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Research Article

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Research on the Fluctuation Transfer Path and Suppression Strategy of Key Parameters in the Process of Styrene Production

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Abstract: As an important chemical raw material, the production process of styrene is complicated and needs precise control. In order to deal with the problem that the parameters may fluctuate or get out of control due to interference in production, this study focuses on the transmission of process parameter fluctuations during styrene production. Considering the characteristics of parameter fluctuation and transmission under the disturbance of slow period in the chemical process, the multi-equipment units and multi-class parameters in the whole process of styrene production were studied. Firstly, Aspen Dynamics is used for dynamic simulation to obtain dynamic data sets under normal and different disturbance conditions. Then, the transfer entropy analysis and graph theory are used to explore the transfer mechanism of the wave, and the transfer path and potential source of the wave are identified. Based on the analysis results of transfer entropy, the LSTM model was built to accurately predict the fluctuation trend of key parameters, and the PID control of the fluctuation source was carried out accurately, thus the parameter fluctuation phenomenon in the whole styrene production process was suppressed. This study not only provides a new theoretical perspective for the parameter fluctuation analysis and control of styrene production process, but also provides a reference for the safety production management of other production processes in the chemical industry.

Keywords: styrene production, Parameter fluctuation transfer, Transfer entropy, LSTM, Predictive control.

1. Introduction

Styrene is an important chemical raw material and main product, used in the production of synthetic resin, synthetic rubber, ion exchange resin, medicine and dyes and other fields. Chemical processes involve complex physical and chemical reactions, which are difficult to be accurately described by mathematical models. The production process is continuous and uninterrupted, and any problems in any unit will affect the production performance such as product quality; Products are not counted by piece; The composition of raw materials, the state of production equipment, production process parameters and product quality can not be sensed in real time or fully, and it is difficult to ensure the long-term stable optimization of the entire production process, which has brought challenges to the further development of the chemical industry. There are many key indicators in the chemical production process, which often have a strong nonlinear relationship with other process parameters, and the interrelated information structure brings great challenges to production management. Therefore, it is necessary to analyze the fluctuation transmission of process parameters in the process of styrene production and its influence degree, and to predict and control the trend of its fluctuation transmission. This is of great significance to ensure the stable and safe operation of chemical production in its process.

At present, the data-driven method based on causal analysis is the most widely used in the research of chemical parameter fluctuation transmission analysis. This method is widely favored by scholars at home and abroad

because it involves less mechanism and process knowledge, has low limitation and is easy to implement. Fortela et al. [1] used Granger causality analysis under generalized variance decomposition to study the transitivity of oscillations of process variables in chemical plants caused by perturbations and faults. However, Granger causality analysis requires that the analysis factors are two independent variables, and does not consider the influence of interference factors or nonlinear embeddedness of time series. It is only applicable to linear systems, and the analysis results of nonlinear coupled systems are not reliable. Compared with Granger causality analysis, transfer entropy, as an information theory-based method, can measure the intensity of causality and is more accurate in dealing with the causality inference of high-dimensional nonlinear time series. Therefore, transfer entropy has a significant advantage in the study of causal analysis of time series with nonlinear characteristics. Lindner et al. [2] took the mining field as an example to compare the application of Granger causality and transfer entropy in fault diagnosis of industrial processes, and found that transfer entropy is better in accuracy and precision and can accurately identify the root cause, while Granger causality produces a large number of false associations. In addition, Yang et al. [3] also tried to use directed transfer function and partially directed coherent isofrequency domain methods to find causality, but these methods also have similar shortcomings to Granger causality analysis.

In 2000, Schreiber [4] combined the relevant theories of Information Theory (IT) and graph theory to propose the Transfer Entropy (TE) algorithm, which is used to describe the value of information transmission between variables. This method is based on IT related theory and is suitable for monitoring and analyzing the nonlinear characteristics of signals. And it can detect the directional and dynamic information transfer between variables, so as to effectively measure the intensity of causal transmission and determine the direction of causal transmission. As an information theory method, transfer entropy can effectively reveal the nonlinear coupling and dynamic interaction between different process parameters in the system, and can be directly applied to complex nonlinear systems. Therefore, in recent years, it has been widely used in various complex industrial fields. Abreu et al.[5] used the K2 algorithm of the Bayesian network and transitive entropy to identify the causality between industrial alarm variables. They mainly used transitive entropy to accurately measure the causality between first-order or multi-order autocorrelation variables to identify the causality between variables. Wen[6] proposed a symbolic conditional transfer entropy method based on control charts. This method symbolized the sigma limit of the exponential weighted moving average graph, and then calculated the conditional transfer entropy of the symbolized process data, so as to reveal the causal relationship between the time series of the symbolized process and draw it on the causal graph. By visualizing the propagation path of the disturbance studied, the root cause of process interference is analyzed, and the feasibility of the method is verified in the Tennessee Eastman process.

As industry enters the era of intelligence, accurate prediction of timing information in chemical process has become an important method to avoid risks in chemical industry. At present, the time series forecasting methods of chemical processes are mainly based on statistics, data and data and mechanism [7]. Chemical time series forecasting methods based on statistics have been widely used in chemical production, mainly including autoregressive model [8], moving average model, and autoregressive integral moving average model [9]. However, these methods are generally suitable for working with linear or stationary time series data. With the improvement of mechanization and automation of chemical production process, the pipeline of chemical production is constantly extended, which makes it impractical to establish a model for prediction by statistical method. For complex non-linear chemical processes, more advanced machine learning or deep learning methods are needed. Data-based chemical time series forecasting refers to the use of historical data to model and forecast the chemical process time series data. Zhu et al.[10] proposed a method that combined process simulation with deep learning model to determine the optimal operating conditions of cryogenic devices, and the process simulation software HYSYS collected data to test and verify the network model. Furkan[11] et al. combined artificial neural network with Aspen simulation to develop a simple and easy to implement prediction model. Through the simulation model, parameters such as gasifier diameter, length, gasifier temperature, air/fuel ratio and fuel type were analyzed, and data sets for ANN training were created. Prediction of composition and calorific value of syngas in circulating fluidized bed gasifier.

However, in the field of time series prediction, traditional neural networks are often difficult to deal with nonlinear, high-noise and high-noise data, and their performance is often unsatisfactory due to local

optimization, especially in the face of complex dynamic changes, nonlinear relationships and long-term dependencies. With its powerful time-dependent modeling capabilities, nonlinear processing capabilities, robustness and multi-variable data processing capabilities, LSTM can effectively capture complex dynamic characteristics in chemical processes and provide more accurate and reliable prediction results, thereby helping to optimize production processes, improve efficiency and reduce risks. Bai et al. [12] proposed a prediction model of key alarm variables of chemical processes based on dynamic internal principal component analysis (DiPCA) and LSTM. DiPCA was used to extract the most predictive principal components of process variables from high-dimensional data, and LSTM was used to learn the relationship between key alarm variables and predict the key alarm variables. Han et al. [13] proposed an LSTM combined with Monte Carlo algorithm model, which is well applied to the production prediction and energy structure optimization of ethylene plants in process industry.

Since the emergence and application of PID controller in the 1940s, PID control has been widely used in various industries. Nowadays, PID control is still the primary choice for process control [14]. Especially in the chemical industry, PID control runs through the entire production process. Mateo et al. [15] proposed a hybrid control framework based on the concepts of sliding mode control and internal model, combined the nonlinear PID controller with the sliding surface dynamic sliding mode control method, and applied it to the two nonlinear chemical processes of variable height mixing tank and continuous stirring tank reactor, so as to track the reference trajectory and suppress the interference. Bhookya et al. [16] proposed a PID level controller based on modified gray Wolf optimization algorithm and parameter set, and applied it to the monitoring platform of Internet of Things devices to realize real-time monitoring and control of liquid level in process industry.

Taking ethylbenzene dehydrogenation to styrene as an example, dynamic simulation technology is used to accurately reflect the changes of various parameters in styrene production under disturbed conditions. Based on dynamic simulation data set, a wave transfer model of process parameters in styrene production was constructed by using transfer entropy method and graph theory. Based on this, the coupling relationship between different process parameters and the mechanism of wave transfer were explored, the potential wave source was determined and the path of parameter fluctuation in styrene production system was revealed. According to the analysis results of the wave transfer model, LSTM is used to predict the trend of wave transfer of key parameters, and PID controller is used to put forward the corresponding control strategy.

The rest of this article is organized as follows. Section 2 introduces methods for transferring entropy and LSTM. In section 3, Aspen Dynamics was used to construct a simulation model of the whole process of ethylbenzene dehydrogenation to produce styrene. Taking the temperature of dehydrogenation tank as an example, the transfer entropy method was used to explore the mechanism and path of parameter fluctuation in the whole process of styrene production. In section 4, based on transfer entropy analysis, LSTM model is used to predict the parameter fluctuation trend and PID control is carried out. Finally, Section 5 gives a conclusion.

2. Basic Theory

Transfer entropy

Transfer Entropy (TE), measured and described by information entropy, is a statistic used to quantify the flow of information, and is particularly suitable for describing how information in a system is transferred from one part (or time series) to another. TE is widely used in time series analysis, complex system modeling, neuroscience, economics and other fields. According to Schreiber's definition, its calculation formula is as follows:

$$\begin{aligned} T_{Y|X} &= T\left(Y_{t+1} \mid Y_t, X_t\right) - T\left(Y_{t+1} \mid Y_t\right) \\ &= \sum p(y_{(t+1)}, y_t^{(l)}, x_t^{(k)}) \log_2 p(y_{(t+1)} \mid y_t^{(l)}, x_t^{(k)}) - \sum p(y_{(t+1)}, y_t^{(l)}) \log_2 p(y_{(t+1)} \mid y_t^{(l)}) \end{aligned} \tag{1}$$

In Eq. (2), $p\left(y_{t+1}, y_t^{(l)}, x_t^{(k)}\right)$ denotes the joint probability of y_{i+1}, $y_t^{(l)}$, $x_t^{(k)}$; $p\left(y_{t+1} \middle| y_t^{(l)}, x_t^{(k)}\right)$ is the conditional probability distribution, i.e., the probability distribution of the condition that the known $y_t^{(l)}$, $x_t^{(k)}$conditional on y_{t+1} ; $p\left(y_{t+1} \middle| y_t^{(l)}\right)$ is the conditional probability distribution, i.e., the probability distribution of y_{t+1} conditional on $y_t^{(l)}$ being known; and k, 1 are the temporal embedding dimensions of X_t and Y_t, respectively. The computation of the difference consists of two parts, the subtrahend represents the amount of information transfer to predict the future state of Y when historical data of the source sequence X and the target

sequence Y exist simultaneously. The minuend represents the amount of information transferred about the future state of Y when only the historical data of Y is known. The difference between the two represents the value of the net information transfer from sequence X to Y.

Since the processing object of entropy transfer is time series data, there is often a time delay between two time series data, that is, there is a certain lag in information transmission. The original formula fixed the time interval at 1, which is often contrary to the actual situation, so Bauer has improved the original formula:

$$T_{Y|X} = T\left(Y_{t+h} \mid Y_t, X_t\right) - T\left(Y_{t+h} \mid Y_t\right)$$
$$= \sum p(y_{(t+h)}, y_t^{(l)}, x_t^{(k)}) \log_2 p(y_{(t+h)} \mid y_t^{(l)}, x_t^{(k)}) - \sum p(y_{(t+h)}, y_t^{(l)}) \log_2 p(y_{(t+h)} \mid y_t^{(l)}) \quad (2)$$

The calculation of the difference consists of two parts, and the subtract represents the amount of information transfer to predict the future state of Y when the historical data of the source sequence X and the target sequence Y are present at the same time. The reduction represents the amount of information transmitted to the future state of Y by knowing only the historical data of Y. The difference between the two values represents the transfer value of the net information of the sequence X to Y. Where, h is the prediction time domain of transferring entropy, that is, the information of X_t sequence needs to be propagated to $Y_t$sequence after several units of time. The increase of H parameter makes the transfer entropy more suitable for practical application scenarios.

By simplification, the above formula can be rewritten as:

$$T_{Y|X} = \sum p(y_{(t+h)}, y_t^{(l)}, x_t^{(k)}) \log_2 \frac{p(y_{(t+h)} \mid y_t^{(l)}, x_t^{(k)})}{p(y_{(t+h)}, y_t^{(l)})} \quad (3)$$

Transitive entropy is an asymmetric measure with directivity, which can effectively represent the causal relationship between variables. $T_{X\to Y}$ represents the transfer entropy between variable X and variable Y, and its calculation formula is as follows:

$$T_{X\to Y} = T_{Y|X} - T_{X|Y} \quad (4)$$

The causal relationship between the two is determined by the value of $T_{X\to Y}$, and the larger of these values are defined as the causal intensity coefficient: if $T_{X\to Y} > 0$, it means that the current information is transferred from variable X to variable Y, i.e., X is the cause and Y is the effect, and the causal intensity coefficient is the value of $T_{Y|X}$; if $T_{X\to Y} < 0$, it means that the information is transferred from variable Y to variable X, i.e., Y is the cause and X is the effect, and the causal intensity coefficient is the value of $T_{X|Y}$; if $T_{X\to Y} = 0$ or the value is below the significance level threshold, it means that there is no obvious causal relationship between the variables.

Long short-term memory neural network

Long short-term memory neural network (LSTM) model is an improvement of recurrent neural network (RNN), which can process and predict sequence data effectively, especially for long-term dependence problems. During the training process, RNN will have the problem of gradient disappearance or gradient explosion, and it cannot handle a very long input sequence, that is, RNN has short-term memory problems. LSTM model can solve this problem. LSTM adds a memory unit that can be used to store long-term state in the hidden layer node of RNN to remember long-term dependent information in the sequence. In order to avoid information memory confusion, it also adds a gating unit to control the information remembered by the memory unit, effectively alleviating the problem of gradient disappearance.

The core of LSTM is its gate control mechanism, which is composed of three basic structures: forgetting gate, input gate and output gate, so as to control information flow. The forgetting gate is used to determine the degree of information retention through the input of the current moment and the output of the previous moment. The input gate is used to receive the updated information of the current moment and synchronously update the memory unit by remembering the new information, while the output gate transmits the processed information of the current moment to the next moment.

(1) Forget gate

It calculates the hidden layer state of the previous moment and the current input through the sigmoid function, and outputs a value between [0,1] to determine the degree of retention of the previous memory unit. The output

result is 0, indicating that it is completely forgotten (not retained), and the output result is 1, indicating that it is all retained. The mathematical expression is:

$$f_t = \sigma(W_f \cdot [h_{t-1}, x_t] + b_f) \quad (5)$$

Where f_t is the output of the forgetting gate, σ is the sigmoid activation function, W_f is the weight matrix, h_{t-1} is the hidden state of the previous time, x_t is the input of the current time t, and b_f is the bias term.

(2) Input gate

The function of the input gate is to accept the updated information of the current moment, which is used to remember the new information, and update the memory unit synchronously to determine how much of the input information of the current moment should be written into the memory unit. The mathematical expression is:

$$i_t = \sigma(W_i \cdot [h_{t-1}, x_t] + b_i) \quad (6)$$

$$\tilde{C}_t = tanh(W_C \cdot [h_{t-1}, x_t] + b_C) \quad (7)$$

Where i_t is the output of the input gate, W_i and b_i are the weight matrix and bias term of the input gate respectively, $\tilde{C}_t$ is the state of the candidate memory unit, *tanh* is the *tanh* activation function, W_C and b_C are the weight matrix and bias term of the state of the candidate unit respectively.

(3) Memory unit update

The memory unit state (C_t) of the LSTM is very important, it carries the long-term memory of the network. The forget gate controls the extent to which the memory unit state of the previous moment is discarded, and the input gate controls the extent to which new information is added. The mathematical expression is:

$$C_t = f_t \cdot C_{t-1} + i_t \cdot \tilde{C}_t \quad (8)$$

Where C_t is the memory unit state of the current moment, C_{t-1} is the memory unit state of the previous moment, f_t and i_t are the output of the forgetting gate and the input gate respectively, and $\tilde{C}_t$ is the candidate memory of the current moment.

(4) Output gate

The output gate determines what information is extracted from the memory unit state and outputs the hidden state as the current moment. The mathematical expression is:

$$o_t = \sigma(W_o \cdot [h_{t-1}, x_t] + b_o) \quad (9)$$

$$h_t = o_t \cdot tanh(C_t) \quad (10)$$

Where o_t is the output of the output gate, h_t is the hidden state of the current moment, $tanh(C_t)$ is the result of the state of the memory unit processed by the *tanh* function, W_o and b_o are the weight matrix and bias term of the output gate respectively.

3. Coupling Analysis and Transmission Path Identification of Slow-Varying Parameter Fluctuations

Dynamic simulation of styrene production process

The dynamic simulation of Aspen Dynamics is based on the steady-state model. Exporting the constructed steady-state model to Aspen Dynamics in Aspen Plus requires transferring the steady-state model parameters, process structure, and material/energy balance to the dynamic environment. Dynamic simulation usually requires a control system to manage the dynamic response in the process, configuring a controller for the key variables in the system (such as pressure, temperature, level, etc.), usually choosing a PID controller. Therefore, a dynamic simulation control system for styrene production was constructed in this paper, as shown in Figure 1. The controller detects the controlled variable and adjusts the controlled variable so that the actual value of the controlled variable is close to the initial value. The simulation was run in dynamic mode, and the dynamic response of the system was observed. By comparing the changes of various important parameters in the steady-state and dynamic simulation, it was confirmed that the parameters in the dynamic model (such as time constant, response speed, controller Settings, etc.) were set reasonably without abnormal behavior, and the time changes and dynamic response could be simulated normally.

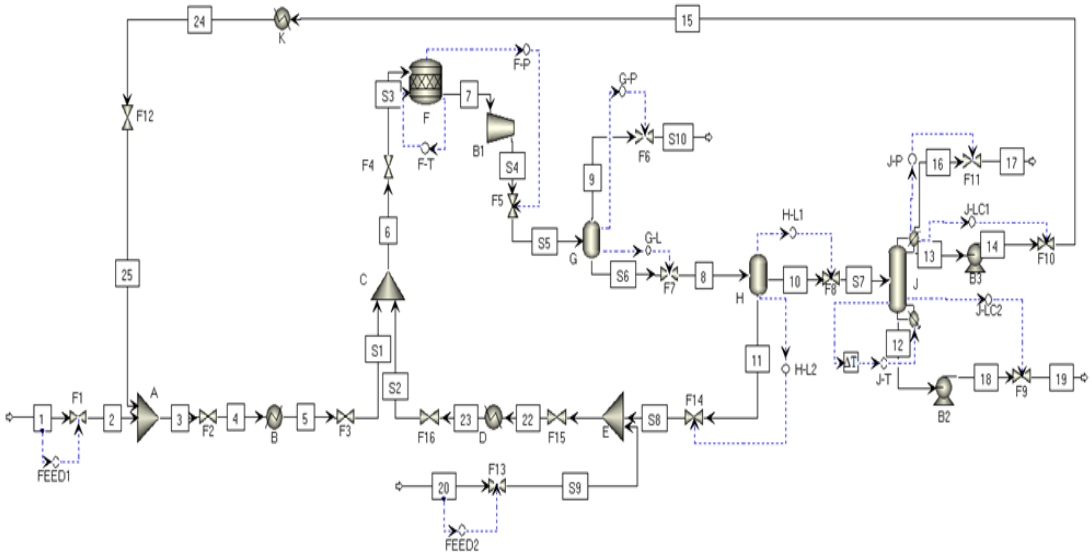


Figure 1: Dynamic simulation flow of ethylbenzene dehydrogenation to produce styrene

Dynamic simulation can simulate disturbance and analyze fault by setting disturbance source and fault mode. On the basis of the dynamic simulation model, parameter disturbance can be further introduced to simulate the changes of input or output flow, pressure and temperature, observe the changes of variables over time and the dynamic response of the system, and calculate the dynamic changes of various equipment and material flow in real time, and the corresponding fluctuation data of each parameter can be output.

Gradual periodic fluctuations

There are many types of slow fluctuation, among which periodic slow fluctuation is the representative. In the process of production, the periodic and repeated fluctuations of parameters are often related to the occurrence of oscillatory faults. The main cause of oscillatory faults is closely related to the feedback mechanism of the control loop. Due to the existence of the control loop, faults will propagate among multiple control loops, resulting in fluctuations in production quality and output. When the external disturbance propagates to the current loop through the coupling between the control loops, the controller will make corresponding adjustments, so that the disturbance can be eliminated in time, as shown in Figure 2. However, due to the unreasonable setting of controller parameters or the presence of viscosity, hysteresis, dead zone and saturation of the control valve, it will lead to the periodic oscillation of abnormal peak value in the loop. Fluctuations generated in the current loop can be further propagated to other loops, resulting in process-wide fluctuations.

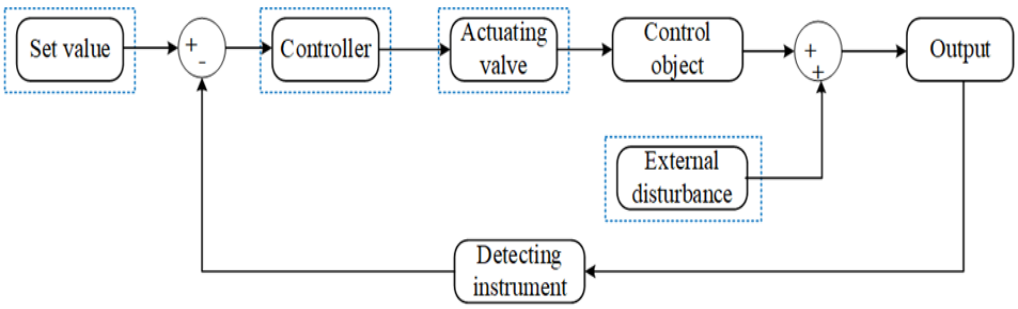
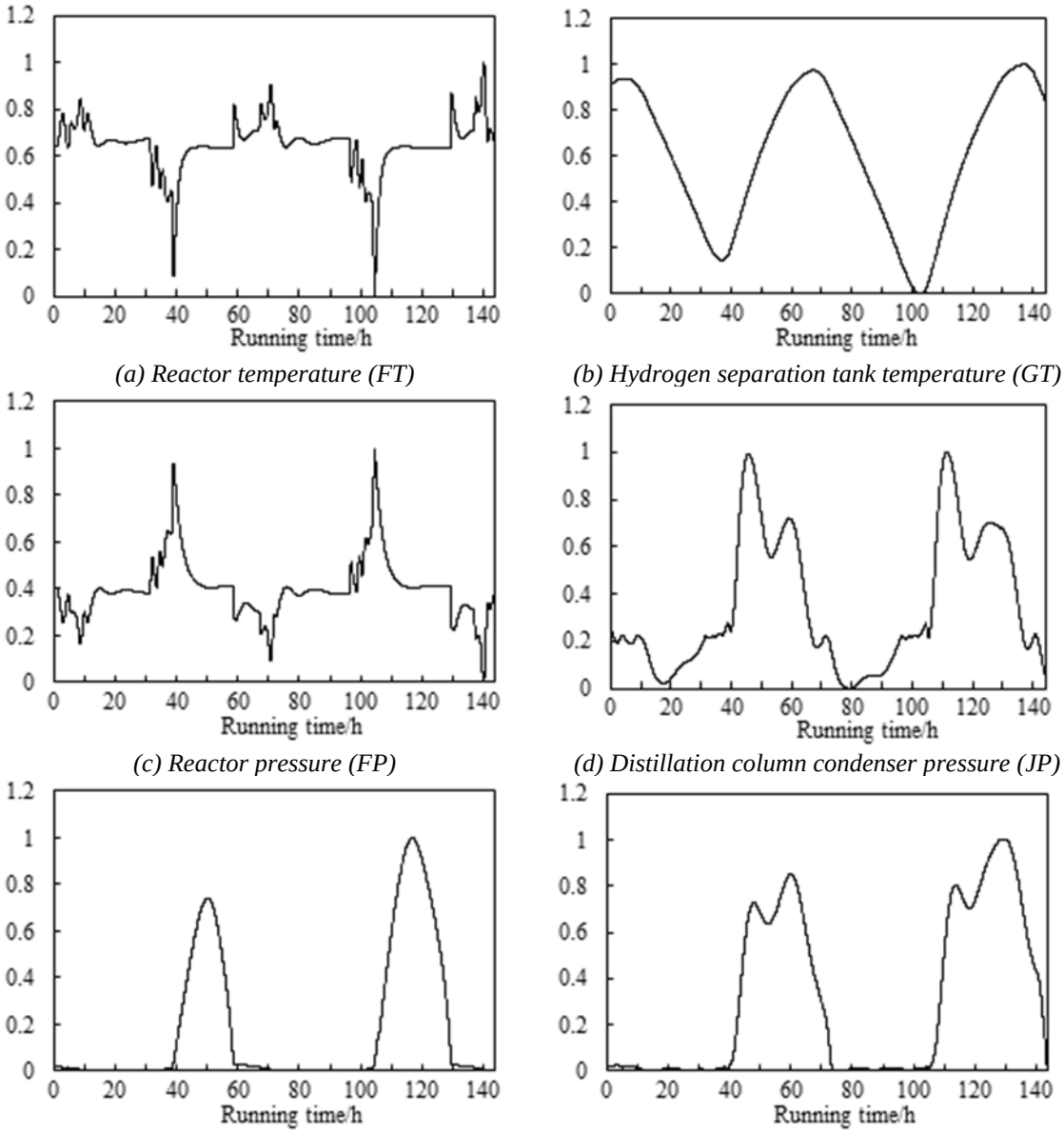


Figure 2: Location of oscillatory faults in the control loop

Due to the special molecular structure of styrene, polymerization is easy to occur. Vaporous styrene monomers tend to polymerize to form stalactite-like polymers, which can block components such as pipes, tanks and valves, affecting the stable and safe operation of production equipment. In the production process, the influence of temperature on styrene is very large, once the temperature meets the conditions will produce polymerization reaction, and the reaction temperature will affect the polymerization reaction speed, as the temperature

continues to increase, the polymerization rate of styrene will continue to increase. Especially in the dehydrogenation solution, if the temperature of the operation process is too high, it will cause a thermal reaction, and these polymers will directly block the outlet pipe of the separator, and the greater the concentration of styrene, the more likely the polymerization reaction will occur. Therefore, this section mainly studies the temperature fluctuation of dehydrogenation separation tank, in order to better control the temperature of styrene production process.

The styrene production dynamic simulation model built above was used to introduce continuous external oscillation disturbance to the process variable dehydrogenation separator temperature in its normal production process, and 14,400 fault data points of each variable were collected. The collected data segment was mainly taken from the fluctuation part of the process data, and the fluctuation rate was calculated separately and normalized. The fluctuation of part of the sampled data is shown in Figure 3.



(a) Reactor temperature (FT) *(b) Hydrogen separation tank temperature (GT)*

(c) Reactor pressure (FP) *(d) Distillation column condenser pressure (JP)*

(e) Distillation column condenser level (JTL) *(f) Distillation column tank level (JSL)*

Figure 3: Schematic diagram of periodic slow-change fluctuation of part of the sampled data

It can be seen from Figure 3 that under the continuous external oscillation disturbance, all parameters in the production system produce obvious periodic responses. The fluctuation of reactor temperature (a) is small at 0h-15h, the whole rises first and then falls, and reaches the peak at 9h; Slight fluctuation from 15h to 30h; 30h-45h

fluctuates greatly, the whole first drops and then rises, 39h reaches the trough, 45h is stable; 59h later, it fluctuated slightly again and entered a new cycle. The reactor pressure (c) and its temperature fluctuate in the opposite direction, but the period and amplitude are basically the same. The temperature of the hydrogen separation tank (b) almost did not plateau, fluctuated downward after 5h, reached the trough after 38h and then rose, and entered a new cycle after 69h. Condenser pressure (d) slight fluctuation in the early stage; 10h-30h fluctuates slightly, the whole first drops and then rises, and reaches the trough around 18h; Slight fluctuation from 30h to 40h; 40h-65h fluctuates greatly, the whole first rises and then falls, reaching the peak around 48h; After 65h, it fluctuated slightly again and entered a new cycle. The fluctuation state of the condenser level (e) and the column tank level (f) in the rectification tower is basically the same, which is basically stable in the early stage, starts to fluctuate upward at about 40h, reaches the peak at about 50h, and then falls back to maintain a stable level, and then fluctuates again to enter a new cycle. But the fluctuation of the tank level lasts longer.

Comprehensive analysis shows that under the influence of the disturbance, the parameters have obvious sustained periodic fluctuations, and the fluctuation amplitude is large and the fluctuation period is long. The monitoring temperature and pressure parameter fluctuation transmission response is faster; However, the fluctuation transmission response of the monitored liquid level parameters has a certain lag, and the lag time is relatively long. This may be because the level change is affected by a variety of factors, such as the flow speed of the liquid, the resistance of the pipeline, etc., resulting in the level change is slower than other parameters. Although there may be some differences in the fluctuation of each parameter in the initial stage, these fluctuation periods gradually converge with the passage of time, and the fluctuation period and amplitude also show a trend of gradual increase. This indicates that the internal dynamic equilibrium state of the system is constantly changing in the face of continuous disturbance, and more frequent and large adjustments are needed to maintain the stable operation of the system.

The fluctuation direction of pressure and temperature in the reactor showed a completely opposite trend, which indicated that the sensitivity of ethylbenzene dehydrogenation to pressure and temperature changes was different. The dehydrogenation of ethylbenzene is a reversible endothermic reaction with increasing volume, so it is beneficial to reduce the reaction pressure or increase the temperature. When the reaction temperature is lowered and the pressure is increased, the reaction will have an adverse effect, resulting in a decrease in the conversion of ethylbenzene, a decrease in the selectivity of styrene, an increase in energy consumption and a heavier equipment burden. However, the period and amplitude of the two are basically the same, which further verifies the existence of dynamic equilibrium in the system. The condenser pressure and liquid level of the distillation column show obvious fluctuation consistency. When the pressure changes, it will directly affect the flow speed and liquid level of the condensate. The change of liquid level can in turn affect the pressure distribution of the condenser.

4. Prediction and Control of Fluctuation Transfer of Key Parameters of Styrene Production

Ethylbenzene dehydrogenation is an important part of styrene production, which is mainly carried out under high temperature conditions, and the reactants will quickly cool to form condensate at the outlet. In the dehydrogenation reaction, there are often cases of abnormal equipment operation leading to production interruption, which seriously affects the production efficiency of styrene, and the production process is continuous, so it will cause a series of chain reactions. Therefore, it is necessary to predict and control the key parameters of ethylbenzene dehydrogenation reactor in order to reduce the fluctuation of chemical parameters and improve the stability and reliability of chemical process.

Construct the prediction and control model of parameter fluctuation transfer

In chemical process control, the dynamic dependence between variables can be effectively captured through TE analysis of the causal relationship between system parameters, especially the influence from process input to output. These causal relationships provide a good input for data-driven predictive control models, and LSTM can make predictions in such complex, non-linear, and time-varying systems. LSTM model can accurately predict the future fluctuation trend through the historical data of the learning process, and provide the basis for the subsequent control decision. PID control is a traditional control method commonly used in chemical process control, which reduces the error between the system output and the set value by adjusting the input of the

system. In actual production, based on transfer entropy analysis and LSTM prediction, real-time control parameter adjustment and optimization of PID controller response can reduce fluctuations and improve production stability.

In the study of chemical parameter fluctuation, the model based on TE, LSTM and PID controller can better predict and control the dynamic change of the system. Therefore, this paper proposes a chemical parameter fluctuation predictive control strategy based on TE, LSTM and PID controllers. The design steps are as follows:

Step 1: Transfer entropy analysis.

(1) Data collection and preprocessing: Collect all kinds of real-time data in the chemical process, and preprocess the data to ensure the accuracy of model training. (2) Calculation of transfer entropy: Select important process parameters and calculate the transfer entropy between them. (3) Identify key variables: Identify key factors that affect other variables and analyze their causal relationships. Through transfer entropy analysis, key variables that may cause fluctuations can be discovered in advance, and target variables can be provided for subsequent prediction models and control systems.

Step 2: LSTM model training and prediction.

(1) Selection of input variables: Based on the analysis results of transfer entropy, parameters that have a significant impact on reactor temperature and pressure (target variables) are selected as input variables, which helps to improve the prediction accuracy and reduce the computational complexity. The time series data is divided into training sets and validation sets, and the time window is defined to determine the length of the input data.

(2) LSTM model construction: LSTM prediction network of reactor temperature and pressure was constructed based on historical data. Using historical data for key variables based on transfer entropy analysis as input, select the number of layers and units of the LSTM. The LSTM layer captures the timing features in the input data to train the model to predict the process output, and the output layer predicts the process state in the future time. In order to train the network efficiently, the backpropagation algorithm with Adam optimizer is adopted in this paper. MAE and RMSE were used to evaluate the deviation between the model prediction and the actual value under different experimental schemes, and the weight and structure were optimized by error feedback.

Table 1: Main parameters of LSTM prediction model

parameters	Number of neurons in the input layer	Number of neurons in the output layer	Maximum iterations	Initial learning rate	Discard layer probability
value	4 or 3	1	100	0.005	0.2

(3) Training LSTM model: The training set is used to train the LSTM model. During the training process, the hyperparameters of the LSTM model are adjusted to improve the performance of the model. With the progress of training iteration, MAE and RMSE gradually become stable, which marks the gradual improvement of model performance and stability. Finally, validation sets are used to check the model's ability to generalize, making predictions for reactor temperature and pressure (target variables), respectively.

Step 3: PID controller design based on TE and LSTM.

(1) Determine the control objective: the main control objective of this paper is system stability. According to the LSTM model, the future process changes are predicted, and the relationship between the control variables obtained by the transfer entropy analysis is set. (2) Select a control strategy: determine the control strategy of the PID controller, including the action mode and weight of the proportion, integral and differential parts to meet the control objectives. (3) Experimental verification: Finally, the designed PID controller is implemented into the actual system, and the performance of the PID controller meets the requirements through experiments.

Wave transmission analysis and path identification

The periodic fluctuations of parameters have been preliminarily discussed above. However, the transfer path, internal mechanism and transfer trend of parameter fluctuations still need to be further analyzed by using transfer entropy theory and graph theory. After data denoising and normalization processing, process data is used to calculate the transfer entropy of the fluctuation transfer relationship between variables. The calculation results of the transfer entropy among process variables are shown in Table 2.

Table 2: Transfer entropy values between key process variables

variable	1	2	3	4	5	6
1	×	0.10	0.18	0.16	0.11	0.07
2	0.18	×	0.14	0.13	0.06	0.08
3	0.18	0.10	×	0.12	0.05	0.08
4	0.17	0.11	0.16	×	0.07	0.10
5	0.17	0.08	0.08	0.09	×	0.07
6	0.12	0.08	0.12	0.12	0.06	×

As shown in Table 1, the transfer entropy between various process parameters is compared to determine the direction of fluctuation transmission, and significance level test is conducted to determine the threshold and screen the causality. According to the causality data after selection, a weighted directed network diagram reflecting the interaction between process variables is constructed, as shown in Figure 4. Based on the causality network of parameter fluctuations, the transmission path and source of parameter fluctuations are identified, and the link most susceptible to disturbance is found out. The output $D_{out}(v_i)$ of each node v_i in the network is calculated by the formula:

$$D_{out}(v_i) = \sum_{x_k} T_{x_j|x_k} \quad (11)$$

The larger the output $D_{out}(v_i)$ of a node, the greater the influence of the historical status of the node on the current status of other nodes, indicating that the dynamic change of the node is the cause of the dynamic change of other nodes, and the state variable of the node is the location of the fluctuation source. Further, after the location of the wave source is determined, starting from the state variable where the wave source is located, the branch road with the largest causal intensity coefficient is retained, which is the main propagation path of the wave mode. The output D_{out} of each node in the figure is calculated, as shown in Table 3.

Table 3: Calculation results of output D_{out}t of key parameters

Key parameter	Value of D_{out}
①F_T	0
②G_T	0.46
③F_P	0
④J_P	0.33
⑤J_{TL}	0.17
⑥J_{SL}	0.36

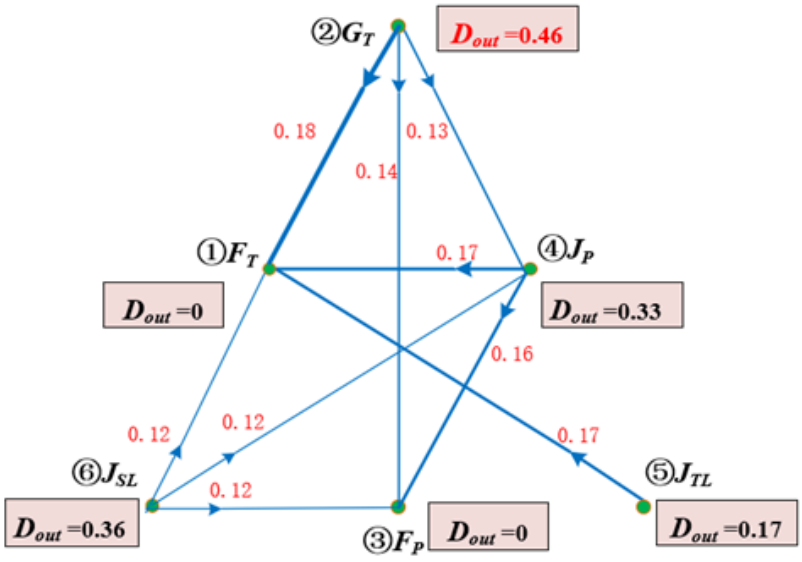


Figure 4: Parameter causality network diagram of periodic slow-change fluctuation

As can be seen from Table 2, the output of process variable G_T is the largest, so G_T is the location of the fluctuation source, which corresponds to the temperature of the hydrogen separation tank in the actual production process, and is consistent with the actual cause of fluctuation, that is, G_T is subject to external oscillation interference. The effectiveness of the proposed method in locating the source of slow-changing periodic fluctuations in chemical processes is verified. At the same time, the output of F_T and F_P is 0, indicating that the influence of the fluctuation of the reactor temperature and pressure on the downstream is smaller than that of the downstream parameter fluctuation on the reactor temperature and pressure. The hydrogen separation tank is the downstream equipment of the reactor, which also proves that the periodic fluctuations generated by G_T are mostly from external oscillation interference. The accuracy of the proposed method in locating the cycle fluctuation source of chemical process was verified again.

On this basis, further research was carried out to predict and control the temperature and pressure of ethylbenzene dehydrogenation reactor under the disturbance scenario.

Parameter optimization and result analysis of LSTM prediction model

Based on the above case, the temperature and pressure of ethylbenzene dehydrogenation reactor under the disturbance scenario were predicted. The time series data of each variable are 14400 pieces respectively. The first 10,000 pieces of data are divided into training sets and the last 4400 pieces are divided into test sets. According to the transfer entropy analysis results in Section 4.2, it can be obtained that:

Model A (temperature prediction): The main key parameters that affect the fluctuation of reactor temperature (F_T) are four variables: temperature of dehydro separation tank (G_T), pressure of distillation column (J_P), liquid level of distillation column condenser (J_{TL}) and liquid level of distillation column reactor (J_{SL}). Therefore, G_T, J_P, J_{TL} and J_{SL} are selected as input variables, and F_T is output variable.

Model B (pressure prediction): The main key parameters affecting the fluctuation of reactor pressure (F_P) are three variables: dehydrogenation separator tank temperature (G_T), distillation column pressure (J_P) and distillation column tank level (J_{SL}). Therefore, G_T, J_P and J_{SL} are selected as input variables, and F_P is output variable.

Model parameter optimization

In the process of constructing and training LSTM prediction model, the setting of hyperparameters is a very important step. In order to optimize the performance of the model, the orthogonal experimental method is used to find the optimal combination of hyperparameters. The effects of the number of hidden layer nodes, activation function and batch size on the prediction results are discussed. Different levels of three factors are considered, namely, the number of hidden layer nodes (50,100,150), activation function (relu, tanh), and batch size (50,100,150). Table 4 lists the details of the orthogonal experiment.

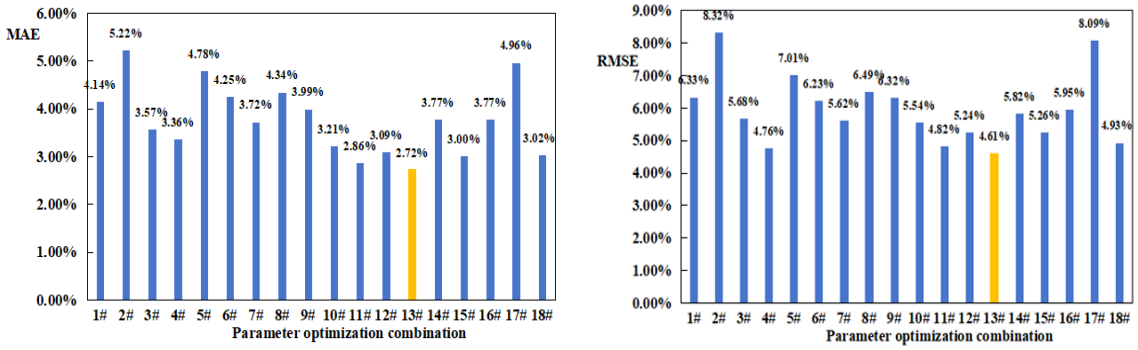
Table 4: Orthogonal test scheme

Group	Optimization parameter			Group	Optimization parameter		
	Number of hidden layer nodes	Activation function	Lot size		Number of hidden layer nodes	Activation function	Lot size
1#	50	tanh	50	10#	50	relu	50
2#	50	tanh	100	11#	50	relu	100
3#	50	tanh	150	12#	50	relu	150
4#	100	tanh	50	13#	100	relu	50
5#	100	tanh	100	14#	100	relu	100
6#	100	tanh	150	15#	100	relu	150
7#	150	tanh	50	16#	150	relu	50
8#	150	tanh	100	17#	150	relu	100
9#	150	tanh	150	18#	150	relu	150

(1) Prediction and evaluation of Model A (temperature of ethylbenzene dehydrogenation reactor)

The prediction performance of model A of each orthogonal test scheme is shown in Figure 6. As can be seen from Figure 5, there are certain differences in network prediction performance under different experimental

schemes. The results show that the MAE and RMSE of scheme 13# are both the minimum values, which are 2.72% and 4.61%, respectively. Therefore, 100 hidden layer node number, relu activation function and 50 batch size were selected as LSTM network parameters for reactor temperature prediction.

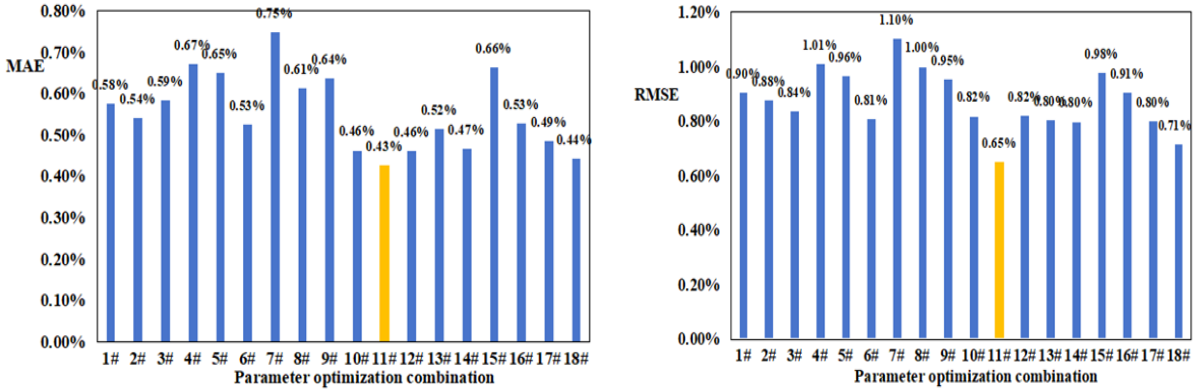


(a) MAE for each test scheme (b) RMSE for each test scheme

Figure 5: Performance evaluation of Model A orthogonal test scheme

(2) Model B prediction evaluation (temperature of ethylbenzene dehydrogenation reactor)

The prediction performance of model B of each orthogonal test scheme is shown in Figure 6. It can be seen that the Settings of different network parameters have different prediction effects on reactor pressure. MAE and RMSE of scheme 11# are both the minimum values, which are 0.43% and 0.65% respectively. Therefore, 50 hidden layer nodes, relu activation function and 100 batch size were selected as LSTM network parameters for reactor pressure prediction.



(a) MAE for each test scheme (b) RMSE for each test scheme

Figure 6: Performance evaluation of Model B orthogonal test scheme

Through the performance evaluation of model A and model B, it is proved that the LSTM model constructed in this paper can effectively predict the temperature and pressure of ethylbenzene dehydrogenation reactor based on transfer entropy analysis. However, under the same orthogonal experiment scheme, the prediction effect of model A and model B is different, and the prediction effect of model B is better than that of model A, indicating that the difference of sample data input to the model will affect the prediction performance of the LSTM model.

Analysis of prediction results

According to the parameter optimization results, the LSTM prediction model (Model A) with the number of hidden layer nodes being 100, the activation function being relu and the batch size being 50 was used to predict the reactor temperature. The LSTM prediction model (Model B) with the number of hidden layer nodes 50, activation function relu and batch size 100 was used to predict the reactor pressure. The prediction results are shown in Figure 7 and Figure 8 respectively.

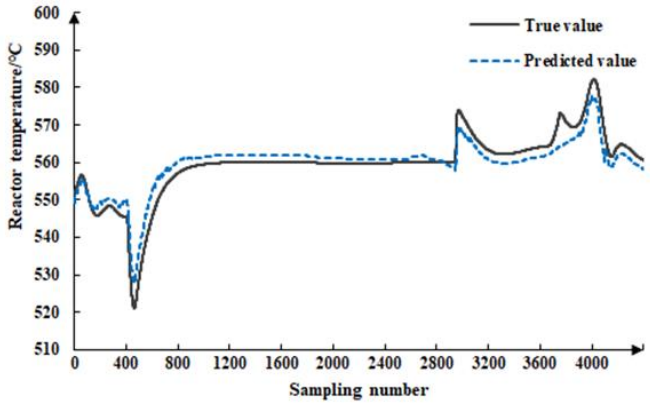


Figure 7: Predicted results of reactor temperature (LSTM Model A)

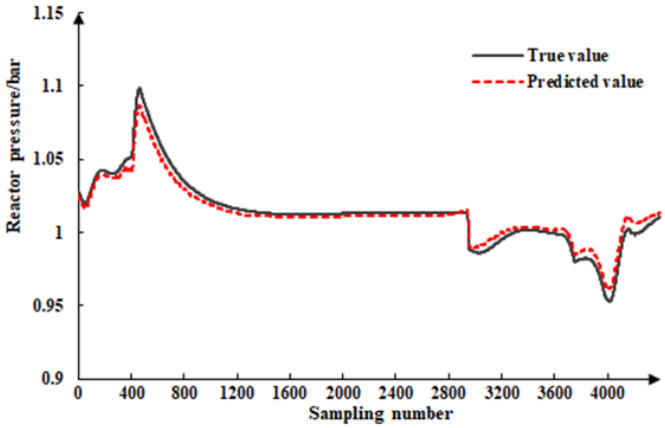


Figure 8: Predicted results of reactor pressure (LSTM Model B)

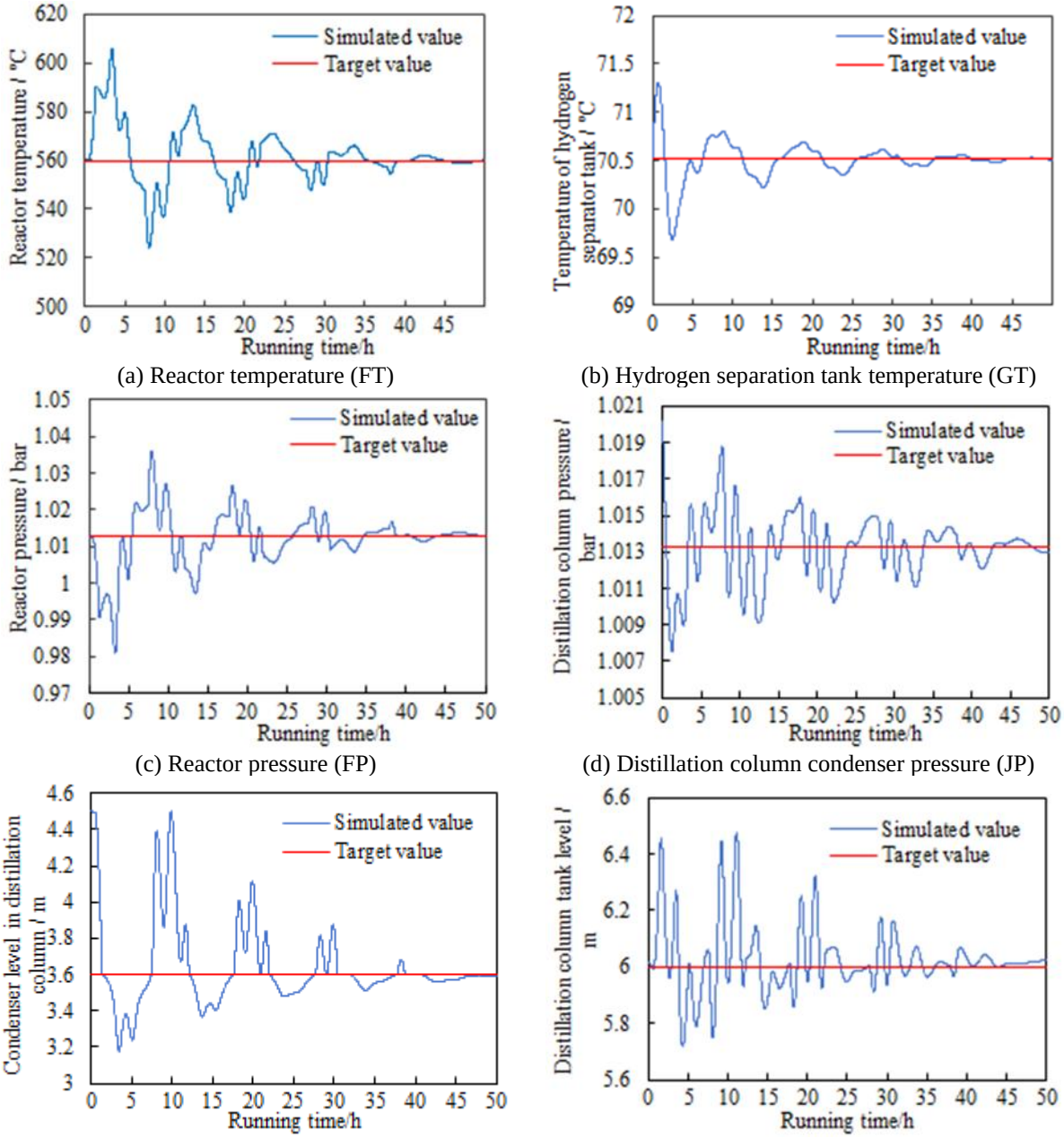
As shown in Figure 7 and Figure 8, the constructed LSTM model has a good prediction effect on the temperature and pressure of the reactor. It can predict the change trend of each index data well, and respond to its fluctuations to achieve accurate prediction. In summary, the LSTM model can better show the relationship between data changes and accurately predict the reactor temperature and pressure, thus providing a reliable data source for the proposal of control strategies.

Design and simulation of PID temperature controller for hydrogen separation tank

Based on the previous research, this paper has obtained the dynamic characteristics of the wave transfer of system parameters through the transfer entropy method, and has effectively predicted the key parameters by constructing the LSTM prediction model. The fluctuation of parameters is predicted in advance based on LSTM model, so that the PID controller can adjust the control parameters more accurately. The feedforward control and feedback control are combined to improve the robustness and stability of the system.

The design of PID controller needs to determine the control target first. In this section, the slow periodic fluctuation of styrene production process is taken as an example, and the fluctuation of key parameters in this scenario is regulated. According to the above analysis results of transfer entropy, the main fluctuation source in this scenario is identified as the temperature of the hydrogen separation tank. Therefore, we choose to add a PID temperature controller for the hydrogen separation tank to control the temperature stability of the hydrogen separation tank and improve the stability of the whole system. According to the dynamic model of Aspen Dynamics above, the target value of PID temperature controller of hydrogen separation tank is set to 70℃. Secondly, the control strategy of PID controller is determined. The PID parameters are initially adjusted by the critical stability method, and the parameters required in the PID adjustment process are calculated. The PID parameters calculated in this paper are proportional gain K_p=1, integral gain T_i=0.05 and differential gain T_d=5. Finally, the designed PID controller is applied to the styrene production system constructed in this paper, and the performance of the PID temperature controller is verified by simulation. The simulation results are shown in

Figure 9. Sets the value of each parameter at normal run time to the reference target value. For example, the temperature of the reactor is 560℃, the temperature of the hydrogen separation tank is 70.5℃, the pressure of the reactor is 1.013bar, the top pressure of the distillation tower is 1.013bar, the liquid level of the distillation tower condenser is 3.6m, and the liquid level of the distillation tower reactor is 6m.



(a) Reactor temperature (FT)

(b) Hydrogen separation tank temperature (GT)

(c) Reactor pressure (FP)

(d) Distillation column condenser pressure (JP)

(e) Distillation column condenser level (JTL)

(f) Distillation column tank level (JSL)

Figure 9: Response curves of key parameters after PID controller

As can be seen from Figure 9, the PID control algorithm designed in this paper can effectively ensure the control accuracy of the control system when the temperature control system has external slow-varying disturbance. By introducing PID temperature controller, the temperature fluctuation of hydrogen separation tank is controlled effectively. Its fluctuation range gradually decreases, and finally accurately approaches the preset target value. At the same time, PID control of the temperature of the hydrogen separation tank also indirectly realizes the control of the periodic fluctuations of other key parameters, and these key parameters gradually tend to the target value with PID control. This further verifies the accuracy and effectiveness of the transfer entropy

method used in this paper to analyze the transfer mechanism of fluctuations between parameters and identify the source of fluctuations.

5. Conclusions

In this paper, a wave transfer model of chemical process parameters was constructed based on transfer entropy and graph theory, and a dynamic simulation model was used to simulate the slow-change cycle disturbance scenario of styrene production process, and data sets were collected and pre-processed. Secondly, the wave transfer between the key parameters under this disturbance is studied, and the transfer entropy between the parameters is calculated to build a network model. Based on this, the potential wave source and the wave transfer path between the key parameters are identified and the causal analysis is carried out. Finally, based on the results of transfer entropy analysis, the parameter prediction and control strategy of using LSTM model and PID controller in styrene production process was further discussed. First, the LSTM prediction model is constructed to accurately predict the future fluctuation trend of key parameters. Then, combined with the causality of prediction results and transfer entropy analysis, a PID temperature controller is introduced and designed to effectively control the temperature of the hydrogen separation tank, which is the source of fluctuation, and indirectly affect other key parameters through the wave transfer mechanism, so that the whole system gradually becomes stable from the slow periodic fluctuation state.

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