

# Discussions on Evaluation of Material Balance in Simulated Moving Bed Chromatography by Orthogonal Collocation Finite Elements Method

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## Abstract

This paper discusses on evaluation of material balance in simulated moving bed chromatography by using the advantage of orthogonal collocation finite elements method (OCFEM) in terms of accuracy of numerical calculation. The tool of OCFEM is differential operator represented by matrix in time and space to make it easy to translate PDEs to algebraic equations, which have high precision numerical calculation ability by high order collocation number. This study presents the dimensionless average concentration profile through the total column, and calculates the yields and purity at raffinate and extract. In conclusion, this discussion showed that the total yield at raffinate and extract is equal to 100% and the mass balance in total columns for each duration of cyclic steady condition is zero.

*Keywords:* Simulated Moving Bed, Chromatography, Orthogonal Collocation Finite Elements Method, differential operator, time and space, high precision, mass balance, yield at raffinate and extract

## Introduction

Simulated moving bed chromate separation is used in the food and pharmaceutical fields, and is one of the methods that can be purified and separated by continuous operation<sup>[1]</sup>. In order to determine the optimal equipment and operating conditions of the simulated moving bed, it was necessary to perform experiments by trial and error, and a highly accuracy simulation technology using a PC was desired. However, it has been pointed out that there are problems in terms of yield and mass balance, which are considered to be caused by the accuracy of the calculations, in the results of numerical simulations using

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differences. In this study, numerical analysis was performed by the orthogonal collocation finite element method (OCFEM) using a differential operator (matrix) in space and time that can be calculated with high accuracy<sup>[3][4][5][6]</sup>. It was found that the total yield of between each cycle was almost 100% under the cyclic steady condition of the raffinate and extract from which the purified components of the simulated moving bed were extracted, while the mass balance throughout the entire column in each cyclic period was almost zero (total balance: on the order of  $10^{-10} \sim 10^{-16}$ ) with the number of cycles 200. It was found that the total yield of raffinate and extract was closer to 100% when the number of periodic cycles was 100 or 200 than when the number of periodic cycles was 50. The total balance, which calculate the sum of the balances of all columns, is almost zero when up to 200 cycles, so the numerical balance is considered to be balanced. These results indicate that the orthogonal collocation finite element method is more accurate than other calculation methods. Using a differential operator matrix of high order, it is possible to perform highly accurate calculations automatically. In this paper, we present the time-average concentration profile and the calculation of the total yield of raffinates and extracts, the results of the periodic steady state of the raffinates and extracts, and the distribution of the mass balance of each column during each cycle under cyclic steady state conditions, and the results of calculating the total balance of all columns. (Fig.1)

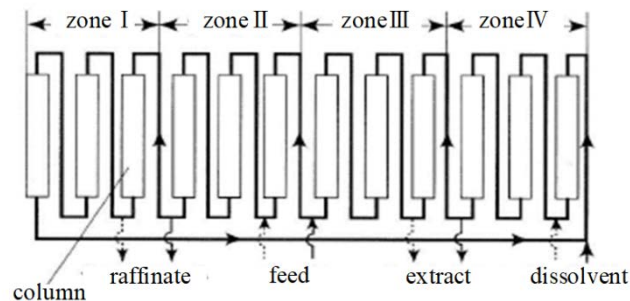


Fig.1 Example of Equipment of simulated moving bed chromate separation [1]

## Differential Operator in Space and Time

### Differential operator in space [2][3][4][5][6]

The partial derivative displayed at each collocation is represented by the product of the differential operator represented by the matrix and the solution vector at the collocation. A differential operator is obtained by differentiating an orthogonal polynomial representing a solution. Orthogonal polynomial fixed the time is represented by following equation.

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$$u = \sum_{i=1}^{N+2} d_i x^{i-1} \quad (1)$$

Differentiating the polynomial (1) to two orders get the following equation (2)(3)

$$\frac{\partial u}{\partial x} = \sum_{i=1}^{N+2} (i-1) x^{i-2} d_i \quad (2)$$

$$\frac{\partial^2 u}{\partial x^2} = \sum_{i=1}^{N+2} (i-1)(i-2) x^{i-3} d_i \quad (3)$$

The solution and differentiate in collocation are represented as follow

$$u_j = \sum_{i=1}^{N+2} x_j^{i-1} d_i \quad (4)$$

$$\left. \frac{\partial u}{\partial x} \right|_j = \sum_{i=1}^{N+2} (i-1) x_j^{i-2} d_i \quad (5)$$

$$\left. \frac{\partial^2 u}{\partial x^2} \right|_j = \sum_{i=1}^{N+2} (i-1)(i-2) x_j^{i-3} d_i \quad (6)$$

Collocation  $x_j$  is the root of N-1 order shifted Legendre polynomial. Representation of eq. (4)(5)(6) by vector and matrix is as follow.

$$\mathbf{u} = \mathbf{Qd} \quad (7)$$

$$\left[ \frac{\partial u}{\partial x} \right] = \mathbf{Cd} \quad (8)$$

$$\left[ \frac{\partial^2 u}{\partial x^2} \right] = \mathbf{Dd} \quad (9)$$

where,

$$\mathbf{d} = [d_i], \quad \mathbf{Q} = [x_j^{i-1}], \quad \mathbf{C} = [(i-1)x_j^{i-2}], \quad \mathbf{D} = [(i-1)(i-2)x_j^{i-3}] \quad (10)$$

From eq. (7)

$$\mathbf{d} = \mathbf{Q}^{-1}\mathbf{u} \quad (11)$$

Substituting eq. (11) to eq. (8)(9) get as following equation

$$\left[ \frac{\partial u}{\partial x} \right] = \mathbf{CQ}^{-1}\mathbf{u} = \mathbf{A}_x \mathbf{u} \quad (12)$$

$$\left[ \frac{\partial^2 u}{\partial x^2} \right] = \mathbf{DQ}^{-1}\mathbf{u} = \mathbf{B}_x \mathbf{u} \quad (13)$$

where,

$$\mathbf{A}_x = \mathbf{CQ}^{-1}, \quad \mathbf{B}_x = \mathbf{DQ}^{-1} \quad (14)$$

$\mathbf{A}_x, \mathbf{B}_x$  are differential operator of one order and two order respectively.  $\mathbf{A}_x, \mathbf{B}_x$  are depend on only the root of sifted Legendre polynomial.

### Induction of differential operator in space by using Lagrange interpolate

Lagrange interpolation using the root of sifted Legendre polynomial is represented by following equation.

$$u(x) = \sum_{i=1}^{N_1+2} l_i(x) u(x_i) \quad (15)$$

$$l_i(x) = \prod_{\substack{k=1 \\ k \neq i}}^{N+2} \frac{x - x_k}{x_i - x_k} \quad (16)$$

The above equation (15) is partial differentiated by x and the partial derivative at the collocations m (number in the x direction) is shown below.

$$\left. \frac{\partial u}{\partial x} \right|_m = \sum_{i=1}^{N+2} l_i'(x_m) u(x_i) \quad (17)$$

$$\left. \frac{\partial^2 u}{\partial x^2} \right|_m = \sum_{i=1}^{N+2} l_i''(x_m) u(x_i)$$

From equation (17), the differential operator (matrix) is represented by equation (18), where ( ' ) and ( '' ) are first-order derivatives and second-order derivatives respectively.

$$\mathbf{A}_x = l_i'(x_m) \quad (17)$$

$$\mathbf{B}_x = l_i''(x_m)$$

**Differential operator in time [3][4][5][6]**

If we fix it in space  $q$  and express the dependent variable  $u$  in space  $q$  with a polynomial with respect to time, we get Equation (18).

$$u^q = \sum_{j=1}^{N_t+1} b_j^q t^{j-1} \quad (18)$$

$u^q$  : The value of the dependent variable for the change in time when the spatial collocation  $q$  is fixed.

$b_j^q$  : Coefficients of the polynomial with respect to time when the spatial collocation  $q$  is fixed.

The first-order derivative of equation (19) with respect to  $t$  yields Equation (20).

$$\frac{\partial u^q}{\partial t} = \sum_{j=1}^{N_t+1} (j-1)t^{j-2} b_j^q \quad (20)$$

$u_i^q$  and first order derivative with respect to  $t$  at time collocation  $i$  are as follow equation.

$$u_i^q = \sum_{j=1}^{N_t+1} b_j^q t_i^{j-1}$$

$$\left. \frac{\partial u^q}{\partial t} \right|_i = \sum_{j=1}^{N_t+1} (j-1)t_i^{j-2} b_j^q \quad (21)$$

Representation by vector and matrix are as follow

$$\mathbf{u}^q = \mathbf{Q}\mathbf{b}^q \quad \mathbf{Q} = [t_i^{j-1}] \quad (22)$$

$$\left[ \frac{\partial u^q}{\partial t} \right] = \mathbf{D}\mathbf{b}^q \quad \mathbf{D} = [(j-1)t_i^{j-2}]$$

First order derivative with respect to  $t$  of  $u$  is as follow

$$\left[ \frac{\partial u^q}{\partial t} \right] = \mathbf{D}\mathbf{b}^q = \mathbf{D}\mathbf{Q}^{-1}\mathbf{u}^q = \mathbf{A}_t \mathbf{u}^q \quad (23)$$

it can be seen from the basic concept of partial derivatives that the differential operators (matrices) of the first order are derived when the space  $q$  is fixed by the same way of thinking as space, but this differential operator (matrix) with respect to time does not depend on the space  $q$ .

Since the differential operator (matrix) of time can be created using the same concept as the differential operator (matrix) of one-dimensional space, it can be obtained by differentiating the one-dimensional Lagrange interpolation formula with orthogonal collocations.

## Model and Formulation by Differential Operator

### Intermittent moving bed model of simulated moving bed chromate separation [1]

The intermittent moving bed model of the simulated moving bed chromatology is equivalent to the operational behavior of real plants and equipment. In simulation of the model, the position of the boundary conditions of R (raffinate), F (raw material: feed), E (extract), and D (eluent: dissolvent) is fixed, and each column is moved in the opposite direction of flow intermittently, simulating that the adsorbent (solid phase) flows in the opposite direction from the flow of the liquid phase.

### System of partial differential equations for advection, diffusion, two-component competitive adsorption and boundary condition equations for R, F, E, D

【chromatography (basic equation)】

Advection diffusion adsorption and desorption equation (dimensionless)

$$\frac{u_s}{u_n} \frac{\partial C_1}{\partial t} + \frac{1-\varepsilon}{\varepsilon} \frac{u_s}{u_n} \frac{\partial q_1}{\partial t} + \frac{\partial C_1}{\partial x} + \frac{1}{P_{en}} \frac{\partial^2 C_1}{\partial x^2} = 0$$

$$\frac{u_s}{u_n} \frac{\partial C_2}{\partial t} + \frac{1-\varepsilon}{\varepsilon} \frac{u_s}{u_n} \frac{\partial q_2}{\partial t} + \frac{\partial C_2}{\partial x} + \frac{1}{P_{en}} \frac{\partial^2 C_2}{\partial x^2} = 0$$

LDF approximation (dimensionless)

$$\frac{\partial q_1}{\partial t} = k_{d1} (q_1^* - q_1) \quad \frac{\partial q_2}{\partial t} = k_{d2} (q_2^* - q_1)$$

Expansion Langmuir eq. (competitive adsorption) (dimensionless)

$$q_1^* = \frac{Q_{sat1} B_1 C_1}{1 + B_1 C_1 + B_2 C_2} \quad q_2^* = \frac{Q_{sat2} B_2 C_2}{1 + B_1 C_1 + B_2 C_2}$$

【Boundary condition】 (dimensionless) Danckwerts boundary condition

① Boundary conditions at the column inlet at the raffinate (R) position.

$$C_{k(3nz+1)} \Big|_{x=0} - \frac{1}{P_{eI}} \left( \frac{\partial C}{\partial x} \right)_{k(3nz+1)} \Big|_{x=0} = \left( -\frac{u_{0R}}{u_{0I}} + \frac{u_{0II}}{u_{0I}} \right) C_{k(3nz)} \Big|_{x=1}$$

Boundary condition at outlet of before column

$$\left( \frac{\partial C}{\partial x} \right)_{k(3nz)} \Big|_{x=1} = 0$$

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- ② Boundary conditions at the column inlet at the position of the raw material feed port (F)

$$C_{k(2nz+1)} \Big|_{x=0} - \frac{1}{P_{eII}} \left( \frac{\partial C}{\partial x} \right)_{k(2nz+1)} \Big|_{x=0} = \frac{u_{0F}}{u_{0II}} C_{kF} + \frac{u_{0III}}{u_{0II}} C_{k(2nz)} \Big|_{x=1}$$

Boundary condition at outlet of before column

$$\left( \frac{\partial C}{\partial x} \right)_{k(2nz)} \Big|_{x=1} = 0$$

- ③ Boundary conditions at the column inlet at the extract (E) position

$$C_{k(nz+1)} \Big|_{x=0} - \frac{1}{P_{eIII}} \left( \frac{\partial C}{\partial x} \right)_{k(nz+1)} \Big|_{x=0} = \left( -\frac{u_{0E}}{u_{0III}} + \frac{u_{0IV}}{u_{0III}} \right) C_{k(nz)} \Big|_{x=1}$$

Boundary condition at outlet of before column

$$\left( \frac{\partial C}{\partial x} \right)_{k(nz)} \Big|_{x=1} = 0$$

- ④ Boundary conditions at the column inlet at the position of the dissolvent supply port (D)

$$C_{k(1)} \Big|_{x=0} - \frac{1}{P_{eIV}} \left( \frac{\partial C}{\partial x} \right)_{k(1)} \Big|_{x=0} = \frac{u_{0I}}{u_{0IV}} C_{k(4nz)} \Big|_{x=1} + \frac{u_{0D}}{u_{0IV}} C_{kD}$$

Boundary condition at outlet of before column

$$\left( \frac{\partial C}{\partial x} \right)_{k(4nz)} \Big|_{x=1} = 0$$

- ⑤ Boundary conditions at the inlet and outlet of columns other than R, F, E, and D

$$C_{k(m)} \Big|_{x=0} - \frac{1}{P_{en}} \left( \frac{\partial C}{\partial x} \right)_{k(m)} \Big|_{x=0} = C_{k(m-1)} \Big|_{x=1}$$

Boundary condition at outlet of before column

$$\left( \frac{\partial C}{\partial x} \right)_{k(m-1)} \Big|_{x=1} = 0$$

where,

- $C_k$  : dimensionless concentration of  $k$  component  
 $C_{k(m)}$  : dimensionless concentration of  $k$  component at  $m$  column  
 $C_{kF}$  : dimensionless feed concentration of  $k$  component  
 $C_{kD}$  : dimensionless desorbent concentration of  $k$  component  
 $q_k$  : dimensionless adsorbed concentration of  $k$  component  
 $q_k^*$  : dimensionless adsorption equilibrium concentration of  $k$  component  
 $t$  : dimensionless time  
 $x$  : dimensionless distance  
 $\varepsilon$  : porosity  
 $P_{en}$  : Pecre number of  $n$  zone  
 $k_{dk}$  : dimensionless overall mass transfer capacity coefficient of  $k$  component  
 $Q_{satk}, B_k$  : dimensionless parameter of Langmuir adsorption equilibrium eq. of  $k$  component  
 $u_n$  : velocity in  $n$  zone  
 $u_s$  : simulated fixed-phase movement speed  
 $u_{0R}$  : velocity in empty column at raffinate(outlet of A component)  
 $u_{0E}$  : velocity in empty column at extract(outlet of B component)  
 $u_{0F}$  : velocity in empty column at feed(inlet mixed substrate)  
 $u_{0D}$  : velocity in empty column at desorbent(dilute liquid)  
 $u_{0n}$  : velocity in empty column in  $n$  zone  
 $nz$  : column number in zone( $nz = 2$ )

### Formulation by Differential operator in time and space of OCFEM Competitive adsorption - advection diffusion model

Advection diffusion adsorption desorption Eq. in  $m$  column :

$$\frac{u_s}{u_n} \mathbf{A}_{tis} \mathbf{C}_{1(m)qs}^{kl} + \frac{1-\varepsilon}{\varepsilon} \frac{u_s}{u_n} \mathbf{A}_{tis} q_{1(m)qs}^{kl} + \mathbf{A}_{xqp} \mathbf{C}_{1(m)pi}^{kl} - \frac{1}{P_{en}} \mathbf{B}_{xqp} \mathbf{C}_{1(m)pi}^{kl} = 0$$

$$\frac{u_s}{u_n} \mathbf{A}_{tis} \mathbf{C}_{2(m)qs}^{kl} + \frac{1-\varepsilon}{\varepsilon} \frac{u_s}{u_n} \mathbf{A}_{tis} q_{2(m)qs}^{kl} + \mathbf{A}_{xqp} \mathbf{C}_{2(m)pi}^{kl} - \frac{1}{P_{en}} \mathbf{B}_{xqp} \mathbf{C}_{2(m)pi}^{kl} = 0$$

LDF approximation - Expansion Langmuir Eq. (Competitive adsorption model) :

$$\mathbf{A}_{tis} \mathbf{q}_{1(m)qs}^{kl} - k_{d1} \left[ Q_{sat1} \frac{B_1 \mathbf{C}_{1(m)qi}^{kl}}{1 + B_1 \mathbf{C}_{1(m)qi}^{kl} + B_2 \mathbf{C}_{2(m)qi}^{kl}} - \mathbf{q}_{1(m)qi}^{kl} \right] = 0$$

$$\mathbf{A}_{tis} \mathbf{q}_{2(m)qs}^{kl} - k_{d2} \left[ Q_{sat2} \frac{B_2 \mathbf{C}_{2(m)qi}^{kl}}{1 + B_1 \mathbf{C}_{1(m)qi}^{kl} + B_2 \mathbf{C}_{2(m)qi}^{kl}} - \mathbf{q}_{2(m)qi}^{kl} \right] = 0$$

element boundary condition :



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$$\mathbf{A}_{xrp} \mathbf{C}_{1(m)pi}^{kl} - \mathbf{A}_{xhp} \mathbf{C}_{1(m)pi}^{(k+1)l} = 0$$

$$\mathbf{A}_{xrp} \mathbf{C}_{2(m)pi}^{kl} - \mathbf{A}_{xhp} \mathbf{C}_{2(m)pi}^{(k+1)l} = 0$$

$$\mathbf{A}_{xrp} \mathbf{q}_{1(m)pi}^{kl} - \mathbf{A}_{xhp} \mathbf{q}_{1(m)pi}^{(k+1)l} = 0$$

$$\mathbf{A}_{xrp} \mathbf{q}_{2(m)pi}^{kl} - \mathbf{A}_{xhp} \mathbf{q}_{2(m)pi}^{(k+1)l} = 0$$

Boundary condition at R,F,E,D :

- ① Boundary conditions at the column inlet at raffinate (R) position

$$\mathbf{C}_{k(3nz+1)li}^{ll} - \frac{1}{P_{eI}} \mathbf{A}_{x1p} \mathbf{C}_{k(3nz+1)pi}^{ll} = \left( -\frac{u_{0R}}{u_{0I}} + \frac{u_{0II}}{u_{0I}} \right) \mathbf{C}_{k(3nz)2i}^{KI}$$

Boundary condition at outlet of before column

$$\mathbf{A}_{x2p} \mathbf{C}_{k(3nz)pi}^{KI} = 0$$

- ② boundary condition at column inlet in feed inlet (F) position

$$\mathbf{C}_{k(2nz+1)li}^{ll} - \frac{1}{P_{eII}} \mathbf{A}_{x1p} \mathbf{C}_{k(2nz+1)pi}^{ll} = \frac{u_{0F}}{u_{0II}} \mathbf{C}_{kF} + \frac{u_{0III}}{u_{0II}} \mathbf{C}_{k(2nz)2i}^{KI}$$

Boundary condition at outlet of before column

$$\mathbf{A}_{x2p} \mathbf{C}_{k(2nz)pi}^{KI} = 0$$

- ③ Boundary condition at column inlet in extracts(E) position

$$\mathbf{C}_{k(nz+1)li}^{ll} - \frac{1}{P_{eIII}} \mathbf{A}_{x1p} \mathbf{C}_{k(nz+1)pi}^{ll} = \left( -\frac{u_{0E}}{u_{0III}} + \frac{u_{0IV}}{u_{0III}} \right) \mathbf{C}_{k(nz)2i}^{KI}$$

Boundary condition at outlet of before column

$$\mathbf{A}_{x2p} \mathbf{C}_{k(nz)pi}^{KI} = 0$$

- ④ boundary condition at column inlet in dissolvent inlet position

$$\mathbf{C}_{k(1)li}^{ll} - \frac{1}{P_{eI}} \mathbf{A}_{x1p} \mathbf{C}_{k(1)pi}^{ll} = \frac{u_{0I}}{u_{0IV}} \mathbf{C}_{k(4nz)2i}^{KI} + \frac{u_{0D}}{u_{0IV}} \mathbf{C}_{kD}$$

Boundary condition at outlet of before column

$$\mathbf{A}_{x2p} \mathbf{C}_{k(4nz)pi}^{KI} = 0$$

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where,

- $\mathbf{C}_{k(m)qs}^{kl}$  : qs vector of concentration  $\mathbf{C}$  of k component in m column of space internal collocation q, time collocation s, in space element k, time element l
- $\mathbf{C}_{k(m)pi}^{kl}$  : pi vector of concentration  $\mathbf{C}$  of k component in m column of space collocation p, time collocation i, in space element k, time element l
- $\mathbf{q}_{k(m)qs}^{kl}$  : qs vector of adsorption concentration  $\mathbf{q}$  of k component in m column of space internal collocation q, time collocation s, in space element k, time element l
- $\mathbf{q}_{k(m)pi}^{kl}$  : pi vector of adsorption concentration  $\mathbf{q}$  of k component in m column of space collocation p, time collocation i, in space element k, time element l
- $\mathbf{A}_{ts}$  : time differential operator (matrix) of i row s column of time collocation
- $\mathbf{A}_{xqp}$  : one order differential operator in space, space internal collocation q row, space collocation p column
- $\mathbf{B}_{xqp}$  : two order differential operator in space, space internal collocation q row, space collocation p column
- $\mathbf{A}_{xrp}$  : one order differential operator in space, space external collocation r row, space collocation p column
- $K$  : space element at outlet of column

Note that the local numbering of the space is 1 for the entrance and 2 for the exit, and the internal collocations are 3~2+NA, and na is the number of internal collocations in the element. In the calculation procedure, each column is formulated with OCFEM, connected using the boundary conditions of the raffinate, raw material feed, extract, and dissolvent inlet, the result of the time component is solved by the overall matrix, and the time change of the concentration in the entire column is calculated by updating the matrix of the time component (time increment).

## Results and Discussion

### Calculate condition

Table 1 and Table 2 show the calculate conditions and various parameters of numerical calculations by OCFEM of the intermittent moving bed model, respectively. One column is divided into 10 elements, and the number of internal points in the element is 6. Referring to the accuracy of the batch chromatographic separation of Okubo and Takamura et al. [6], it is shown that when the number of elements in one column is 10 and the number of internal points in the element is 6, accuracy of results is sufficient (3~4 significant digits) in engineering.  $\Gamma(\text{II})$  (synonymous with GMII) is the slope of the operating line in relation to the flow velocity in zone II. The diffusion coefficient  $D_f$  was calculated at 3.1 cm<sup>2</sup>/min, but this value is assumed to be on the same order as the Pecre number of the batch chromatography, and it is necessary to measure it experimentally as it is diffusion coefficient depends on the diameter of the adsorbed particles, the flow velocity in the column, and the temperature.

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Fig. 2 shows columns in the number of columns 2 in the zone.

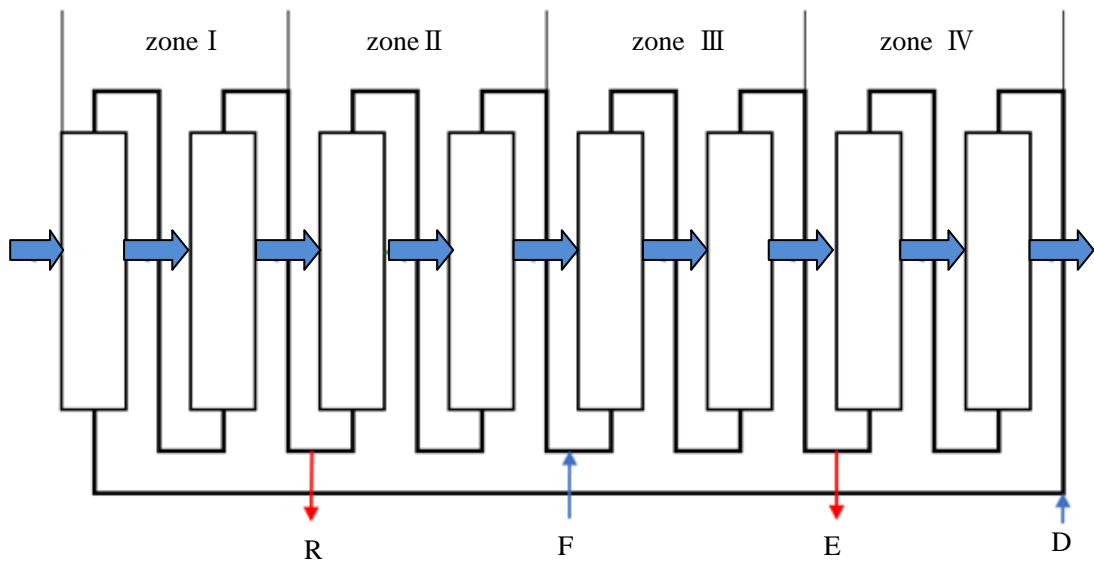
It shows the relationship between the direction of movement (in numerical calculations) and the outlet (raffinate extract) and the supply port (dissolvent feed).

Table-1 Calculate condition

Total column number	Elements number in a column	Internal collocations	$\Gamma(\text{II}); \text{GM}(\text{II})$
8	10	6	1.00
8	10	6	1.05
8	10	6	1.10

Table-2 Parameter

Component	$Q_{\text{sat}}$ (dimensionless)	B(dimensionless)	$D_f$ ( $\text{cm}^2/\text{min}$ )
1(A)	1.429	1.4335	3.1
2(B)	1.25	0.647	3.1



↓ Outlet (Raffinate (A component: strong adsorption), Extract (B Component: weak adsorption))

↑ supply inlet (Feed, Dissolvent)

➡ moving direction of column

Fig-2 Relationship of column and column moving direction, and outlet • inlet

**Yield and purity in raffinate and extract**

Tables 3 and 4 show the yield and purity of raffinates and extracts in 50,100 cycles. As shown in Table 5, the number of cycle and the total yield of raffinate and extract in the case of GMII.1.05 is 98.2121% in 50 cycles, which is not close to 100%, but 99.9978% in 100 cycles, and 100.000% in 200 cycles, approaching 100%. In the case of GMII.1.05, the periodic vibration cycle of raffinates and extracts up to 100 cycles is shown in Fig. 3 ~ Fig. 4. It can be seen that the periodic cycle oscillation of the raffinate in the case of GMII.1.05 cannot be said to be periodic steady at the number of cycles 50. Under these conditions, it can be seen that the number of periodic cycles should be at least 100.

Table-3 Yield and purity of component A, B in raffinate and extract at cycle 50

zcolu	GMII	Component	Concentration		Yield		Purity	
			R	E	R	E	R	E
2	1.00	A	0.000763	0.101372	0.269432%	99.582728%	0.27 %	99.57 %
		B	0.282216	0.000443	99.605520%	0.434917%	99.73 %	0.43 %
	1.05	A	0.040395	0.113659	11.934847%	86.277250%	10.63 %	99.80 %
		B	0.339771	0.000227	100.386909%	0.172603%	89.37 %	0.20 %
	1.10	A	0.114021	0.113872	29.560973%	70.431904%	22.84 %	99.78 %
		B	0.385135	0.000246	99.850146%	0.152314%	77.16 %	0.22 %

Table 4 Yield and purity of component A, B in raffinate and extract at cycle 100

zcolu	GMII	Component	Concentration		Yield		Purity	
			R	E	R	E	R	E
2	1.00	A	0.000766	0.101521	0.270185%	99.729317%	0.27 %	99.57 %
		B	0.282110	0.000440	99.568090%	0.431958%	99.73 %	0.43 %
	1.05	A	0.046175	0.113761	13.642555%	86.355264%	12.02 %	99.80 %
		B	0.337884	0.000226	99.829383%	0.171328%	87.98 %	0.20 %
	1.10	A	0.114044	0.113874	29.567071%	70.433214%	22.85 %	99.78 %
		B	0.385127	0.000246	99.847932%	0.152296%	77.15 %	0.22 %

Table-5 Total yield at 50, 100, 200 cycle and Purity at 200 cycle

zcolu	GM II	Component	Total yield			Purity(200cycle)	
			50cycle	100cycle	200cycle	R	E
2	1.00	A	99.8522%	99.9995%	99.9995%	0.27%	99.57%
		B	100.0404%	100.0000%	99.9999%	99.73%	0.43%
	1.05	A	98.2121%	99.9978%	100.0000%	12.02%	99.80%
		B	100.5595%	100.0007%	100.0000%	87.98%	0.20%
	1.10	A	99.9929%	100.0003%	100.0003%	22.85%	99.78%
		B	100.0025%	100.0002%	100.0002%	77.15%	0.22%

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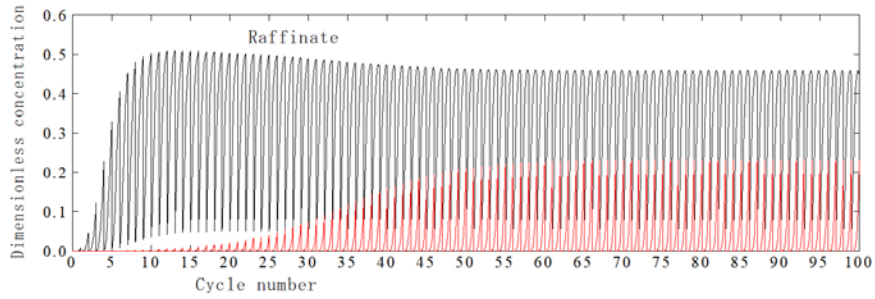


Fig-3 Cyclic vibration in Raffinate of GM II 1.05

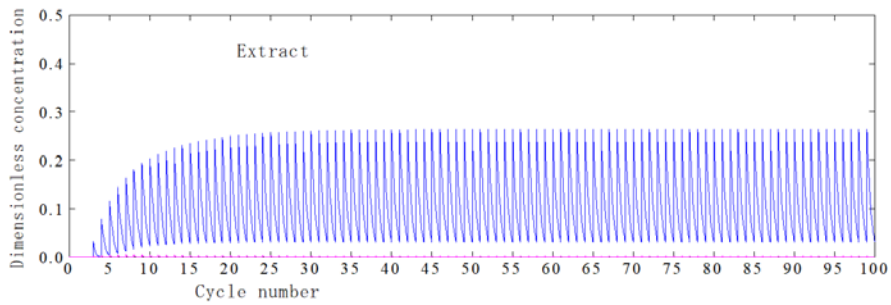


Fig-4 Cyclic vibration in Extract of GM II 1.05

**Time-averaged dimensionless concentration distribution of components A and B across the column**

Fig-5 shows the time-averaged dimensionless concentration distribution of components A and B in the periodic steady state (number of cycles 200) at each GMII (1.00, 1.05, 1.10). From the purity of Table 5, it can be said that the operating conditions of GMII.1.00 are good.

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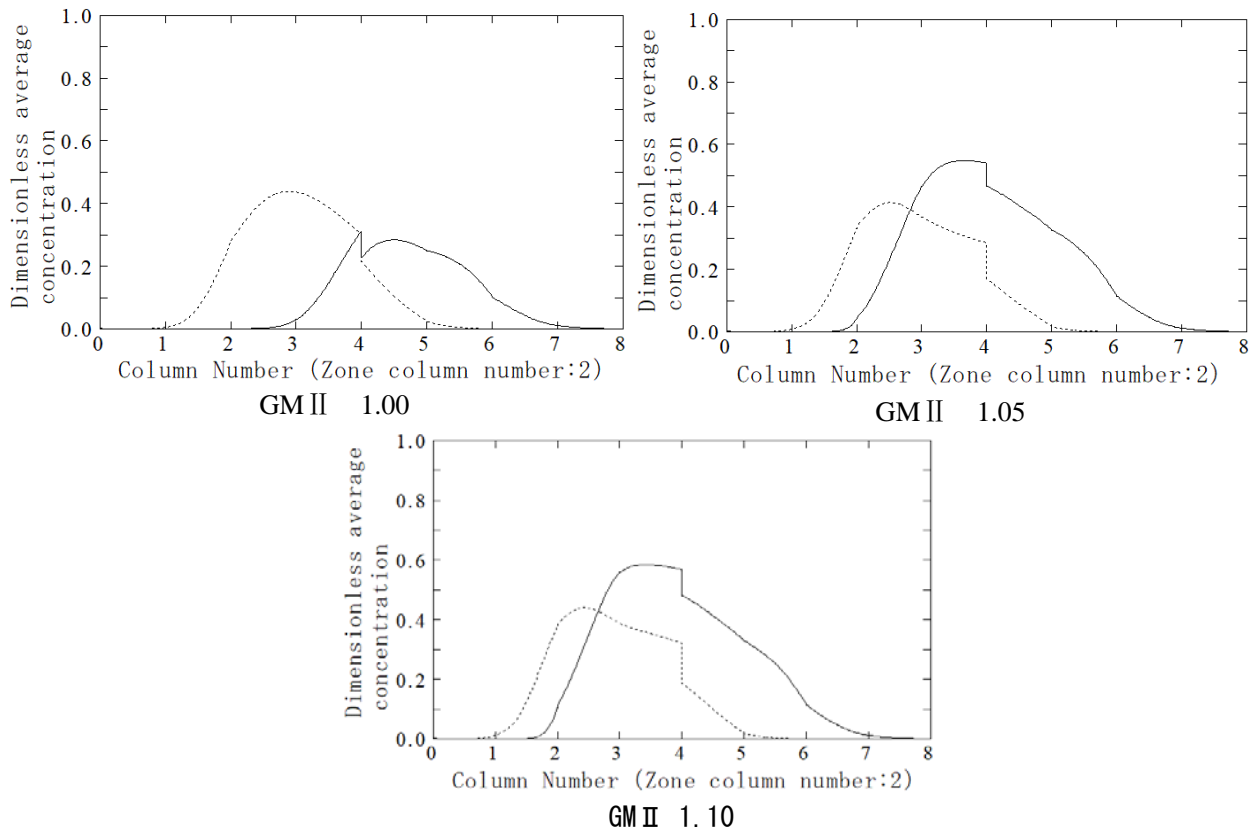


Fig-5 Distribution of time average dimensionless concentration of component A, B

**Balance distribution of components A and B of each column in the periodic state and total balance of all columns**

The total balance of all columns is the sum of the periodic steady-state steps (one cycle) of each column. The mass balance of each step (1 cycle) is (the amounts of components in the column at the end of the step) - (the amounts of components in the column at the beginning of the step). The amounts of components in the column at the end step are integrated over the length of one column. (Total amount in liquid and amount adsorbed) The amounts of components in the column at the start step is integrated in the same way. The total balance is the sum of all columns of the mass balance calculated for each column.

Fig. 6 ~ 7 show the balance distribution of components A and B of each column in the 50 and 100 periodic states, and the numerical value of the total balance of all columns. Table-6 summarizes the total balance for 50, 100, and 200 cycles. In Fig. 6, Fig. 7, and Table 6, the total balance is on the order of

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$10^{-4} \sim 10^{-5}$  when the periodic cycle (ncyc) is 50, and the total yield of the A component of raffinate extract is 98.2121% in GM(

II-1.05 and the case of GMII.1.05

yield of the A component of raffinate and extract is 99.9978%, indicating that ncyc=100 is sufficient. In the case of the operating conditions 1.00 for GMII in Table 6, the total balance was on the order of  $10^{-5} \sim 10^{-6}$  with ncyc=50, and in the case of GM

II-1.10, total balance was

ncyc=50. As shown in Tables 5 and 6, if the total balance is on the order of  $10^{-6}$  or less, the total yield is close to 100%, and it is considered sufficient.

From the above, it was shown that if the total balance of all columns is on the order of  $10^{-6} \sim 10^{-7}$  or less, the total yield of R and E will be close to 100%. Although it depends on other conditions, it was found that it is good to repeat calculations until the periodic cycle ncyc = 100.

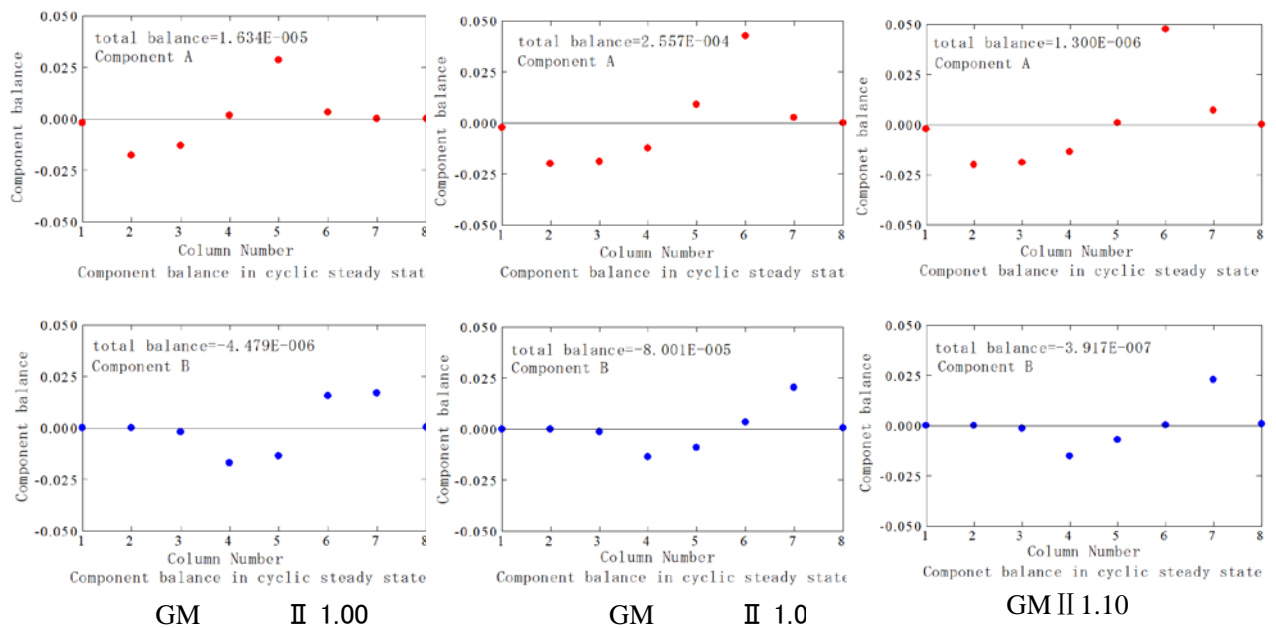


Fig-6 Balance distribution of each column and Total balance at cycle 50

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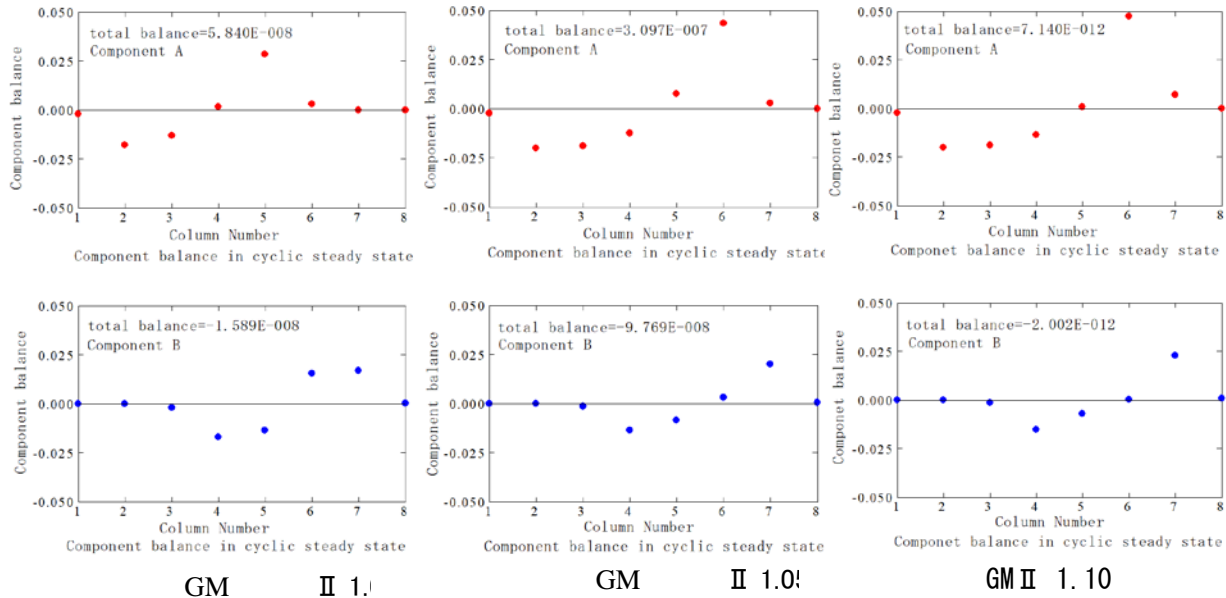


Fig-7 Balance distribution of each column and Total balance at cycle 100

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Table-6 Total balance at each cycle

	component	Total balance		
		50cycle	100cycle	200cycle
GM II 1.00	A	1.634E-05	5.840E-08	7.621E-13
	B	-4.479E-06	-1.589E-08	-2.073E-13
GM II 1.05	A	2.557E-04	3.097E-07	3.669E-13
	B	-8.001E-05	-9.769E-08	-1.147E-13
GM II 1.10	A	1.300E-06	7.140E-12	9.489E-16
	B	-3.917E-07	-2.002E-12	-1.388E-16

## Conclusions

For the design of simulated moving bed chromatography, we programmed an intermittent moving bed model by OCFEM (orthogonal collocation finite element method). The reliability of the program depends on the reliability of the numerical computation method used in the computational program and the reliability of the intermittent moving layer model of the two-component competition.

In this paper, we discuss the accuracy problems of OCFEM, which is a numerical computation method. The reason why the total yield of raffinate and extract was 98.2121% at cycle 50 and not 100% when the



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operating condition GMII was 1.05 was that it was not accurate to the periodic steady state at cycle 50. It was shown that when the number of cycles was 100 the total yield of the raffinate and extract was almost 100%. From the above, it was concluded that the orthogonal collocation finite element method can perform calculations with high accuracy.

## Acknowledgement

In writing this paper, I would like to express my gratitude to Dr. Kazuo Okada of Organo Co., Ltd. for his various opinions.

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