Online Sequential Extreme Learning Machine Based Soft-sensor Model of SMB Chromatographic Separation Process

Cheng Xing, Jie-Sheng Wang *, Qing-Da Yang, Yong-Cheng Sun, Yi-Peng ShuangGuan

Abstract—**Simulated moving bed chromatography (SMB) is a proven and efficient separation tool for the complex separation needs of a variety of industries. On the basis of analysis on the SMB chromatographic separation, the appropriate indexes were selected to optimize and control the separation process. Taking the component purity and yield of extract and residual solution as prediction objects, the soft-sensor modeling was conducted based on online sequential extreme learning machine (OS-ELM), online sequential reduced kernel extreme learning machine (OS-RKELM) and regularized online sequential extreme learning machine (ReOS-ELM). The results show that different limit learning functions can effectively realize the accurate prediction of key economic and technical indexes, and can meet the real-time, efficient and robust operation of SMB chromatographic separation process.**

Index Terms—**SMB chromatography separation, Soft-sensor modeling, Extreme learning machine, Online sequence ELM**

I. Introduction

SMB chromatography is a new separation technology with broad application prospects [1], it simulates counter-current flow between the two phases through periodic operation of multiple columns to achieve continuous feed supply and product removal [2]. The SMB chromatography separation mechanism is complex, the parameters are numerous, it is difficult to run at the best operating point for a long time [3]. Due to the limitations of field conditions and the lack of mature detection devices, it is difficult to obtain the key economic and technical indicators, and it is difficult to realize the direct quality closed-loop control [4-5], while the soft sensing technology can effectively realize the prediction of key indexes in complex industrial processes [6].

Extreme Learning Machine is a network with single hidden layer proposed by Professor Huang in 2006 [7-8]. In Ref. [9], a new damage identification method for aircraft composite structures based on I-ELM was proposed to solve the problem of difficulty in effectively identifying aircraft composite structures. Ref. [10] introduced the idea of online learning on the basis of IF-ELM algorithm and proposed the algorithm of IFOS-ELM without inverse matrix. After calculating the appropriate number of hidden layer nodes, new data was added to enhance the real-time learning ability of the algorithm. Ref. [11] proposed an improved version of EM-ELM based on regularization method, namely IR-ELM. It can quickly and recursively update output weights as new hidden nodes are added. In Ref. [12], OS-ELM algorithm is improved from the aspects of non-Gaussian noise robustness and hidden layer structure sparsity, and is applied to channel balancing of OFDM system. Ref. [13] proposes an online sequential reduction kernel extreme learning machine (OS-RKELM). It can avoid the tedious fine tuning. Ref. [14] proposes an improvement of OS-ELM based on dual-objective optimization method. This method minimizes the empirical error and obtains a small norm of network weight vector. Deep learning techniques can be used to process large amounts of data and achieve better results. However, these methods lead to long training times, and prediction accuracy is also important.

This paper presents a soft sensing modeling method for SMB chromatographic separation process based on online sequential extreme learning machine. The rest is arranged as follows. In Section 2, the SMB chromatographic separation process is described. Section 3 introduces the online sequential extreme learning machine. The forth section carries out the simulation experiments. Finally, the conclusion of the paper is given.

II. Principle review and modeling

The SMB chromatographic separation technique aims to mimic the motion of the stationary phase adsorbent by continually alternating the positions of the feed and discharge ports. This method employs a loop configuration composed of multiple interconnected chromatographic columns. By sequentially moving the raw material inlet and the raffinate outlet in the direction of the mobile phase, SMB

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effectively replicates counter-current flow between the mobile phase and stationary phase, leading to the separation of two components. Using the separation of two components as an example, the fundamental principle of SMB chromatographic separation is illustrated in Fig. 1 [15-16]. Suppose components A and B are the substances to be separated, with component A having a stronger adsorption affinity than component B. The eluent, labeled D, functions as the desorbent, and the extract, marked E, is the desired product. The feed is denoted as F, and the raffinate as R. The entire system is divided into four zones (I, II, III, IV, or 1, 2, 3, 4) according to the entry and exit points of the liquid and their respective roles. Each zone has a specific function in the overall separation process.

To develop the model, several auxiliary variables were selected guided by the process flow and preexisting knowledge. These variables are used to enhance the accuracy and reliability of the soft-sensor model. The information is shown in Table I.

(1) Fluid throughput of feed liquid injection inlet and injection pump (F pump), and unit is ml/min.

(2) Fluid throughput of the rinsing pump at the rinsing liquid inlet (D pump), and unit is ml/min.

(3) Time to switch the valve, and unit is min.

Determine the following variables as the output variables of the soft-sensor model.

(1) Integrity of the target substance in the effluent from port E (If there is an impurity effluent from port E, purity < 1).

(2) Degree of impurity in the outlet R (if there is a target outlet R, purity < 1).

(3) Mass recovery of the target object at port E/the injection mass of the target object can be obtained by the yield of the target object at port E.

(4) Quality of impurity outflow at port R/quality of impurity injection, impurity yield at port R.

III. Proposed Methodology

A. Online Sequential Extreme Learning Machine (OS-ELM)

Liang et al. proposed online sequential Extreme Learning Machine (OS-ELM) on the basis of ELM in 2006. The training algorithm has the following characteristics.

(1) Training samples can be learned one by one, or they can be learned block by block with fixed length or variable length.

(2) At any given time, only single or single blocks of newly arrived observations will be seen and learned, not entire past data.

(3) Once the learning process of a specific single or block training sample is completed, the training sample or block will be discarded. OS-ELM is divided into an initialization phase and an online learning phase.

In the initialization stage, OS-ELM initializes the output weight β through a small set of offline training samples. In the online learning phase, OS-ELM updates the output weight β by using single or multiple samples obtained in real time.

(1) Initialization phase

Suppose there are N_0 random training sample $\{(x_i, t_i)\}_{i=1}^{N_0}$ in the initialization phase, where $x_i \in R^n$ is the i input vector and $t_i \in R^n$ is the associated expected value $\beta_0 = \min_{\beta}\|H_0\beta_0 - T_0\|$. Based on the idea of extreme learning machine, initialize and obtain:

$$H_0 = \begin{bmatrix} G(w_1,b_1,x_1) G(w_2,b_2,x_1) \cdots G(w_L,b_L,x_1) \\ G(w_1,b_1,x_2) G(w_2,b_2,x_2) \cdots G(w_L,b_L,x_2) \\ \vdots \quad \vdots \quad \ddots \quad \vdots \\ G(w_1,b_1,x_{N_0}) G(w_1,b_1,x_{N_0}) \cdots G(w_L,b_L,x_{N_0}) \end{bmatrix}_{N_0 \times L}$$
$$T_0 = \begin{bmatrix} t_1^T \\ t_2^T \\ \vdots \\ t_{N_0}^T \end{bmatrix}_{N_0 \times m} \tag{1}$$

According to the least square method, get:

$$\beta_0 = H_0^{\delta} T_0 \tag{2}$$

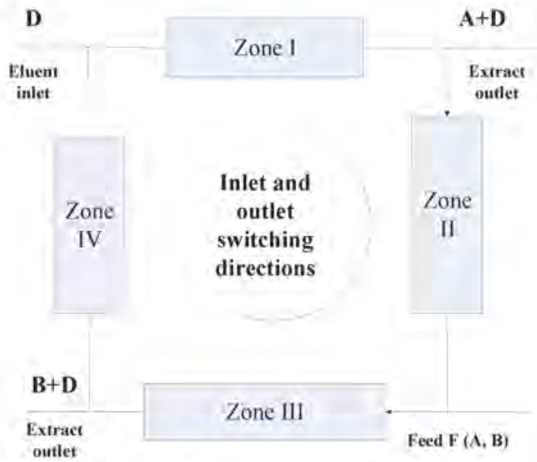

Fig. 1 Operating principle of SMB chromatographic separation process

Table I. Units and ranges of selected variables

Name	Injection pump flow capacity (F pump)	Injection pump flow capacity (D /pump)	Switch time	Purity of target substance in N port	Impurity purity in M port	Yield of target at port N	Yield of impurity at port M
Unit	ml/min	ml/min	min	mg/ml	mg/ml	%	%
Range	0-1	0-1	0-1	11-20	0-1	0-100	0-100

Using the Moore-Penrose generalized inverse matrix calculation method, the generalized inverse matrix of N_0 is N_0^{δ} :

$$N_0^{\delta} = \left(H_0^T H_0\right)^{-1} H_0^T \tag{3}$$

Then get:

$$\beta_0 = K_0^{-1} H_0^T T_0 \tag{4}$$

$$K_0 = H_0^T H_0 \tag{5}$$

(2) Online learning phase

Suppose that N_1 new samples $\{(x_i, t_i)\}_{i=N_0+1}^{N_0+N_1}$ enter the model after the completion of the initialization stage, then the updated output weight meets the following requirements:

$$\beta_1 = \min_{\beta} \left\| \begin{bmatrix} H_0 \\ H_1 \end{bmatrix} \beta - \begin{bmatrix} T_0 \\ T_1 \end{bmatrix} \right\| \tag{6}$$

According to the calculation method of generalized inverse and the least square method, it can be calculated:

$$\beta_1 = K_1^{-1} \left\| \begin{bmatrix} H_0 \\ H_1 \end{bmatrix} \beta - \begin{bmatrix} T_0 \\ T_1 \end{bmatrix} \right\| \tag{7}$$

where:

$$K_1 = \begin{bmatrix} H_0 \\ H_1 \end{bmatrix}^T \begin{bmatrix} H_0 \\ H_1 \end{bmatrix} = H_0^T H_0 + H_1^T H_1 = K_0 + H_1^T H_1 \tag{8}$$

$$\begin{bmatrix} H_0 \\ H_1 \end{bmatrix}^T \begin{bmatrix} H_0 \\ H_1 \end{bmatrix} = K_1 \beta_0 - H_1^T H_1 \beta_0 + H_1^T T \tag{9}$$

Therefore, formula $\beta_1 = K_1^{-1} \left\| \begin{bmatrix} H_0 \\ H_1 \end{bmatrix} \beta - \begin{bmatrix} T_0 \\ T_1 \end{bmatrix} \right\|$ can be written as:

$$\beta_1 = \beta_0 + K_1^{-1} H_1^T \left(T_1 - H_1 \beta_0\right) \tag{10}$$

Through the generalization of the above process, it is assumed that the current output weight has been updated for k time to obtain β_k and K_k . When the N_k data enters the model, the following recursive formula is established:

$$K_{k+1} = K_k + H_{k+1}^T H_{k+1} \tag{11}$$

$$\beta_{k+1} = \beta_k + K_{k+1}^{-1} H_{k+1}^T \left(T_{K+1} - H_{k+1} \beta_k\right) \tag{12}$$

According to Woodbury's formula:

$$\begin{aligned} K_{k+1}^{-1} &= \left(K_k + H_{k+1}^T H_{k+1}\right)^{-1} \\ &= K_k^{-1} - K_k^{-1} H_{k+1}^T \left(I + H_{k+1} K_k^{-1} H_{k+1}^T\right)^{-1} H_{k+1} K_k^{-1} \end{aligned} \tag{13}$$

Let $K_{K+1}^{-1} = P_{k+1}$, then the online update method of OS-ELM is as follows:

$$P_{k+1} = P_k - P_k H_{k+1}^T \left(I + H_{k+1} P_k H_{k+1}^T\right)^{-1} H_{k+1} P_k \tag{14}$$

$$\beta_{k+1} = \beta_k + P_{k+1} H_{k+1}^T \left(T_{k+1} - H_{k+1} \beta_k\right) \tag{15}$$

The above derivation process is the algorithm principle of OS-ELM. Firstly, it initializes the output weight of OS-ELM through β_0 few training samples. After the initialization, it enters the online sequential training stage and adjusts the output weight through some online samples that enter the model in real time.

B. Online Sequential Reduced Kernel Extreme Learning Machine (OS-RKELM)

In numerous real-world scenarios, data often arrives in block after block (note: The arrival of data samples one after another is a special case of block after block) or in sequence. In addition, GKLEM, like most batch learning methods, does not handle big data well when the data set is scaled up. Therefore, OS-RKELM, an online sequential simplified kernel Extreme learning machine (OS-Rkelm), is proposed. Given a large initial training set :

$$\varphi_0 = \left\{ (\mathrm{X}_i, t_i) \middle| \mathrm{X}_i \in R^m, t_i \in R^{\varsigma} \right\}_{i=1}^{N_0}$$

Where, L mapping sample X_L is randomly selected from the training set, and the initial output weight is:

$$\beta^{(0)} = \mathrm{Z}_0^{-1} \mathrm{K}_0^T \mathrm{T}_0 \tag{16}$$

where, $\mathrm{Z}_0 = \mathrm{I}/C + \mathrm{K}_0^T \mathrm{K}_0, \mathrm{K}_0 = \kappa(\mathrm{X}_0, \mathrm{X}_L)$.

Suppose another data block $\varphi_0 = \{(\mathrm{X}_i, t_i)\}_{i=N_0+1}^{N_0+N_1}$ is arrived, where N_1 represents the number of data samples in the new data block arrived, then the output weight $\beta^{(1)}$ is:

$$\beta^{(1)} = \mathrm{Z}_1^{-1} \begin{bmatrix} \mathrm{K}_0 \\ \mathrm{K}_1 \end{bmatrix}^T \begin{bmatrix} \mathrm{T}_0 \\ \mathrm{T}_1 \end{bmatrix} \tag{17}$$

where, $\mathrm{Z}_1 = \dfrac{1}{C} + \begin{bmatrix} \mathrm{K}_0^T & \mathrm{K}_1^T \end{bmatrix} \begin{bmatrix} \mathrm{K}_0 \\ \mathrm{K}_1 \end{bmatrix}, \mathrm{K}_1 = \kappa(\mathrm{X}_1, \mathrm{X}_L)$.

For sequential learning, $\beta^{(1)}$ will be expressed as a function of $\beta^{(0)}$, Z_1, K_1, and T_1. Now Z_1 can be written as

$$\mathrm{Z}_1 = \frac{\mathrm{I}}{C} + \begin{bmatrix} \mathrm{K}_0^T & \mathrm{K}_1^T \end{bmatrix} \begin{bmatrix} \mathrm{K}_0 \\ \mathrm{K}_1 \end{bmatrix} = \mathrm{Z}_0 + \mathrm{K}_1^T \mathrm{K}_1 \tag{18}$$

$$\begin{aligned} \begin{bmatrix} \mathrm{K}_0 \\ \mathrm{K}_1 \end{bmatrix}^T \begin{bmatrix} T_0 \\ T_1 \end{bmatrix} &= \mathrm{K}_0 T_0 + \mathrm{K}_1^T T_1 \\ &= \mathrm{Z}_0 \mathrm{Z}_0^{-1} \mathrm{K}_0^T K_0 + \mathrm{K}_1^T \mathrm{T}_1 \\ &= \left(\mathrm{Z}_1 - \mathrm{K}_1^T \mathrm{K}_1\right) \beta^{(0)} + \mathrm{K}_1^T \mathrm{T}_1 \\ &= \mathrm{Z}_1 \beta^{(0)} - \mathrm{K}_1^T \mathrm{K}_1 \beta^{(0)} + \mathrm{K}_1^T \mathrm{T}_1 \end{aligned} \tag{19}$$

Substitute Eq. (18)-(19) into Eq. (17), and $\beta^{(1)}$ is derived from the following formula:

$$\begin{aligned} \beta^{(1)} &= \mathrm{Z}_1^{-1} \left(\mathrm{Z}_1 \beta^{(0)} - \mathrm{K}_1^T \mathrm{K}_1 \beta^{(0)} - \mathrm{K}_1^T \mathrm{T}_1 \right) \\ &= \beta^{(0)} + \mathrm{Z}_1^{-1} \mathrm{K}_1^T \left(\mathrm{T}_1 - \mathrm{K}_1 \beta^{(0)} \right) \end{aligned} \tag{20}$$

In general, when $(k+1)-th$ block of dataset A reaches:

$$\varphi_{k+1} = \{(\mathrm{X}_i, t_i)\}_{i=\left(\sum_{j=0}^{k} N_j\right)+1}^{\sum_{j=0}^{k+1} N_j} \tag{21}$$

where, $k \geq 0$ and N_{k+1} represent the middle observation number $(k+1)$ of the block, then obtain:

$$\begin{aligned} \mathrm{Z}_{k+1} &= \mathrm{Z}_k + \mathrm{K}_{k+1}^{\mathrm{T}} \mathrm{K}_{k+1} \\ \beta^{(k+1)} &= \beta^{(k)} + \mathrm{Z}_{k+1}^{-1} \mathrm{K}_{k+1}^{\mathrm{T}} \left(\mathrm{T}_{k+1} - \mathrm{K}_{k+1} \beta^{(k)} \right) \end{aligned} \tag{22}$$

where, $\mathrm{K}_{k+1} = \kappa(\mathrm{X}_{k+1}, \mathrm{X}_L), \mathrm{X}_{k+1} = \{\mathrm{X}_i\}_{i=\left(\sum_{j=0}^{k} N_j\right)+1}^{\sum_{j=0}^{k+1} N_j}$. Get:

$$\mathrm{T}_{k+1} = \begin{bmatrix} t^{\mathrm{T}}_{\sum_{j=0}^{k} N_j + 1} \\ \vdots \\ t^{\mathrm{T}}_{\sum_{j=0}^{k+1} N_j} \end{bmatrix} \tag{23}$$

Calculate $\beta^{(k+1)}$ by using Z_{k+1}^{-1} instead of Z_{K+1}. The updated equation for Z_{k+1}^{-1} is then derived using Woodbury's equation [17] :

$$\begin{aligned} \mathrm{Z}_{k+1}^{-1} &= \left(\mathrm{Z}_k + \mathrm{K}_{k+1}^{\mathrm{T}} \mathrm{K}_{k+1} \right)^{-1} \\ &= \mathrm{Z}_k^{-1} - \mathrm{Z}_k^{-1} \mathrm{K}_{k+1}^{\mathrm{T}} \left(1 + \mathrm{K}_{k+1} \mathrm{Z}_k^{-1} \mathrm{K}_{k+1}^{\mathrm{T}} \right)^{-1} \mathrm{K}_{k+1} \mathrm{Z}_k^{-1} \end{aligned} \tag{24}$$

Suppose $G_{k+1} = \mathrm{K}_{k+1}^{-1}$, then the equation $\beta^{(k+1)}$ for updating can be derived as:

$$\begin{aligned} G_{k+1} &= G_k - G_k^{-1} \mathrm{K}_{k+1}^{\mathrm{T}} \left(1 + \mathrm{K}_{k+1} G_k \mathrm{K}_{k+1}^{\mathrm{T}} \right)^{-1} \mathrm{K}_{k+1} G_k \\ \beta^{(k+1)} &= \beta^{(k)} + G_{k+1} \mathrm{K}_{k+1}^{\mathrm{T}} \left(\mathrm{T}_{k+1} - \mathrm{K}_{k+1} \beta^{(k)} \right) \end{aligned} \tag{25}$$

The overall steps are as follows: First select the kernel function (including kernel type and parameter Settings) and map sample number L .The new data sample $\varphi = \{(\mathrm{X}_i, t_i) | \mathrm{X}_i \in R^m, t_i \in R^{\lambda}, i = 1,2,...\}$ then arrives in turn.

Therefore, OS-RKELM consists of two phases, namely the initialization and the online learning. In the first phase, the initial data set block can be used for training. The initial data set can be either $N_0 > L, N_0 = L$ or $N_0 < L$, because the regularization parameter I/C ensures that Z_0 is full rank. After the first phase, the second phase proceeds in a piece-by-piece or block-by-block mode as needed.With the exception of the data point in X_L, once a data point is learned, it can be discarded. There is no need for memory or archiving of data samples. OS-RKELM is an online kernel-based algorithm.

C. Regularized Online Sequential Extreme Learning Machine (ReOS-ELM)

Suppose there is an initial training data set with N_0 training mode $(x_j, t_j) \in R^n \times R$, where $x_j = [x_{j1}, x_{j2}, \cdots, x_{jn}]^{\mathrm{T}}$. For the single hidden layer neural network with n input node and 1 output node, the jth input mode corresponds to the jth output:

$$o_j = \sum_{i=1}^{L} \beta_i G(\omega_i, b_i, x_j), j = 1, \cdots, N_0 \tag{26}$$

where, for hidden nodes, L represents the number, i represents the nth, $G(\cdot)$ represents the active function. β_i and b_i are the output weight connecting the ith hidden layer and the output node respectively and the hidden bias of the ith hidden node.

OS-ELM is a novel online learning algorithm, whose outstanding feature is that the input weights and hidden deviations are randomly selected. To obtain the output weight, minimize the defined error function:

$$\left\| \mathrm{H}_0 \beta_0 - \mathrm{T}_0 \right\|^2 \tag{27}$$

The data collected in the training process often contains noise, and Eq. (27) may lead to poor generalization ability and over-fitting. Compared with OS-ELM, REOS-ELM can minimize empirical errors as far as possible to obtain the small norm of the network weight vector. The following cost function is considered:

$$\left\| \mathrm{H}_0 \beta_0 - \mathrm{T}_0 \right\|^2 + \lambda \left\| \beta_0 \right\|^2 \tag{28}$$

where, λ is the regularization factor. The formula of β_0 is as follows:

$$\beta_0 = P_0 H_0^{\mathrm{T}} \mathrm{T}_0 \tag{29}$$

$$P_0 = \left(\mathrm{H}_0^{\mathrm{T}} \mathrm{H}_0 + \lambda \mathrm{I}_L \right)^{-1} \tag{30}$$

where, I_L is the identity matrix, the size of I_L is L , $T_0 = [t_1, \cdots, t_{N_0}]^{\mathrm{T}}$, and:

$$H_0 = \begin{bmatrix} G(\omega_1, b_1, x_1) & \cdots & G(\omega_L, b_L, x_1) \\ \vdots & \vdots & \vdots \\ G(\omega_1, b_1, x_{N_0}) & \vdots & G(\omega_L, b_L, x_{N_0}) \end{bmatrix} \tag{31}$$

So the kth block is obtained as:

$$N_k = \{(\mathrm{X}_i, t_i)\}_{i=\sum_{j=0}^{k+1} N_j + 1}^{i=\sum_{j=0}^{k} N_j} \tag{32}$$

The weight updating in REOS-ELM is similar to the recursive least squares (RLS) algorithm.

$$P_k = P_{k-1} - \frac{P_{k-1} H_k^T H_K P_{k-1}}{I N_k + H_k P_{k-1} H_k^T} \tag{33}$$

$$\beta_k = \beta_{k-1} + P_k H_k^T \left(T_k - H_k \beta_{k-1} \right) \tag{34}$$

where, I_{N_k} is the identity matrix, and the size of I_{N_k} is N_k ; T_k and H_k are respectively the target of the kth arrival training data and the hidden layer output of the kth arrival training data.

IV. Simulation Experiment and Result Analysis

Based on the online sequential extreme learning machines, a soft-sensor model was established for the purity of target object in outlet E effluent, purity of impurity in outlet R effluent, yield of target object at outlet E and yield of impurity at outlet R in SMB chromatography separation process.The number of hidden layer nodes of ELM neural network model is set to 30.After sorting out the historical data related to the simulated process of moving bed chromatography separation, 1000 groups of representative data were selected, then 900 groups of data were randomly selected as the training set, the remaining 100 groups were selected as the test set to detect the predictive performance of the soft sensor model.

In order to better compare the prediction performance of the soft sensor model, four specific indicators listed in Table II are selected, which are maximum error (MPE), sum of residual squares (SSE), mean absolute percentage error (MAPE) and root mean square error (RMSE), where $\hat{y}$ is the estimated value and y is the actual value.

The auxiliary variables of the soft sensing model of SMB chromatographic separation process established by error index are the flow rate of raw liquid inlet pump (F pump), the flow rate of flushing liquid inlet pump (D) and valve switching time. The purity of the target object in the outflow at port E, the purity of the impurity in the outflow at port R, the yield of the target object at port E and the yield of the impurity at port R are output as soft sensor models. The nonlinear relationship between them is fitted by the online sequence extreme learning machine, so as to establish the prediction model of the corresponding economic and technical indicators. The simulation results are shown in Fig. 2-9.

Fig. 2 is the predicted output comparison curve when the purity of target substance in the effluent at port E in SMB chromatographic separation process is OSELM, OSRKELM, ReOSELM and ELM, and Fig. 3 is the prediction error comparison curve. Fig. 4 is the predicted output comparison curve of impurity purity in outlet R effluent during SMB chromatographic separation process under OSELM, OSRKELM, ReOSELM and ELM conditions, and Fig. 5 is the predicted error comparison curve. Fig. 6 is the prediction output comparison curve of the yield of the target at port E in the SMB chromatographic separation process under OSELM, OSRKELM, ReOSELM and ELM, and Fig. 7 is the prediction error comparison curve. Fig. 8 is the prediction output comparison curve of the yield of impurities at port R during SMB chromatographic separation under OSELM, OSRKELM, ReOSELM and ELM conditions, and Fig. 9 is the prediction error comparison curve. Table III shows the comparison of predicted performance data.

The results show that the soft sensing model based on OSELM has high accuracy in predicting the key economic and technical indexes of SMB chromatographic separation process. But the results are different for different online sequential extreme learning machines. As can be seen from the above simulation charts, the purity of the target object in the outflow solution at E, the purity of the impurity in the outflow solution at port R, the yield of the target object at port E and the yield of the impurity at port R have small errors and high prediction accuracy when using OSELM to establish the soft sensing model.

V. Conclusion

A soft-sensor model was constructed for the SMB chromatographic separation process, considering the model inputs as the flow rate of the raw material liquid inlet pump (F pump), the flow rate of the flushing liquid inlet pump (D pump), and the valve switching time. The desired outputs of the model were determined to be the degree of contamination in the desired compound in the outflow liquid at port E, degree of impurity concentration in the outflow liquid at port R, the yield of the target compound at port E, and the yield of the impurity at port R. A soft-sensor model of SMB chromatographic separation process based on online sequential extreme learning machine was established. The simulation results show that for the purity of the target object in the outflow liquid of E, the purity of the impurity in the outflow liquid of R, the yield of the target object at E and the yield of the impurity at R, the error is small and the prediction accuracy is high. At the same time, the established soft-sensor model exhibited notable capability in accurately predicting the economic and technical indexes within the SMB chromatographic separation process.

TABLE II. SPECIFIC INDICATORS

Name	Calculation method
MPE	$MPE = \max\left\{\left(\hat{y}-y\right), 0\right\}$
SSE	$SSE = \sum_{i=1}^{n}\left(\hat{y}_i - y_i\right)^2$
$MAPE$	$MAPE = \frac{\sum \frac{\left\|\hat{y}_i - y_i\right\|}{y_i} \times 100}{n}$
$RMSE$	$RMSE = \left[\frac{1}{n}\sum_{i=1}^{n}\left(\hat{y}_i - y_i\right)^2\right]^{\frac{1}{2}}$

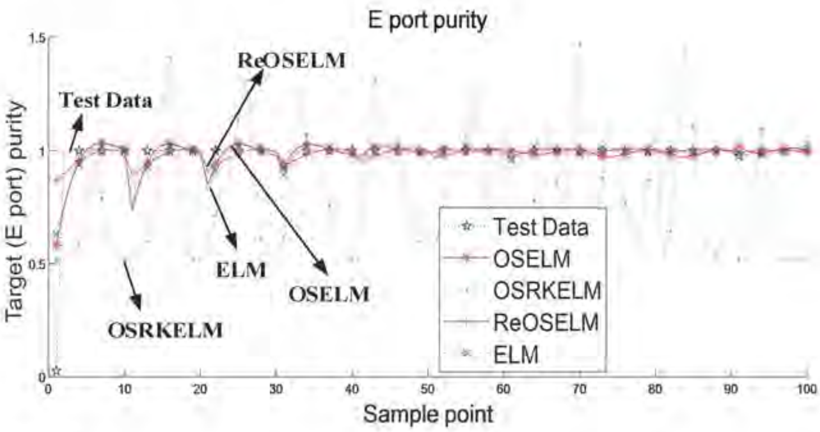

Fig. 2 Purity prediction results of E port

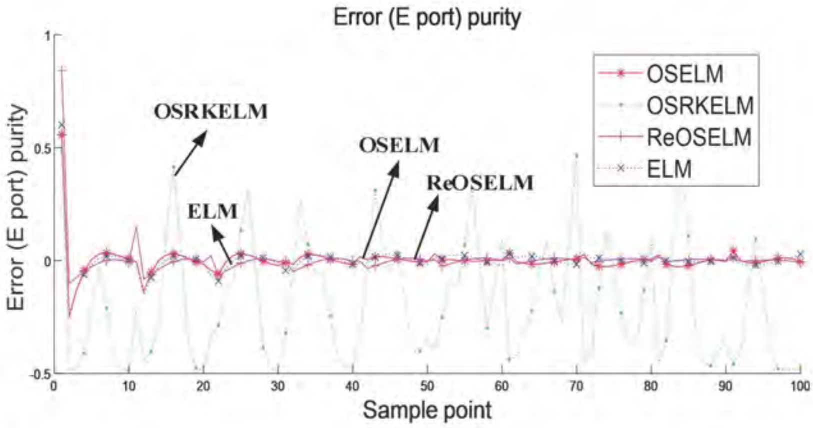

Fig. 3 Prediction error of E-port purity.

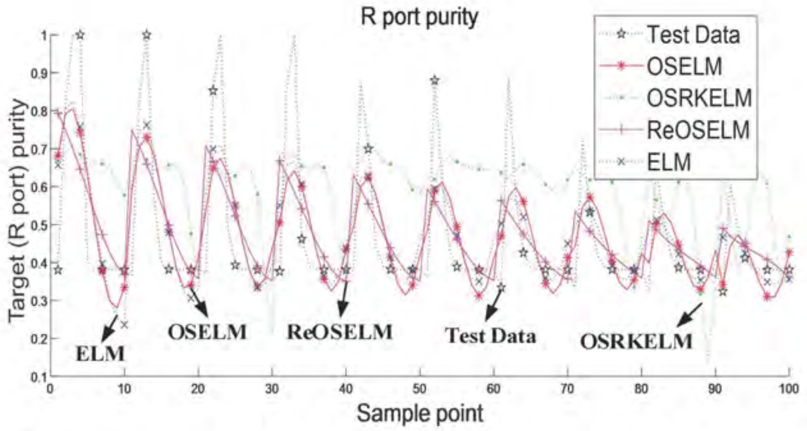

Fig. 4 Purity prediction results of R port.

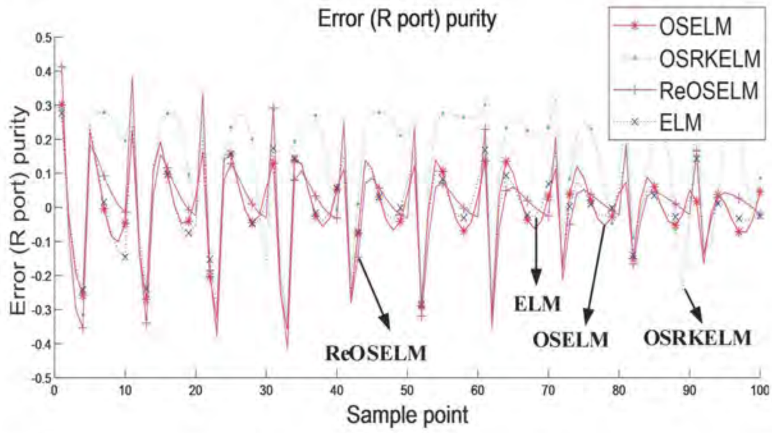

Fig. 5 Prediction error of R-port purity.

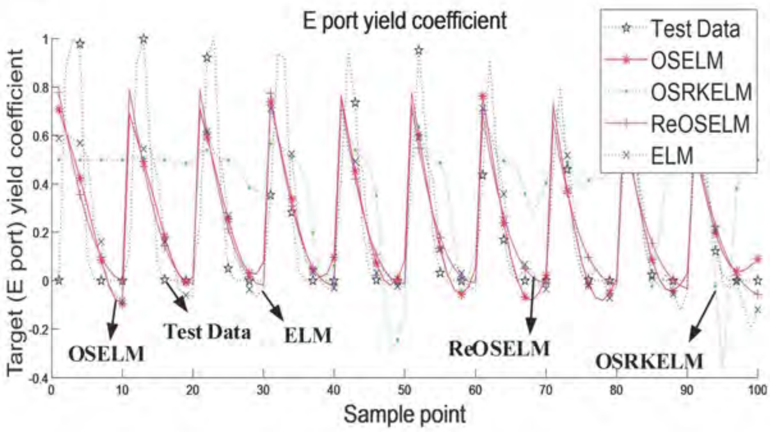

Fig. 6 Predicted yield results of E port.

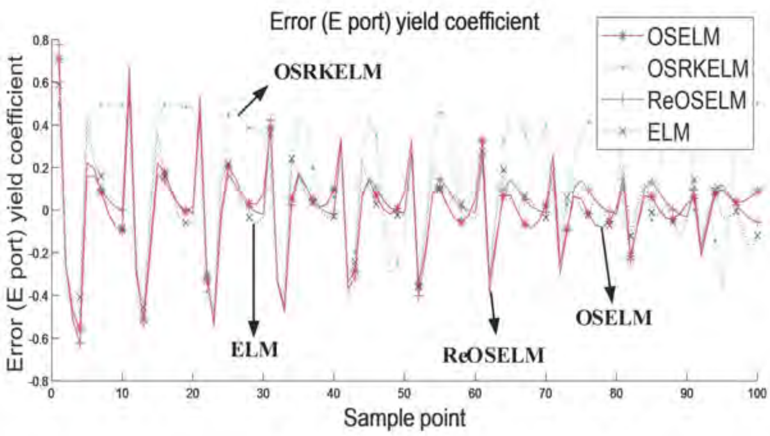

Fig. 7 Yield prediction error of E port.

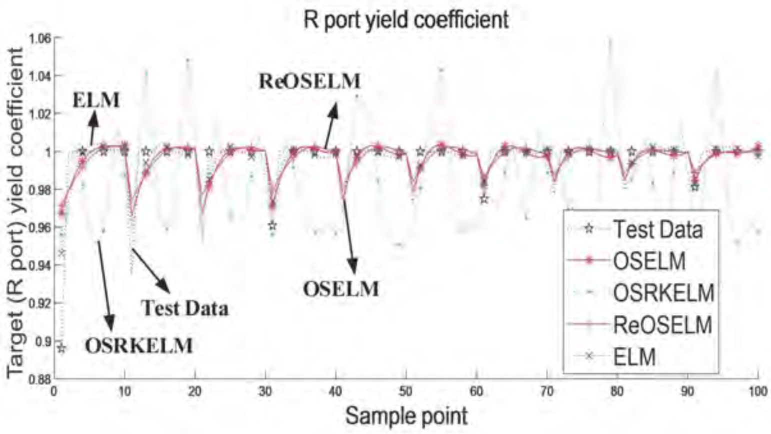

Fig. 8 Prediction results of R-port yield.

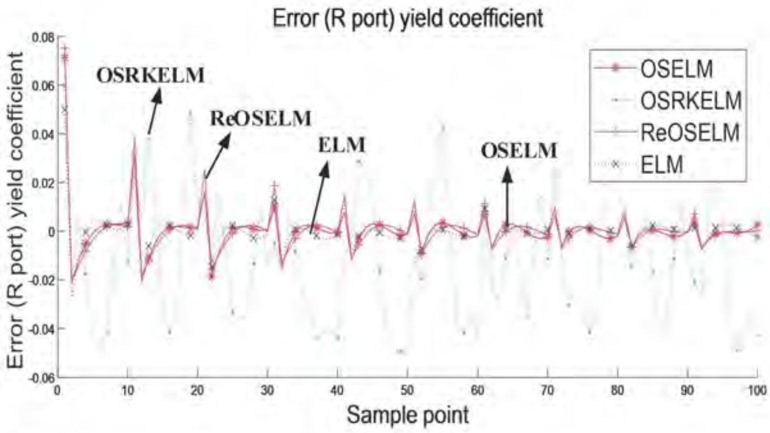

Fig. 9 Prediction error of R-port yield.

TABLE III. COMPARISON OF PREDICTIVE PERFORMANCE INDEXES OF SOFT SENSING MODELS

Performance index		RMSE	SSE	MAPE	MPE
N-port purity	OSELM	0.0665	0.4425	0.9748	0.5570
	OSRKELM	0.3222	10.3783	0.7120	0.4876
	ReOSELM	0.0884	0.7808	0.0352	0.8423
	ELM	0.0711	0.5051	0.0523	0.6018
M-port purity	OSELM	0.1222	1.4928	0.5279	0.3344
	OSRKELM	0.2211	4.8885	0.2949	0.3562
	ReOSELM	0.1487	2.2105	0.5284	0.4136
	ELM	0.1248	1.5568	0.4624	0.3582
N-port yield	OSELM	0.2017	4.0701	0.3203	0.5863
	OSRKELM	0.3516	12.3639	0.5197	0.4998
	ReOSELM	0.2222	4.9395	0.3513	0.7753
	ELM	0.2103	4.4229	0.2419	0.7070
M-port yield	OSELM	0.0078	0.0060	0.0060	0.0499
	OSRKELM	0.0291	0.0848	0.0498	0.0597
	ReOSELM	0.0107	0.0114	0.0066	0.0753
	ELM	0.0096	0.0092	0.9861	0.0712

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