)|. \tag{13}$$

3. Experiment and Deconstruction of Chemical Process Flow

3.1. Instance Destructuring. In the field of machine learning, the confusion matrix is used to judge the quality of the model. The confusion matrix that presents the four indicators together is shown in Table 1.

In order to verify the feasibility of the method based on deep learning, the test set about chemical process flow is divided into four categories, and the number of tests is set to 10, 20, 30, and 40 times, and case studies are carried out [21, 22]. The key evaluation indicators of the deep learning model in the first type of test set are shown in Table 2.

From the information in Table 2, the training effect of the model in this study is very good. When the number of tests is 10, the four indicators of the model all reach 100% efficiency, which shows that the model has a very good performance in terms of precision, accuracy, and recall. When the number of tests is added to 20, the precision rate of the model is 77%, the accuracy rate is 95%, and the recall rate is 100%, which are basically above 75%. When the number of tests reaches 30, the precision of the model is 100%, the accuracy rate is 95%, and the recall rate is 71%, which is a good testament to the excellent potential of this model.

The following are the key evaluation indicators of the deep learning model of the second type of test set, as shown in Table 3.

As shown in Table 3, the training effect of this model is better. Although the performance of each indicator has not reached 100%, it is basically more than 60%. When the number of tests is added to 20, the precision rate of the model is 65%, the accuracy rate is 93%, and the recall rate is 67%, which is basically above 60%. When the number of tests reaches 30, the precision rate of the model is 87%, the accuracy rate is 83%, and the recall rate is 85%, and the performance is still very good. When the number of tests reaches 40, the model has a precision rate of 67%, a precision rate of 95%, and a recall rate of 65%.

The following are the key evaluation indicators of the deep learning model of the third type of test set, as shown in Table 4.

As shown in Table 4, the training effect of the model is basically good. Although the performance of each indicator has not reached 100%, it is basically more than 60%. When the number of tests is added to 10, the precision of the model is 100%, the precision is 100%, and the recall is 100%. When the number of tests reaches 20, the precision of the model is 91%, the accuracy rate is 98%, and the recall rate is 100%, and the performance is still very good. When the number of tests reaches 30, the model has a precision rate of 86%, a precision rate of 88%, and a recall rate of 65%.

The following are the key evaluation indicators of the deep learning model of the fourth type of test set, as shown in Table 5.

As shown in Table 5, the training effect of this model is good. Although the performance of each indicator has not reached 100%, it is basically more than 60%. When the number of tests is added to 10, the precision of the model is 100%, the precision is 100%, and the recall is 100%. When the number of tests reaches 20, the precision of the model is 100%, the accuracy is 100%, and the recall rate is 100%, and the performance is still very good. When the number of tests reaches 30, the precision of the model is 100%, the accuracy is 97%, and the recall rate is 81%. This is a good illustration of the excellent performance of this model.

Table 1: Confusion matrix table.

Confusion matrix		True value	
		Positive	Negative
Predicted value	Positive	TP	FP
	Negative	FN	TN

Table 2: The key evaluation indicators of the first type of test set.

Test times	Accuracy (%)	Accuracy (%)	Recall (%)	$F1$-score (%)
10	100	100	100	100
20	77	95	100	87
30	100	95	71	83
40	100	100	100	100

Table 3: The key evaluation indicators of the second type of test set.

Test times	Accuracy (%)	Accuracy (%)	Recall (%)	$F1$-score (%)
10	100	91	61	76
20	65	93	67	87
30	87	83	85	89
40	67	95	65	73

Table 4: Key evaluation indicators of the third type of test set.

Test times	Accuracy (%)	Accuracy (%)	Recall (%)	$F1$-score (%)
10	100	100	100	100
20	91	98	100	96
30	86	88	65	71
40	77	91	91	82

Table 5: Key evaluation indicators of the fourth type of test set.

Test times	Accuracy (%)	Accuracy (%)	Recall (%)	$F1$-score (%)
10	100	100	100	100
20	100	100	100	100
30	100	97	81	89
40	83	95	91	86

3.2. Deconstruction Based on Deep Learning. In order to further verify the superiority of our method compared to other methods, people conducted a comparative experiment between the deep learning method and other methods [23]. And in order to get more intuitive data, the accuracy of these methods was quantitatively compared. They were placed under the same conditions for ten repetitions. The result is shown in Figure 7.

The information can be obtained from Figure 7, the accuracy of the method in this study is higher than 94% in 10 experiments, which is higher than the other three methods, and the effect obtained by the method in this study is very stable. When the number of tests is 1, the accuracy of this method is 97, the accuracy of method 1 is 93, the accuracy of method 2 is 92, and the accuracy of method 3 is 94. When the number of tests is 4, the accuracy of this method is 95, the accuracy of method 1 is 93, the accuracy of method 2 is 91, and the accuracy of method 3 is 92. When the number of tests is 8, the accuracy of this method is 96, the accuracy of method 1 is 91, the accuracy of method 2 is 92, and the accuracy of method 3 is 92. When the number of tests is 10, the accuracy of this method is 95, the accuracy of method 1 is 94, the accuracy of method 2 is 93, and the accuracy of method 3 is 93.

This shows that the proposed method can obtain richer information than shallow networks by expressing highly abstract features of diagnostic data. This advantage will be more obvious in industrial occasions with many variables, complex data relationships, and high nonlinearity [24]. It is worth noting that although method 1 achieves high accuracy in the tenth experiment, the model is too random, and the diagnostic results fluctuate greatly, and it is easy to fall into a local optimum.

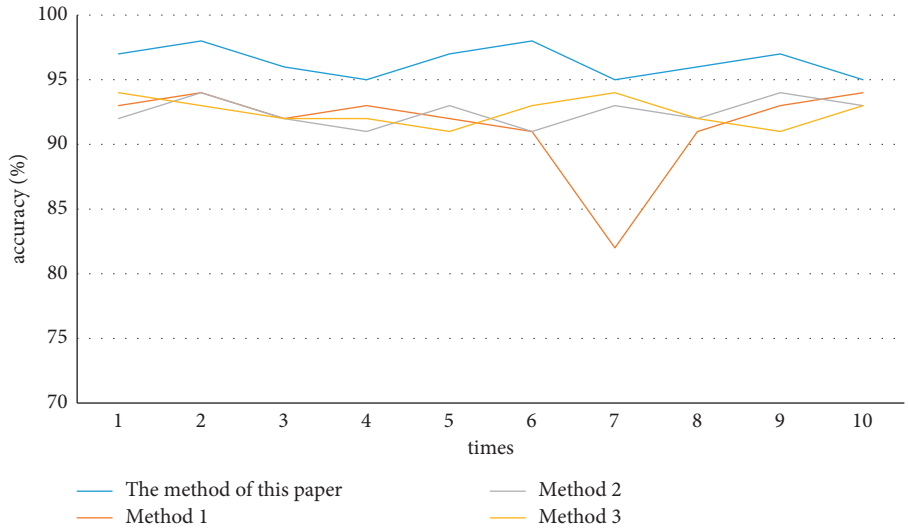

Figure 7: Comparative experimental results.

In order to further verify that the proposed deep model can solve the defect that the traditional multi-layer neural network is easy to fall into the local optimal solution, the sixth and eighth experiments are analyzed in detail, and the results are shown in Figure 8.

The information can be obtained from Figure 8. In two experiments, the proposed method has achieved relatively ideal classification results in about 100 iterations. However, method 1 falls into the local optimal solution early in the sixth experiment, and the classification error stays at about 0.3. Therefore, although the multi-hidden layer neural network can also obtain a relatively ideal classification effect, the classification error sometimes converges. Sometimes it falls into a local optimum, and the diagnosis results fluctuate wildly, which obviously cannot achieve satisfactory results in industrial occasions where the comprehensive performance of the diagnosis model is high. Therefore, the proposed deep fault diagnosis method can not only extract complex abstract information in complex industrial data, but also has a great improvement in model classification accuracy compared with shallow networks. Moreover, it overcomes the limitation that the traditional multi-hidden layer neural network is easy to fall into the local optimal solution, so it can be well adapted to the detection and diagnosis of complex chemical processes.

In order to verify the reliability of our method, people applied the deep learning algorithm in four test sets of chemical process flow design, and conducted two experiments [25]. The number of training sessions is set to 100 times. The result is shown in Figure 9.

It can be seen from Figure 9 that although a larger batch update amount has a faster convergence rate in the early stage of the fine-tuning process, as the number of iterations increases and the objective function approaches, the training process oscillates or even diverges. The smaller batch update amount, although the convergence speed is slightly slower, can gradually converge to a lower range with the increase in training times. In the parameter combination that has not been optimized enough, the error on the test set can be similar to or even better than that of the optimization model based on deep learning. A model with a larger learning rate must have a faster convergence rate, but in the later stage, there will be oscillations and the phenomenon of falling into a local optimum. A model with a lower learning rate converges more slowly at the beginning of training. In order to overcome this problem, this study adopts a training method of using a larger learning rate in the early stage of training and lowering the learning rate in the later stage of training. After the training of the model is completed, the test set data is input into the diagnostic model to obtain the prediction result, and the result is compared with the label data of the test set. If the diagnostic rate does not meet the requirements, it must return to the pre-training step to reset the model parameter combination to train a new model. If the diagnostic performance is good, the model will be used in the online stage. This is a good proof that deep learning algorithms are very suitable for chemical process design.

In order to better verify the accuracy of the method in this study, in the chemical data set, the method in this study is compared with the other two methods [26]. The result is shown in Figure 10.

The information can be obtained from Figure 10, which shows the classification improvement effect of different methods on the model. The proposed method is largely better than random selection, and with the increase in the number of iterations, the performance improvement effect is greater until a convergence value. After 10 iterations, the design accuracy of the three methods reached 99.76%, 99.48%, and 98.2%, respectively. After active learning, the model classification accuracy was improved by nearly 1.5%. However, although the active learning criterion based on information entropy has greatly improved the classification performance of the model, the results are similar to those obtained from industrial datasets. From the graphs of the number of false positive points and the false positive rate of the model under different methods, it can be found that the

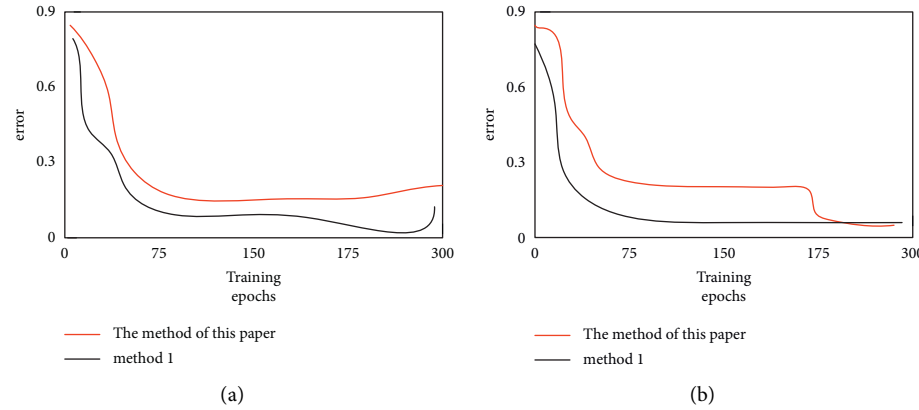

Figure 8: Specific analysis. (a) The 6th experiment. (b) The 8th experiment.

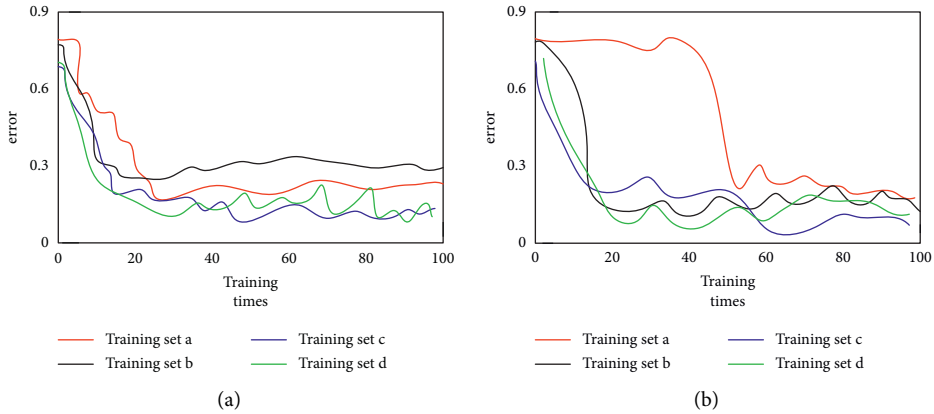

Figure 9: Error Curve. (a) The first experiment. (b) The second experiment.

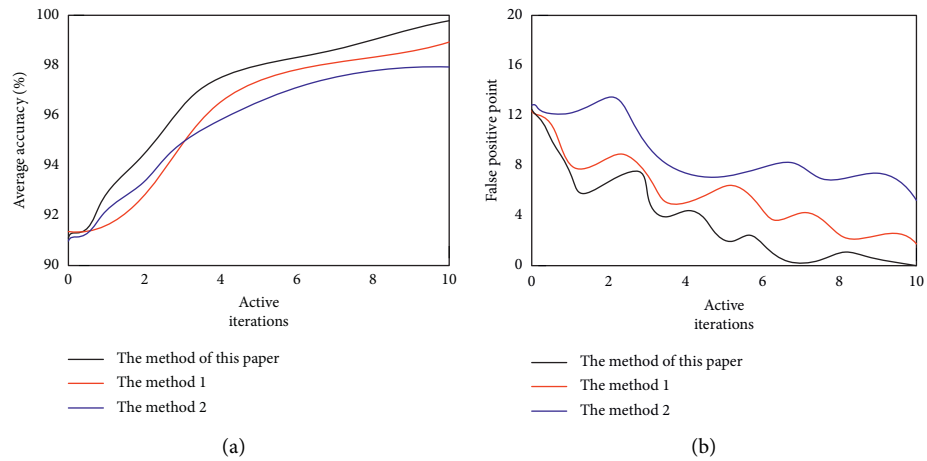

Figure 10: Experimental results of chemical data set. (a) Classification accuracy. (b) Number of false positive samples.

proposed method is not only better than the traditional method in overall accuracy but also reduces the occurrence of false positives. It is worth noting that although there is a certain fluctuation in the false positive phenomenon in the process of increasing the number of iterations (such as a sudden increase in the false positive rate in the second iteration), with the increase of the number of iterations, the suppression effect of the proposed method on false positives tends to be stable, and is generally better than other methods.

In the above experiments, the advantages of the proposed method are illustrated from the perspectives of model depth and sample selection criteria. From the perspective of

model depth, the effects of deep learning-based methods and other shallow models in chemical process design are compared, and the results show that the method proposed in this study is superior to the existing shallow models in terms of precision and accuracy. At the same time, the article further verifies the necessity of feature learning and expression in the proposed method by comparing different models. From the perspective of active learning sample selection criteria, the traditional deep network model and the active deep network model combined with information entropy are compared. The results show that the proposed method can not only efficiently use the labeled samples to improve the classification accuracy of the model but also suppress the false positive phenomenon of the diagnostic results to a large extent. Therefore, deep learning has great potential in chemical process design.

4. Conclusion

In this study, the design of chemical process flow is studied and analyzed by the deep learning method. And it is concluded that the application of this method is of great help to the design of chemical process flow, which greatly improves the accuracy and precision of process design, and makes the whole design have a better effect. Therefore, further research on the design of deep learning in this process can be considered. However, due to the limited length of the article, it cannot cover all aspects, and there are not many examples used in the research, which is also the limitation of this article. Looking forward to further research with more real data in the future is to discover more ways to help design chemical processes. At the same time, people should also firmly believe that there will be more research materials on this topic in the future, and the design of chemical process flow will become more and more scientific and accurate.

Data Availability

Data sharing is applicable to this article as no datasets were generated or analyzed during the current study.

Disclosure

The authors confirm that the content of the manuscript has not been published or submitted for publication elsewhere.

Conflicts of Interest

There are no potential conflicts of interest in this study.

Authors' Contributions

All authors have seen the manuscript and approved it to submit for publication.

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