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Optimization for adsorption separation process of simulated moving bed based on moving asymptotes algorithm

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The Simulated Moving Bed (SMB) is a continuous multi–column chromatographic process that has become an attractive technology for complex separation tasks that are regularly encountered in the areas of pharmaceuticals, fine chemicals and biotechnology. This paper focuses on the implementation of the control concept to SMBs operating. Based on moving asymptotes algorithm, the optimizing strategy is carried out for improvements of the extract and raffinate purity, the productivity and the solvent consumption. The feasibility of the moving asymptotes is verified by the triangle theory. The simulation results illustrate that the moving asymptotes method is fast in convergence and the optimal solutions are distributed uniformly.

Key words: Adsorption separation process, Simulated moving bed, Equilibrium diffusion model, Moving asymptotes, Optimizing strategy

INTRODUCTION

The Simulated Moving Bed (SMB) separation technology is a kind of continuous chromatographic separation technique for scale production, which is with the advantages of strong separation ability, small appearance and low operation costs. It has a large range of applications in the areas of the petroleum chemical industry, fine chemical industry and sugar industry [1,2]. Recently, due to the strong coupling and the mechanism complexity in the SMB separation process, many researches carried out the modeling, the model solving and optimizing of SMB separation process in order to give the theoretical guidance for the product development, the process of industrialization and the application range can be expanded accordingly. The commonly used SMB chromatography models[3] are General Rate Model (GRM), Lumped Pore Diffusion Model (PORM), Ideal Model (IM), Equilibrium Dispersive Model (EDM) and Transport Dispersive Model (TDM). Comparing with other models, EDM has higher practicability. During the simulation process, EDM ignores the influence of mass transfer resistance, whose calculation speed is faster than GRM and PORM, the considered factors of which are more comprehensive than IM. Therefore, it has a large range of applications[4]. By using EDM, the influence of changing feed flow rate on SMB separation technology was researched[5]. On the other hand, SMB model is very difficult to be solved for its style of partial differential equations. Therefore, the general solution method is to transfer the partial differential equations to ordinary differential equations by using discrete methods, such as orthogonal collocation finite element method, Galerkin method and CE/SE method[6]. In reference [7], the adsorption isotherm model was simulated by using CE/SE method; the advantages and disadvantages of the finite difference method and orthogonal collocation finite element method were discussed. By comparing with other methods, the orthogonal collocation finite element method is not only convenient and fast, but also flexible and accurate in the processing of stiff problems. There are many operation conditions that affect the chromatographic separation performance in SMB process, such as switching time, flow rate of the area, and the size of the column. Therefore, the optimization analysis of SMB is a hot research topic in this area. Marco Mazzotti firstly proposed the triangle theory[8] which is under the ideal status, hence the axial dispersion and mass transfer resistance were not considered and there must be accuracy problem in real applications. In recent years, the genetic algorithm or particle swarm optimization is used for SMB process design[9, 10]. The genetic algorithm needs copy, crossover and mutation operations in the process, thus its efficiency must be affected. And the particle swarm optimization algorithm is with shortcomings like easily falling into local optimal solution, being prone to unstable and slow in convergence in the actual operation of the process.

In this paper, the equilibrium diffusion model of SMB chromatographic separation process is firstly solved by using orthogonal collocation finite

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element method. Then, the optimization strategy is proposed based on the method of moving asymptotes [11]. Finally, the simulation is carried out in the operation optimization of SMB chromatographic separation process. The simulation results show that the proposed optimization method can improve the economic benefits of SMB operation and guide the process operation.

BASIC PRINCIPLE OF SMB

SMB is composed by a plurality of chromatographic columns with the valves and the pipelines in series, principle of which is to simulate the movement direction of the solid phase to achieve the solid phase and fluid phase countercurrent motion by periodically opening and closing the valve to switch import and export positions [12-14]. Fig. 1 shows the operation process of SMB in which the solid arrow indicates the location of imports and exports for current cycle, the dotted arrow indicates that for the next cycle. SMB chromatographic separation process can be divided into four zones, as shown in Fig 1. The feed solution and the elution are imported between zone 2 and 3, zone 1 and 4, respectively. The extraction and raffinate are collected between zone 1 and 2, zone 3 and 4 respectively. The function of zone 1 is mainly to realize the regeneration of the adsorbent, and the strong absorption component is desorbed from the solid phase. The effect of zone 2 is to desorb the weak adsorption components and adsorb the strong adsorption components, the purpose is to make the extract contain only strong absorption components, and do not contain weak adsorption components. Zone 3 is opposite to zone 2, so that the liquid contains only the weak absorption of components, and does not contain strong absorption component. The effect of zone 4 is the regeneration of the elution solution, the weak adsorption components are desorbed from the fluid phase [15]. By selecting the reasonable design parameters, the type of adsorbent, elution solution and operating parameters, the raffinate contains only the weak adsorption component B, the extract contains only the strong adsorption component A, so as to achieve the purpose of continuous separation.

EQUILIBRIUM DIFFUSION MODEL OF SMB CHROMATOGRAPHIC SEPARATION

The mathematical model of SMB chromatographic separation is coupled by a series of single chromatographic column model and node model [16].

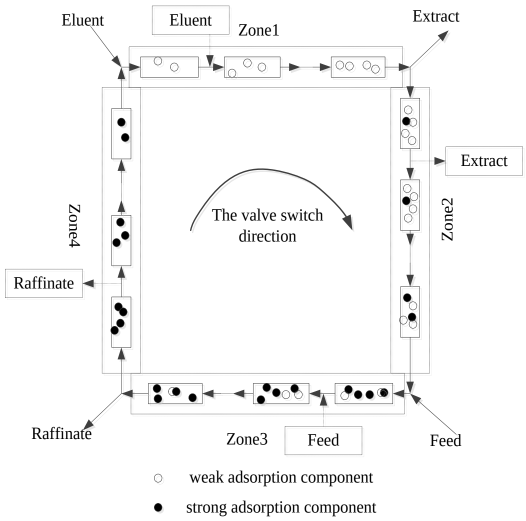

Fig.1. Operation schematic diagram of SMB

Because EDM has a higher practicability, and the computer simulation speed of which is fast, therefore, the EDM single column chromatographic model is adopted in this paper. There are two assumptions as follows [17]: (1) The flow and the solid phase reach the equilibrium state instantaneously. (2) The effect of axial diffusion and non equilibrium is integrated into the axial diffusion coefficient. The effect of molecular diffusion, eddy diffusion and mass transfer resistance on the model is considered, the influence of interphase mass transfer resistance is ignored. The diffusion of the fluid phase and solid phase is instant and reach an equilibrium state, thus its influence is not considered.

The mathematical description of EDM is as follows:

$$\frac{\partial c_i}{\partial t}+F_a\frac{\partial q_i}{\partial t}+u\frac{\partial c_i}{\partial x}=D_a\frac{\partial^2 c_i}{\partial x^2} \tag{1}$$

Initial condition is:

$$c_i(x,0)=q_i(x,0)=0 \tag{2}$$

Boundary condition is:

1） $$c_i(t,0)=\psi_i(t) \tag{3}$$

2） $$uc_i(t,0)+D\frac{\partial c_i}{\partial x}\Big|_{0,t}=uc_k(t) \tag{4}$$

$$\frac{\partial c_i}{\partial x}\Big|_{x=L}=0 \tag{5}$$

where $\psi_i(t)$ is inlet concentration of the ith chromatographic column, $c_k(t)$ is known.

Adsorption isotherm equation is:

$$q_i(x,t)=f[\mathrm{c}(x,t)] \tag{6}$$

The equilibrium relationship between the nodes can be obtained by the mass conservation relation:

$$Q_4 + Q_D = Q_1, c_{i,4}^{out} Q_4 = c_{i,1}^{in} Q_1 \quad (7)$$

$$Q_1 - Q_E = Q_2, c_{i,1}^{out} = c_{i,2}^{in} \quad (8)$$

$$Q_2 - Q_F = Q_3, c_{i,2}^{out} Q_2 + c_{i,F} Q_F = c_{i,3}^{in} Q_3 \quad (9)$$

$$Q_3 - Q_R = Q_4, c_{i,3}^{out} = c_{i,4}^{in} \quad (10)$$

OPTIMIZATION STRATEGY OF SMB

Principle of moving asymptotes

Moving Asymptotes (MA) is an optimization method based on convex function. In 1987, Svanberg firstly proposed the method, which uses the sub problem with convex functions and separable variables to approximate the original problem [11]. For this algorithm, the selection principle of the approximate function is that the private function is replaced by the first order derivative of the current iteration point. The method of moving asymptotes is used to optimize the multi-objective problem and the implicit problem is converted into a convex approximation sub problem. The optimization model is as follows:

Considering the optimization problem P,

$$\text{MIN} \quad f_0(X) \quad X \in R^n \quad (11)$$

$$\text{S.T.} \quad f_i(X) \le f_i^* \quad i = 1, \ldots, m \quad (12)$$

$$x_{ja} \le x_j \le x_{jb} \quad j = 1, \ldots, n \quad (13)$$

where $f_0(X)$ is the objective function, $X = (x_1, \ldots, x_n)^T$ is the design variable, $f_i(X) \le f_i^*$ is behaviour constraint, and $x_{ja} \le x_j \le x_{jb}$ is technical constraint.

The method to solve the problem P is to construct the sub problem. The solution of the original problem is approximated by the sub problem. The detailed algorithm procedure is as follows:

Step 1: Choose the initial point x^0, let $k = 0$.

Step 2: Give the iteration point x^k, and calculate $f_i(X^k)$ and $\nabla f_i(X^k)$, $i = 1, \ldots, m$.

Step 3: The established sub problem is used to approximate the original problem, which means that $f_i(X)$ is replaced by $f_i^k(X)$, and the establishment of sub problem $f_i^k(X)$ needs the data calculated in step 2.

Step 4: Solve sub problem. The optimal solution of the sub problem is taken as the next iterative point, i.e. *k=k+1*, and return to step 2.

Construction of sub problem

In the process of using moving asymptotes algorithm for solving optimization problem, the key point is to construct and solve sub problem. In the kth iterative of the algorithm, the sub problem is constructed as follows:

$$\text{MIN} \quad f_0^k(X) \quad X \in R^n \quad (14)$$

$$\text{S.T.} \quad f_i^k(X) \le f_i^* \quad i = 1, \ldots, m \quad (15)$$

$$x_j^\alpha \le x_j \le x_j^\beta \quad j = 1, \ldots, n \quad (16)$$

where *i=0, 1, ..., m.*

$$f_i^k(X) = r_i^k + \sum_{j=1}^{n} \left(\frac{p_{ij}^k}{U_j^k - x_j^k} + \frac{q_{ij}^k}{x_j^k - L_j^k} \right) \quad (17)$$

$$r_i^k = f_i(X^k) - \sum_{j=1}^{n} \left(\frac{p_{ij}^k}{U_j^k - x_j^k} + \frac{q_{ij}^k}{x_j^k - L_j^k} \right) \quad (18)$$

$$p_{ij}^k = \begin{cases} (U_j^k - x_j^k) \dfrac{\partial f_i(X)}{\partial x_j} & \dfrac{\partial f_i(X)}{\partial x_j} > 0 \\ 0 & \dfrac{\partial f_i(X)}{\partial x_j} \le 0 \end{cases} \quad (19)$$

$$q_{ij}^k = \begin{cases} -(x_j^k - L_j^k) \dfrac{\partial f_i^k(X)}{\partial x_j} & \dfrac{\partial f_i^k(X)}{\partial x_j} < 0 \\ 0 & \dfrac{\partial f_i^k(X)}{\partial x_j} \ge 0 \end{cases} \quad (20)$$

where $\partial f_i^k(X) / \partial x_j$ is the value at $X = X^k$, which is a variable changing with the iteration point x_j^k, and satisfies $L_j^k < x_j^k < U_j^k$. At $x = x^k$, there is

$$f_i^k(x^k) = f_i(x^k) \quad (21)$$

$$\frac{\partial f_i^k}{\partial x_j} = \frac{\partial f_i}{\partial x_j} \quad i = 1, \ldots, m, \ j = 1, \ldots, n \quad (22)$$

In the sub problem, if x_j^k is close to L_j^k or U_j^k, the value of f_i^k will increase sharply. Therefore, $x_j^k = L_j^k$ or $x_j^k = U_j^k$ is the asymptote. The solution after each iteration is maintained between L_j^k and U_j^k, the values of which are changed between the iterations, it is equivalent to the movement of asymptote, thus L_j^k and U_j^k are called moving asymptotes.

The second partial derivative of f_i^k at $X = X^k$ is:

$$\frac{\partial^2 f_i^k}{\partial (x_j)^2} = \frac{2 p_{ij}^k}{(u_j^k - x_j)^3} + \frac{2 q_{ij}^k}{(x_j - l_j^k)^3} \quad (23)$$

Simplify the equation (23), we obtain

$$\frac{\partial^2 f_i^k}{\partial (x_j)^2} = \begin{cases} \dfrac{2 \partial f_i / \partial x_j}{u_j^k - x_j} & \partial f_i / \partial x_j > 0 \\ 0 & \partial f_i / \partial x_j > 0 \\ \dfrac{-2 \partial f_i / \partial x_j}{x_j - l_j^k} & \partial f_i / \partial x_j > 0 \end{cases} \quad (24)$$

It is easy to see that the function f_i^k is a convex function. In addition, the next iterative point always exists between the lower bound of L_j^k and upper bound of U_j^k. In view of this situation, it is able to obtain a good effect of approximation by regulating the boundary values during the running process of the algorithm. By comparing the method of moving asymptotes with other optimization algorithms, its advantages are very obvious, sub problem is constructed with convexity and separable independent variable.

Solution of sub problem

In the method of moving asymptotes, sub problem we constructed needs to be solved by an algorithm, here Lagrange function is selected.

For equations (14) - (16), the number of iterations is omitted by *k*, and the simplified form is as follows:

$$\text{MIN} \quad r_0 + \sum_{j=1}^{n} \left(\frac{p_{0j}}{U_j - x_j} + \frac{q_{0j}}{x_j - L_j} \right) \tag{25}$$

$$\text{S. T} \quad \sum_{j=1}^{n} \left(\frac{p_{ij}}{U_j - x_j} + \frac{q_{ij}}{x_j - L_j} \right) \le b_i \quad i = 1,...,m \tag{26}$$

$$\alpha_j \le x_j \le \beta_j \qquad j = 1,...,n \tag{27}$$

Where $\alpha_j = max\{x_j^{\alpha}, \alpha_j\}$, $\beta_j = min\{x_j^{\beta}, \beta_j\}$, $L_j < \alpha_j \le \beta_j < U_J$, and $b_i = f_i^* - r_i$.

The sub problem is a variable separable convex function, and the dual method can be used to solve the problem. The sub problem is constructed as a Lagrange function, which is:

$$l(x, y) = f_0^k(X) + \sum_{i=1}^{m} y_i f_i^k(X) \tag{28}$$

Substitute sub problem (25) into（28）, we have

$$l(x, y) = r_0 - Y^T B + \sum_{j=1}^{n} \left(\frac{p_{0j} + Y^T P_j}{U_j - x_j} + \frac{q_{0j} + Y^T Q_j}{x_j - L_j} \right) \tag{29}$$

The following equation can be obtained by simplifying the equation（29）.

$$l(x, y) = r_0 - Y^T B + \sum_{j=1}^{n} l_j(x_j, Y) \tag{30}$$

$B = (b_1,...,b_m)^T$, $P_j = (P_{1j},...,P_{mj})^T$, $Q_j = (Q_{1j},...,Q_{mj})^T$ and $Y = (y_1,..., y_m)^T$.

where Y is the multiplier of Lagrange's function.

$$l_j(x_j, y) = \frac{p_{0j} + Y^T P_j}{U_j - x_j} + \frac{q_{0j} + Y^T Q_j}{x_j - L_j} \tag{31}$$

If $y_i \ge 0$, the dual objective function can be constructed as:

$$w(Y) = r_0 - Y^T B + \sum_{j=1}^{n} w_j(Y) \tag{32}$$

Where,

$$w_j(Y) = \min_{x_j}\{l_j(x_j, Y); \alpha_j \le x_j \le \beta_j\} \tag{33}$$

The minimum value of x_j is determined by *Y*, it can be expressed as $x_j(Y)$. If $y_i \ge 0$, then $p_{0j} + Y^T P_j \ge 0$ and $q_{0j} + Y^T Q_j \ge 0$. Hence, $l_j(x_j, Y)$ is convex function.

Therefore, assume that there is at least one positive term in $p_{0j} + Y^T P_j$ and $q_{0j} + Y^T Q_j$, and the first order derivative of $l_j(x_j, Y)$ on x_j is:

$$l_j^{'}(x_j, Y) = \frac{p_{0j} + Y^T P_j}{(U_j - x_j)^2} - \frac{q_{0j} + Y^T Q_j}{(x_j - L_j)^2} \tag{34}$$

The second order derivative of $l_j(x_j, Y)$ on x_j is:

$$l_j^{''}(x_j, Y) = \frac{2(p_{0j} + Y^T P_j)}{(U_j - x_j)^3} + \frac{2(q_{0j} + Y^T Q_j)}{(x_j - L_j)^3} \tag{35}$$

The second order derivative of $l_j(x_j, Y)$ on x_j is positive, so the first order derivative of $l_j(x_j, Y)$ on x_j is increasing function. The conclusion about the minimum value of $x_j(Y)$ can be gotten as follows:

(1) If $l_j^{'}(\alpha_j, Y) \ge 0$, then $x_j(Y) = \alpha_j$;

(2) If $l_j^{'}(\beta_j, Y) \le 0$, then $x_j(Y) = \beta_j$;

(3) If $l_j^{'}(\alpha_j, Y) < 0$ and $l_j^{'}(\beta_j, Y) > 0$,then $x_j(Y)$ has a unique solution. The form of the solution is shown in the following form:

$$x_j(Y) = \frac{(p_{0j} + Y^T P_j)^{1/2} L_j + (q_{0j} + Y^T Q_j)^{1/2} U_j}{(p_{0j} + Y^T P_j)^{1/2} + (q_{0j} + Y^T Q_j)^{1/2}} \tag{36}$$

Substitute $x_j(Y)$ into the following function $w(Y)$, we have:

$$w(Y) = r_0 - Y^T B + \sum_{j=1}^{n} \left(\frac{p_{0j} + Y^T P_j}{U_j - x_j(Y)} + \frac{q_{0j} + Y^T Q_j}{x_j(Y) - L_j} \right) \tag{37}$$

Hence, the first order partial derivative of $w(Y)$ on y_i is obtained:

$$\frac{\partial w}{\partial y_i} = -b_i + \sum_{j=1}^{n} \left(\frac{p_{ij}}{U_j - x_j(Y)} + \frac{q_{ij}}{x_j(Y) - L_j} \right) \tag{38}$$

Then, the dual problem of the sub problem is equivalent to the maximum value of the dual function $w(Y)$ when $y_i \ge 0$.

SMB optimization strategy

Maximizing extraction and raffinate purity

In the separation of SMB, the high purity of product is the most basic requirement in the process. In this optimization problem, the feed flow rate Q_F and the elution flow rate Q_D are fixed values. Based On this basis, the concentration of the extraction and raffinate reach to maximum.

In this paper, the flow rate of zone 2 is taken as one of the control variables, and another one is the switching time t^* . The mathematical model of the optimization problem is:

$$\text{Max} \quad P_1 = X_E(Q_{II}, \ t^*) \tag{39}$$

$$\text{Max} \quad P_2 = X_R(Q_{II}, \ t^*) \tag{40}$$

The optimization problem also ensures that the purity of the product reaches a certain constraint, such as

$$X_A \geq 98\% \tag{41}$$

$$X_B \geq 98\% \tag{42}$$

Decision variables are as follows:

$$2min \leq t^* \leq 4min \tag{43}$$

$$30mL/min \leq Q_{II} \leq 45mL/min \tag{44}$$

$$Q_F = 3.64mL/min \tag{45}$$

$$Q_D = 21.15mL/min \tag{46}$$

$$Q_I = 56.83mL/min \tag{47}$$

The optimization is carried out by using the method of moving asymptotes, the distribution of Pareto optimal solution set is shown in figure 2. The simulation results show that the moving asymptotes algorithm converges to Pareto solution set, which has better dispersion degree and more uniform distribution.

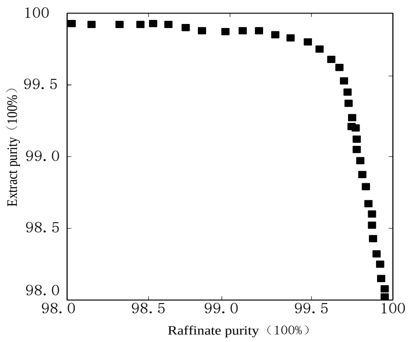

Fig. 2. Optimal solution distribution of MA

In order to ensure the accuracy of the algorithm of moving asymptotes in SMB optimization, the triangle theory is used to verify the algorithm. Based on the balance theory, m_2 and m_3 are fixed values under ideal conditions. However, due to the existence of the diffusion coefficient and mass transfer resistance in the separation process of actual production, m_2 and m_3 is moving from high to low with the Pareto optimal solution.

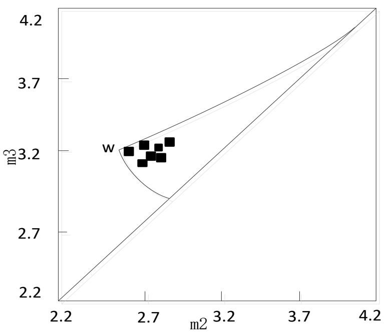

Fig. 3. m2- m3 plane of MA

The corresponding positions of operation points of SMB after optimization on $m_2 - m_3$ plane are shown in figure 3. It can be seen from the figure that the optimization results of proposed algorithm remain in complete separation region, and the calculation results meet the triangle theory.

Maximizing productivity and minimizing solvent consumption

From an economic point of view, SMB solvent consumption and productivity are important economic indicators. In this paper, the flow rate of feed Q_F and the flow rate of zone 1 Q_1 are fixed values to minimize the solvent consumption and maximize the productivity. Because the flow rate of feed Q_F and the flow rate of zone 1 Q_1 are given, therefore, according to the relationships between the flow rate in each zone, three of the operation parameters Q_D , Q_R , Q_E , Q_2 , Q_3 and Q_4 are independent, Q_D , Q_R , Q_E and t^* are taken as control variables. Therefore, the mathematical description of this optimization is as follows:

$$\text{Max} \quad P_1 = P_r(Q_D, Q_R, Q_E, t^*) \tag{48}$$

$$\text{Min} \quad P_2 = SC(Q_D, Q_R, Q_E, t^*) \tag{49}$$

The optimization problem also ensures that the purity of the product reaches a certain constraint, which is:

$$X_A \geq 98\% \tag{50}$$

$$X_B \geq 98\% \tag{51}$$

Decision variables and fixed parameters:

$$2min \leq t^* \leq 4min \tag{52}$$

$$10mL/min \leq Q_D \leq 40mL/min \tag{53}$$

$$5mL/min \leq Q_R \leq 20mL/min \tag{54}$$

$$10mL/min \leq Q_E \leq 30mL/min \tag{55}$$

$$Q_F = 3.64mL/min \tag{56}$$

$$Q_I = 56.83mL/min \tag{57}$$

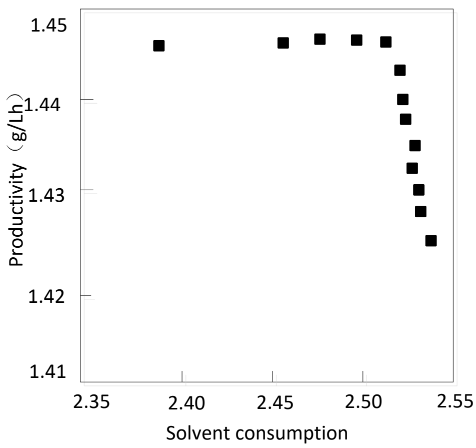

Fig. 4. Optimal solution distribution of MA

Moving asymptotes algorithm is used to solve this problem, figure 4 shows the Pareto optimal solution set distribution. We can get that when the solvent consumption is increased, the productivity will be reduced accordingly.

Figure 5 shows the position of optimized operating point in the $m_2 - m_3$ plane, the optimization results maintain complete separation region. The decision variables distribution diagram of moving asymptotes method is shown in figure 6, the control solutions of variables are uniformly distributed, and the number of optimal solutions are satisfied.

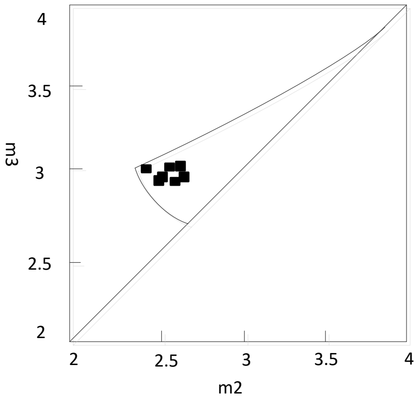

Fig. 5. m2- m3 plane of MA

CONCLUSION

In this paper, According to moving asymptotes algorithm, extract purity, raffinate purity, productivity and solvent consumption are optimized and simulated. The feasibility is verified by triangle theory. The simulation results show that the algorithm has a fast convergence speed, and the optimal solutions are well-distributed. The SMB optimization strategy can be used for SMB separation process design and operation guidance.

The limitation of this study is that it is based on the separation of the two components, and the algorithm has some space to improve. Our future work will continue to improve the optimization algorithm to realize the online optimization control of the various modified simulated moving bed.

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Symbol description:

c_i : Concentration of component *i* in fluid phase

q_i : Concentration of component *i* in solid phase

u : Superficial velocity

ε : Column porosity

h : Space step

A : Strong adsorption component

B : Weak adsorption component

D_a: Axial diffusion coefficient

F_a: Phase rate

H_i: Henry's constant of component *i*

L: Column length

Q: Flow rate

Subscripts

1,2,3,4: denote zone 1,2,3 and 4 respectively

i: Component

E: Extraction

F: Feed

R: Raffinate

D: Elution

Superscripts

*: Equilibrium value

in: Entry value

out: Export value

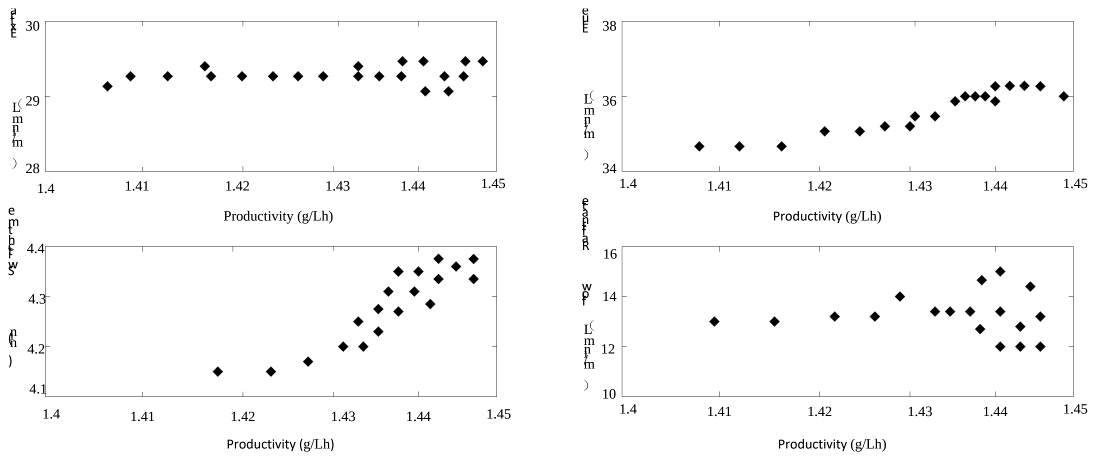

Fig. 6. Control variable distribution of MA\

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