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# An Automatic Advanced Fuzzy Controller for Simulated Moving Bed

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**ABSTRACT** Simulated moving bed (SMB) is one of the most successful technologies in chromatographic separation, which is widely used in chemical industry and food industry. There are many parameters that can affect the separation effect of SMB, and the sensitivity is very strong, so the effective control is always a difficulty problem for SMB. In this paper, a self-tuning advanced fuzzy controller is proposed to control the purity of the SMB outlet, and the study finds it has smaller steady-state error and better adaptability of in SMB when compares with the traditional and advance fuzzy type controller.

**INDEX TERMS** Chromatographic, SMB, fuzzy, control.

## **I. INTRODUCTION**

Chromatography is an indispensable and important technology in the manufacturing process of chemical products and biomedicine. The principle is to use the distribution difference between the static phase and the mobile phase to separate the mixture. The accuracy of separation is related to the quality and availability of products. Therefore, how to use an effective and accurate separation technology has always been an important problem to be solved by the biochemical industry. Nowadays, the use of SMB (simulated moving bed) technology with continuous feed for chromatography has been recognized as the most advanced technology. SMB is a continuous process technology that can improve the efficiency of adsorbent in the adsorption bed. This SMB technology with multiple columns reduces the solvent and water content consumption, as well as improving the production capacity; it is recognized as the cleanest manufacturing technology in the biomedical industry [1]–[3].

The compounds to be separated are first dissolved in the solvent, and then injected into the column under high pressure. Driven by the mobile phase, each component penetrates through the fixed phase in the column. The degree of movement of each component depends on its distribution

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state. Some components have little force (adsorption force) with the fixed phase, and are flushed out of the column quickly, while some components have greater force with the fixed phase, and they will be flushed out slowly [4], [5].The process shown in figure 1.



**FIGURE 1.** Simulated moving bed operation process.

SMB device is divided into four regions: Zone I (elution zone) is the adsorption section of component A. The strongly adsorbed component B is separated from the solid phase

adsorbent by eluent D. The fresh eluate enters from the bottom of zone I, contacts with the adsorbent, and discharges component B to obtain the extract. Zone II (rectification zone) is the refining zone of component B and desorption zone of component A. The liquid entering the zone II from zone I has strong adsorption capacity, so A in the adsorbent is continuously replaced by B and enters zone III along with the flowing liquid and fresh feed (A and B);Zone III (attached) is the desorption zone of component A. Component A is discharged from the outlet of the raffinate through the downward flowing liquid to obtain the raffinate; Zone IV (secondary fine zone) is the partial desorption area of desorber D, which aims to recover partial desorber D.

However, in order to improve the output of material separation, the precision and intelligent control of multi column SMB has always been a big problem in the industry. Technicians often set some initial control parameters of SMB through some by their experience, but this way which makes SMB often not run in the best state. Therefore, how to make SMB run in the best state has become a target for many researchers. The main difficulty of the research lies in the is due to its complexity and nonlinearity of SMB., m Multi column SMB includes several control variables such as flow velocity of multiple sections and switching time of valves, system parameters such as size, length and porosity of pipeline itself, and non controllable parameters such as the aging of adsorbent and fluctuation of feed concentration, which make the control of SMB system quite complicated. In addition, the control purpose of SMB is different from that of traditional one control. Its control objective is not to minimize the control output error, but is to make the concentration of separated substances reach a certain proportion, that is, the so-called separation purity requirement. Thus, the traditional control theory is inapplicable to SMB system, and it is not easy to achieve, so it still stays in simple PLC control.

### **II. LITERATURE REVIEWS**

In terms of controller, many scholars have developed and designed corresponding types of controllers for specific materials. A simple P controller proposed by Kloppenburg and Gilles [6] is used to control the real-time online SMB by using the difference of UV spectrum waveform as the tuning of control parameters. A nonlinear state estimator based on the real moving bed model (TMB) is proposed by Wang *et al.* [7] and is used to design the control mechanism of SMB. In reference [8], the design and optimal control of a single column chromatography separation process and its optimal control is are proposed. The monitoring system on the real-time line is used to detect the UV signal value, and then generate the prediction of chromatography separation state, so as to provide the controller with reference and send the best control signal to control the single column chromatography tube. In reference [9], Toumi and Engell propose a nonlinear model predictive controller which is designed based on the concept of optimal control. It can deal with the complex hybrid (continuous/discrete) dynamics of the RSMB plant

able pressure drop) into account. The efficiency of the control concept is proven in experiment. In reference [10], Suvarov et al propose an adaptive controller. By adjusting the flow rate and switching period, the spatial position of adsorption and desorption waves can be tuned up, and then the purity and yield of raffinate and extraction port can be adjusted. In reference [11], Yan *et al.* applied apply the model predictive control method to SMB Chromatographic Separation process. The researchers established a state space model to model the production. By changing the relevant parameters, the output response curve of the production model was is obtained, and the parameters were are optimized. Finally, the simulation results showed that the system was is successfully controlled based on each control cycle and given production interval. In order to optimize the performance of the control system, Li *et al.* [12] proposed a control method based on piecewise affine model in the process of SMB Chromatographic Separation. The simulation results show that the method is feasible, and the actual yield curve of target substances and impurities can fit the set target yield value [12].

and takes hard process constraints (e.g. the maximal allow-

In the practical application of SMB, Coelho *et al.* [13] adopt a mathematical optimum method to predict the performance of a real SMB unit, and achieve the 97% separation purity control for the TIA and GCA material. Natarajan and Lee [14] propose repetitive model predictive control (RMPC) technique on SMB process, and it performs in continuous chromatographic separation of a phenylalanine —tryptophan mixture. Carlos and Alain [15] present a new method to control the separation process of simulated moving bed chromatography. The method combines wave theory with multi model predictive control (MPC). Wave theory provides a theoretical framework for the formulation of control law, and rolling time domain MPC is used to determine the appropriate controller parameters Sharma *et al.* [16] propose a multilinear modeling method to establish the mathematical modeling of the whole nonlinear dynamic system of SMB in the way of Bayesian weighting. Neto *et al.* [17] propose an adaptive nonlinear model predictive control method for enantioseparation of praziquantel. In the control framework, the main concern of this model is to solve the amount of computation and the speed of solving is fast enough in this model. In [18], Wei et al not only concentrate on separation purity but also on the efficiency, and put forward a two-steps method: feeding, purification and recovery. Maruyama *et al.* [19] propose bypass simulated moving bed (BP-SMB) chromatography. This method is characterized by multiple purification of the extract and raffinate port materials, and it is used in the production of corn syrup (HFCS). The separation of HFCS shows that BP-SMB operation is of little advantage in productivity, but it is flexible and robust. Nogueira *et al.* [20] propose a new strategy to identify the optimal transfer function of TMB / SMB. The most sufficient transfer function is used in the controller to overcome the problems related to the dynamic behavior of the process. The results show that this method can easily identify the transfer function of the optimal

#### **TABLE 1.** Parameters of SMB system.



operation point of the process, and MPC can control the process in both cases of servo and regulator. Matos *et al.* [21] apply the PSO method to optimize the productivity and the eluent consumption of the separation of the bi-naphthol enantiomers in a True Moving Bed (TMB) device. The results show that the desired optimization is achieved. Other controller research on SMB can be found in literature [22]–[29].

Generally speaking, the research on SMB intelligent controller design is not mature, and there is still room for improvement in the existing research work. The main manifestations are as follows: Firstly, in practical application, it is mainly aimed at specific separation substances and industrial equipment and thus does not have universality. Besides, experiments are carried out on physical machines, and the cost of the experiment is relatively high, For example, for the separation of sugars in the food industry, it may not be suitable for the separation in the chemical industry. Secondly, the research on the robustness and adaptability of the controller is insufficient. With the change of environmental parameters, the result is easy to lead to the failure of separation effect. In the practical application of SMB, it often needs to be adjusted according to the changes of equipment and environment. When approaching the control target, the traditional fuzzy control force will become smaller. However, because of the particularity of SMB system, it is periodic

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switching. In the experiment, the steady-state value is smaller than the target value; when introducing the error acceleration, an advance fuzzy controller is used and the steady-state value is larger than target value. Therefore, a more intelligent automatic control technology is needed. In this paper, in the framework of computer simulation, based on the discrete dynamic system of SMB, an automatic advanced fuzzy controller is proposed to control the purity separation of SMB, and the steady-state error and the adaptive performance of the controller under the change of parameters are observed. The results show that, compared with the traditional fuzzy controller and the advanced fuzzy controller, the controller has less steady error and better adaptive ability.

The research framework of this paper is as follows.: Firstly, for real-time control, the SMB process model is discrete by finite difference method; Secondly, the feasibility of finite difference method is observed by computer simulation; Thirdly, automatic advance fuzzy controller is used to control SMB system; Finally, compared with the traditional and advance fuzzy controller.

#### **III. SMB MATHEMATICAL MODEL**

For SMB, the balance of mobile and solid phase is:

<span id="page-2-0"></span>
$$
\frac{\partial C_{ij}}{\partial t} = D_i \frac{\partial^2 C_{ij}}{\partial x^2} - v_j^* \frac{\partial C_{ij}}{\partial x} - \frac{1 - \varepsilon}{\varepsilon} k_i (q_{ij}^* - q_{ij}) \tag{1}
$$

$$
\frac{\partial q_{ij}}{\partial t} = k_i (q_{ij}^* - q_{ij}) \tag{2}
$$

The parameters meaning is shown in table1. Formula [\(2\)](#page-2-0) substituted into  $(1)$ , it gets as follows:

$$
\frac{\partial C_{ij}}{\partial t} = D_i \frac{\partial^2 C_{ij}}{\partial x^2} - v_j^* \frac{\partial C_{ij}}{\partial x} - \frac{1 - \varepsilon}{\varepsilon} \frac{\partial q_{ij}}{\partial t} \tag{3}
$$

The adsorption equilibrium of the two enantiomers is expressed by linear isotherms.

$$
q_{ij} = H_i C_{ij} \tag{4}
$$

Purity formulas are:

$$
\bar{C}_{E,B} = \frac{C_{E,B}}{C_{E,A} + C_{E,B}}
$$
(5)

$$
\bar{C}_{R,A} = \frac{C_{R,A}}{C_{R,A} + C_{R,B}}\tag{6}
$$

 $\bar{C}_{E,B}$  represents extract material *B* of purity,  $\bar{C}_{R,A}$  represents raffinate material *A* of purity,  $\overline{C}_{E,B}$  represents extract material *B* of concentration, and  $\overline{C}_{R,A}$  represents raffinate material *A* of concentration. In order to eliminate periodic fluctuations and achieve a better control, we take the average purity of a switching cycle as the output, and the formula is as follows:

$$
\bar{C}_{E,B,t} = \frac{\int_{t-T}^{t} C_{E,B,t} dt}{T_{\theta}} \tag{7}
$$

$$
\bar{C}_{R,A,t} = \frac{\int_{t-T}^{t} C_{R,A,t} dt}{T_{\theta}}
$$
(8)

## **IV. SIMULATION**

The simulated digitization system contains 8 packed columns which was  $2 - 2 - 2 - 2$  model, that is, each zone has two columns. The relationship between flow rate and velocity shown in as formula [\(10\)](#page-4-0),*r* is the radius of the column.

$$
v_j = \frac{Q_j}{\varepsilon \pi r^2} \tag{9}
$$

Using finite difference method to solve the PDEs, setting the time step is 0.1 seconds, and the length of the string in space is divided into 50 parts, the mathematical of dynamic model is shown in appendix. The initial parameters of system are shown in table 2, the volume flow rate of zones are given here, while the velocity is used in the actual iterative calculation formula.

#### **TABLE 2.** The initial parameters for SMB.



All the digitization calculations are conducted in MATLAB R2016a on a PC equipped with Intel core i7-3770K 3.53GHz and 16GB RAM running Windows 10.

The simulation separated concentration ratio show in figure 2 which was not under control. Figure 3 shows the axial concentration variation between the two materials. It can be seen that the finite difference method can also simulate the SMB system very well. Compared with the traditional finite element method, this method is conducive to control and optimization [17]. Therefore, on the basis of the dynamic model, the next step is to control the purity of SMB.

## **V. AUTOMATIC ADVANCE FUZZY CONTROLLER DESIGN**

SMB control process is very sensitive and complex, it is necessary to adjust the magnitude of the single pole value of the action force in the controlled process. In traditional fuzzy controller design, the error membership function usually like figure 4. From figure 4 we can find when the error is small, the force is too small, the speed and efficiency of control are not high. It is necessary to adjust the output force under different parameters and targets to ensure that the force can be applied even when the error is relatively small. In this paper, will use the automatic adjustment controller is used to act on the SMB system.





**FIGURE 2.** The concentration separation results of outlets.



**FIGURE 3.** The concentration separation results of outlets.

Set  $e_{i-1} = -|k \times e|, e_{i+1} = |k \times e|,$  and set  $k < 1$ this ensures that when the error is negative, the error will only fall on the interval  $(e_{i-2}, e_{i-1})$ , and when the error is



**FIGURE 4.** Central value of error membership function  $(e_{i-2}, e_{i-1}, e_i, e_{i+1}, e_{i+2}) = (-1, -0.5, 0, 0.5, 1).$ 



**FIGURE 5.** Central value of automatic adjust error membership function  $(e_{i-2}, e_{i-1}, e_i, e_{i+1}, e_{i+2}) = (-1, -0.2, 0, 0.2, 1).$ 

positive, then the error will only fall on interval  $(e_{i+1}, e_{i+2})$ . The figure 3 shows the automatic adjust the magnitude of the force. The location of  $e_i$  is shown in figure 5.The reason for this is to ensure that the error will only correspond to *NS*, *NB* or *PS*, *PB*, then reference to the rule base, it will correspond to the single pole value of *PS*, *PB* or *NS*, *NB* force, no matter how small the system error, the force will also be applied to the controlled system, not likely when the error of the system is very small, no force will be exerted on the system. At the same time, it is necessary to modify the unipolar value of the attribute function of the force, just like such as the following three cases:

(1) When the value of the corresponding rule base is greater than 0, it is revised according to the following equation.

<span id="page-4-0"></span>
$$
u_{ij} = u_{ij}^*(1 - e^{-|\beta x|}) + \alpha \tag{10}
$$

(2) When the value of the corresponding rule base is less than 0, it is revised according to the following equation.

$$
u_{ij} = u_{ij}^*(1 - e^{-|\beta x|}) - \alpha \tag{11}
$$

(3) When the value of the corresponding rule base is equal 0, it is not revised the force of attribution function.

$$
u_{ij} = u_{ij} \tag{12}
$$



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**FIGURE 6.** The control block diagram of SMB.

Parameter



**FIGURE 7.** Desire  $B = 0.9$ , desire  $A = 0.9$ . Switch = 180s.

In the automatic advanced fuzzy type controller, the input variables contain error, first-order error difference and second-order error, the formula is as follows:

$$
e_1 = desired \ B - C_{E,B} \tag{13}
$$

 $e_2 = desired A - C_{RA}$  (14)

$$
e_3 = e_1 + e_2 \tag{15}
$$



**FIGURE 8.** Desire B = 0.95, desire  $A = 0.93$ , Switch = 178s.

$$
\Delta e_1 = e_1(k) - e_1(k-1) \tag{16}
$$

$$
\Delta e_2 = e_2(k) - e_2(k-1) \tag{17}
$$

$$
\Delta e_3 = \Delta e_1 + \Delta e_2 \tag{18}
$$

$$
\Delta^2 e_1 = \Delta e_1(k) - \Delta e_1(k-1) \tag{19}
$$

$$
\Delta^2 e_2 = \Delta e_2(k) - \Delta e_2(k-1) \tag{20}
$$

$$
\Delta^2 e_3 = \Delta^2 e_1 + \Delta^2 e_2 \tag{21}
$$

where  $e_1$ ,  $\Delta e_1$  and  $\Delta^2 e_1$  are the input of the zone I controller,  $e_2$ ,  $\Delta e_2$  and  $\Delta^2 e_2$  are the input of the zone II controller,  $e_3$ ,  $\Delta e_3$  and  $\Delta^2 e_3$  are the input of the zone III controller.

The fuzzy system defines five linguistic variable values on input variable contains errors, first-order error and second-order error: *NB*, *NS*, *ZE*, *PS*, *PB*. Then defines the control parameter flow rate  $\Delta Q_I$ ,  $\Delta Q_{II}$ ,  $\Delta Q_{III}$ , taking the single pole fuzzification value where the center value  $i$ s(A,B,C,D,E,F,G,H,I) = (0.18,0.12,0.08,0.05,0,-0.05,-0.08,- $0.12, -0.18$ ) for  $\Delta Q_I$ .(A,B,C,D,E,F,G,H,I) = (0.0007,0.0006,



**FIGURE 9.** Desired B = 94%, desired A = 96%, Switch time = 180s.

 $0.0005,0.0004,0, -0.0004,-0.0005,-0.0006, -0.0007)$  for  $\Delta Q_{II}$ . (A,B,C,D,E,F,G,H,I) =

 $(0.12, 0.1, 0.07, 0.04, 0, -0.04, -0.07, -0.1, -0.12)$  for  $\Delta Q_{III}$ . All membership functions are triangular function due to easy to implement, it has advantages for practical application [22].

Then, we draw on the kinematics principle to formulate the corresponding fuzzy rule table as follows:

The fuzzifying equation is as follows:

$$
V = T(u_1, u_3, u_5) \times y_1 + T(u_1, u_3, u_6) \times y_2
$$
  
+ 
$$
T(u_2, u_3, u_5) \times y_3 + T(u_2, u_3, u_6) \times y_4
$$
  
+ 
$$
T(u_1, u_4, u_5) \times y_5 + T(u_1, u_4, u_6) \times y_6
$$
  
+ 
$$
T(u_2, u_4, u_5) \times y_7 + T(u_2, u_4, u_6) \times y_8
$$
 (22)  

$$
W = T(u_1, u_3, u_5) + T(u_1, u_3, u_6) + T(u_2, u_3, u_5)
$$
  
+ 
$$
T(u_2, u_3, u_6) + T(u_1, u_4, u_5) + T(u_1, u_4, u_6)
$$
  
+ 
$$
T(u_2, u_4, u_5) + T(u_2, u_4, u_6)
$$
 (23)



**FIGURE 10.** Desired B = 96%, desired A = 94%, Switch time = 180s.

The value  $u_1$ ,  $u_2$  obtained for fuzzifying acceleration, value  $u_3$ ,  $u_4$  obtained for fuzzifying error, value  $u_5$ ,  $u_6$  obtained for fuzzifying error speed.  $y_1 \cdots y_8$  corresponding to the unipolar value of the attribution function of the regular library force. *T* is product t-norm. Finally, the power of fuzzification is:

$$
U = \frac{V}{W} \tag{24}
$$

The control parameters flow rate of zones I,II and III are set as follows table:

The control structure of automatic advance fuzzy type I controller in SMB system is shown in fig. 6.

#### **VI. EXPERIMENTS RESULTS**

In this section, firstly we use the automatic advance fuzzy controller to control the purity of SMB system, Fig. 7 and fig. 8 show the control results. In the experiment showed in fig.7, the switching time is 180 second and the desired purities of materials A and B are  $A = 0.90$  and  $B = 0.90$ .



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**FIGURE 11.** Under the change of adsorbent parameters  $H_A = 0.01 \rightarrow 0.03$ .

**TABLE 3.** Fuzzy rule for  $\Delta Q_i$  when  $\Delta^2 e(k) > 0$ .

 $\Delta Q_i$ 

$\Delta^2 e$	PS	${\cal PB}$	PS	PB	PS	P B	PS	PB	PS	$\overline{PB}$
$\epsilon$ Δe		NB		N <sub>S</sub>		ZE		PS		PB
NB	$\boldsymbol{A}$	$\boldsymbol{A}$	$\boldsymbol{A}$	$\boldsymbol{A}$	$\boldsymbol{A}$	$\boldsymbol{A}$	$\mathcal{C}$	B	D	$\mathcal{C}_{0}^{0}$
N <sub>S</sub>	$\boldsymbol{A}$	$\boldsymbol{A}$	$\boldsymbol{B}$	$\boldsymbol{A}$	$\overline{C}$	$\boldsymbol{B}$	E	D	$\overline{F}$	$\cal E$
ZE	$\boldsymbol{A}$	$\boldsymbol{A}$	$\mathcal{C}_{0}$	$\mathcal{C}$	E	E	G	G		Ι
PS	$E_{\rm}$	$\boldsymbol{F}$	$\overline{F}$	G	H	$\overline{I}$	I	$\overline{I}$		I
PB	F	G	H							

The actual purities produced by SMB are  $A = 0.8977$  and  $B = 0.9088$ . In the experiment showed in fig.8, the switching



FIGURE 12. Under the change of feed port concentration  $\bm{\mathsf{C}}_{\bm{\mathsf{f}}} = 4.5 \rightarrow 5.2.$ 



**TABLE 4.** Fuzzy rule for  $\Delta Q_i$  when  $\Delta^2(k) = 0$ .

time is 178 second and the desired purities of materials A and B are  $A = 0.93$  and  $B = 0.95$ . The actual purities produced by SMB are  $A = 0.9319$  and  $B = 0.9519$ .

Next, we compare the automatic advance fuzzy controller with other controllers. Fig. 9 and fig. 10 show the comparison





**FIGURE 13.** Under the change of switch time  $\theta = 178s \rightarrow 182s$ .

## **TABLE 5.** Fuzzy rule for  $\Delta Q_i$  when  $\Delta^2 e(k) < 0$ .



results. The effects of the controller on the change of adsorbent parameters, feed concentration and switch time are observed, fig.11, fig. 12 and fig. 13 show the separation results; each group of experiments is divided into two

#### **TABLE 6.** Controller parameters setting.

$\mathsf{Zone}$	$\alpha \rightarrow$	B÷	lΨ $k \in$
I₽	$0.015 -$	$30\degree$	$0.95 -$
H₽	$0.001 \div$	20e	$0.95 -$ l٥
НЬ	0.01e	25e	$0.95 -$ l₽

**TABLE 7.** First and second group experiments.



experiments, including the control of the purity target of material B was 92%, and 96%, and material A was 93%, and 97%.

In the first and second group of experiments, the switching time parameter is 180 seconds. The control results data show in the table 7.It can be seen from the table and figure 9, 10 that the steady-state error of automatic advanced fuzzy controller is between traditional fuzzy and advance fuzzy. But automatic advanced fuzzy controller has the least fluctuation, the highest stability and the fastest convergence speed.

In the third group of experiments in fig. 11, it can be observed that under the change of adsorbent parameters, automatic advance fuzzy is the most stable. In the purity control of A, the fluctuation of advanced fuzzy and traditional controller is highest, and the automatic advance fuzzy is the smoothest.

In the fourth group of experiments in fig. 12, it can be observed that under the change of feed port concentration, the results are similar to the experiments in fig.10.

From the fifth group of experimental results, it can be observed that under the change of switching time, the traditional fuzzy controller appears ill conditioned characteristics, and the volatility of control results is relatively large by advance fuzzy type controller in raffinate port, but the automatic advance fuzzy controller is also stable.

# **VII. CONCLUSION**

In this paper, the automatic advanced fuzzy controller is used to control the purity of SMB. The purity of traditional fuzzy controller in steady state is usually lower than the target value, while the steady-state value of advanced fuzzy controller is often higher; and the steady-state error of automatic advanced fuzzy controller is more than that of traditional fuzzy controller but less than that of advanced fuzzy controller. The automatic advanced fuzzy controller has strong robustness

and adaptability to the changes of system parameters such as adsorption parameters and feed port concentration, and is the most stable one among the three controllers. But no matter which controller is used, the fluctuation of raffinate liquid outlet is relatively large. For further consideration, the adaptive fuzzy neural network with strong learning ability can be used to control the system by combining neural network technology, or the convolution neural network can be used to estimate the system parameters firstly, and then the fuzzy technology can be used for control.

## **APPENDIX**

In order to obtain the concentration data of two materials varying with time and space, it is necessary to discredited and numerically simulate the diffusion equation of materials in a simulated moving bed.

Set  $t_k = t_0 + \bar{k}s$ ,  $x_l = x_0 + lh$ ,  $F = \frac{1-\varepsilon}{\varepsilon}$ 

$$
\frac{\partial^2 C_{i,j}}{\partial x^2}(x_l, t_k) = \frac{C_{i,j}(x_{l+1}, t_k) - 2C_{i,j}(x_l, t_k) + C_{i,j}(x_{l-1}, t_k)}{h^2}
$$
\n(A1)

$$
\frac{\partial C_{i,j}}{\partial x}(x_l, t_k) = \frac{C_{i,j}(x_{l+1}, t_k) - C_{i,j}(x_l, t_k)}{h}
$$
(A2)

$$
\frac{\partial C_{i,j}}{\partial t}(x_l, t_k) = \frac{C_{i,j}(x_l, t_{k+1}) - C_{i,j}(x_l, t_k)}{s}
$$
(A3)

$$
\frac{\partial q_{i,j}}{\partial t}(x_l, t_k) = H_i \frac{\partial C_{i,j}}{\partial t}(x_l, t_k)
$$
  
  $i = 1, 2, j = 1, \cdots 8$  (A4)

 $C_{i,j}(x_l, t_k)$  denote as  $C_{i,j}(l, k)$ , substituted into SMB system, we can get:

$$
(1 + FH_i)C_{i,j}(l, k+1) = \left(\frac{Ds}{h^2} - \frac{v_j^*s}{h}\right)C_{i,j}(l+1, k) + \left(\frac{v_j^*s}{h} - \frac{2Ds}{h^2} + 1 + FH_i\right) - C_{i,j}(l, k)\frac{Ds}{h^2}C_{i,j}(l-1, k)
$$
(A5)

The initial conditions of partial differential equations need to be discredited to generate initial solubility and boundary solubility constraints.

Boundary condition is:

(i) 
$$
C_{i,j}(x, 0) = C_{0,i,j}(x)
$$
 (A6)

(ii) 
$$
\frac{\partial C_{i,j}(x,t)}{\partial x}|_{x=l_n} = 0
$$
 (A7)

(iii) 
$$
D_i \frac{\partial C_{i,j}(x, t)}{\partial x} |_{x=0} = v_j [C_{i,j}(0, t) - \bar{C}_{i,j}^{\text{sec}t}(t)]
$$
 (A8)

Section I, 1<sup>st</sup> column:

$$
\bar{C}_{i,j}^{\text{I}}(t) = \frac{Q_{IV}C_{i,j-1}(l_{n-1}, t)}{Q_{I}} \tag{A9}
$$

Section III,1<sup>st</sup> column:

$$
\bar{C}_{i,j}^{\text{III}}(t) = \frac{Q_{II} C_{i,j-1}(l_{n-1}, t) + Q_f C_{f,i}}{Q_{III}} \tag{A10}
$$



Any other column:

$$
\bar{C}_{i,j}^{\text{sec}t}(t) = C_{i,j-1}(l_{n-1}, t)
$$
\n(A11)

where  $C_f$  is the feed stream concentration, Q is volume flow rate,  $C_{0,i,j}$  is initial concentration,  $\bar{C}_{i,j}^{\text{sec }t}$  is the column inlet concentration with superscript sec  $t = I, II, III, IV, l$  is column length. We can get from formula (A7):

$$
C_{i,j}(n+1,k) = C_{i,j}(n,k)
$$
 (A12)

It can get from formula (A8):

$$
D_i[\frac{C_{i,j}(1,k) - C_{i,j}(0,k)}{h}] = v_j^*[C_{i,j}(0,k) - \bar{C}_{i,j}^{\text{sec }t}(k)]
$$
\n(A13)

So can get:

$$
C_{i,j}(1,k) = \left(\frac{hv_j^*}{D_i} + 1\right)C_{i,j}(0,k) - \frac{hv_j^*}{D_i}\bar{C}_{i,j}^{\sec t}(k) \quad (A14)
$$

set  $M = \frac{v^*s}{h}$ ,  $N = \frac{Ds}{h^2}$  $\frac{Ds}{h^2}$  it get the next two boundary equation:

$$
(1 + FH_i)C_{i,j}(1, k+1) = (1 + FH_i + M - 2N - \frac{MN}{M + N})
$$

$$
\times C_{i,j}(1, k) + (N - M)C_{i,j}(2, k)
$$

$$
-\frac{M^2}{M + N} \bar{C}_{i,j}^{\text{sec } t}(k) \tag{A15}
$$

$$
(1 + FH_i)C_{i,j}(l, k+1) = (N - M)C_{i,j}(l+1, k)
$$

$$
+(M-2N+1+FHi)Ci,j(l, k)
$$

$$
-NCi,j(l-1, k) l \neq 1, n
$$
(A16)

$$
(1 + FHi)Ci,j(n, k + 1) = (1 + FHi - N)Ci,j(n, k) - NCi,j(n - 1, k)
$$
 (A17)

denote the matrix *A*, as shown at the top of the page.

So the Iterative equation is:

$$
C_{i,j}(k+1) = AC_{i,j}(k) + w(k)
$$
 (A18)

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