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REDUCED-ORDER DISTILLATION MODEL USING COLLOCATION METHOD WITH CUBIC SPLINES

Sang Yeol CHOI, Heung Shik KIM, Kwang Soon LEE*, Ki Pung YOO and Won Hong LEE

Department of Chemical Engineering, Sogang University,
C. P. O. Box 1142, Seoul, Korea
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Abstract—A simple and compact form of reduced-order distillation model especially suitable for real-time applications is proposed. For this purpose, a modular collocation approach with the cubic spline interpolation function is developed and applied to an underlying distillation model which is constructed based on the McCabe and Thiele assumptions plus constant tray holdups.

To evaluate the performance of the model, numerical simulations are carried out for the case of dynamics as well as steady states. As a consequence, it is found that the proposed reduced-order model gives better approximation than those obtained by the conventional reduced-order model with the Lagrange interpolation function.

INTRODUCTION

Although various novel separation techniques have drawn much attention in recent years, conventional separation processes such as distillation still retain very important position in chemical and petrochemical industries. Distillation, however, inevitably consumes large extra amount of energy and also has been known as a nontrivial process to control due to significant interactions in it. For these reasons, distillation has been considered as one of the major challenges for advanced control and on-line optimization in chemical engineering.

For successful implementation of advanced control and on-line optimization, it need scarcely be said that the most important step is to have a well-tuned distillation model in a manageable form. In this respect, various reduced-order modeling techniques have been proposed for distillation process. Some of them are modal analysis [1], compartmental modeling [2, 3], and others [4]. In most of the works, however, attentions have been placed only on obtaining perturbed dynamic models, aiming at the design of control system, where the knowledge of steady-state conditions are presumed. Unfortunately, these models are of no help in on-line distillation optimization. Toward versatile implementations to dynamic as well as steady-state, Cho and Joseph [5, 6] proposed a different type of reduced-order model for multistage separation processes utilizing the concept of collocation. They also extended the idea of collocation to reduced-order modeling of distillation processes in their later work [7]. The method by collocation has been further refined by Stewart et al. [8] and thereafter used in distillation optimization by Swartz and Stewart [9]. The original idea of Cho and Joseph, however, when directly applied to distillation processes, may give rise to serious modeling error near the feed stage. It is because they tried to use a single polynomial, which is smooth in nature, to approximate an entire profile of a distillation variable, while the profiles are usually supposed to change largely at the feed stage as one might experience in distillation studies. Recently, Kim et al. [10] have conducted separate collocations for rectifying and stripping sections, respectively, and named it as MPA (Modular Polynomial Approximation). By utilizing the MPA, they could neatly solve the troubles in Cho and Joseph's work and could get better results without increasing model complexity.

As an extension of the MPA, a new reduced-order distillation model based on collocation with the cubic splines instead of the Lagrange interpolation function is proposed in this work. In the modeling process, a simplified dynamic distillation model based on the McCabe and Thiele assumptions [11] is setup first. The proposed model is parameterized by the relative volatilities and the liquid-phase holdups, which govern the mixture separability and column dynamics, re-

*To whom correspondence should be addressed.

spectively, for posterior tuning. Performance of the proposed model is evaluated by comparing with that of the original MPA through numerical simulations.

FORMULATION OF THE UNDERLYING DISTILLATION MODEL

Rigorous description of distillation dynamics usually requires a large number of nonlinear differential equations together with complicated and tedious vapor-liquid equilibrium relationships. Even then, prediction by such a rigorous model very often deviates from real behaviors, mostly due to inevitable ambiguity of the parameters such as tray efficiencies, amount of internal reflux, heat loss to environment and so forth. Adjustment of such parameters using field data, therefore, becomes a necessary step to make the model a practical process simulator. As the other extreme, the pure empirical ones such as transfer function or ARMAX(Auto Regressive Moving Average with eXogenous inputs) models are mathematically simple but valid only for a limited region about certain operating conditions.

Considering the both aspects of the above two extremes, one of the plausible approaches is to use a simplified physical model with appropriately chosen tuning parameters for posterior correction. For binary distillation columns where nonideality is not so excessive, we can assume constant liquid and vapor phase molar flow rates for each of the rectifying and stripping sections without serious deterioration of the model [11]. In this case, the relative volatilities instead of detailed thermodynamic relationships can be used as reasonable expressions for vapor-liquid equilibria. These assumptions significantly simplify the model description. Since the relative volatilities play a key role in determining the degree of separation, deviation from the rigorous model can be moderated to a large extent if we take relative volatilities as tuning parameters and adjust them properly. The dynamic part of a distillation model can be simplified if we take only the mixing dynamics into account while leaving the liquid holdup as another tunable constant. This simplification can be justified since the hydraulic dynamics in a tray is usually faster than the mixing dynamics.

Based on the above reasonings, we assume the followings in the underlying distillation model.

1. The column separates a binary mixture and has a total condenser.

2. In each of the rectifying and stripping sections of the column, liquid and vapor flow rates are constant.

3. Phase equilibria are expressed by relative volatilities, α_r and α_s for the rectifying and stripping sections, respectively.

4. Liquid holdup in each tray is constant and has H_r and H_s in the rectifying and stripping sections, respectively.

5. Liquid holdups in the condenser and the reboiler are perfectly regulated, and have constant values, H_c and H_b, respectively.

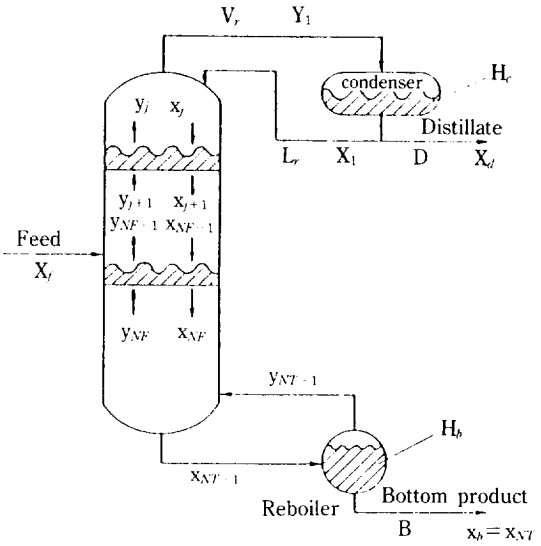

Fig. 1. Schematic diagram of a binary distillation column.

Figure 1 shows the simplified distillation column with the above assumptions. Using the notations shown in Fig. 1, the dynamic model of the column can be described by the following equations.

For the condenser

$$H_c dx_1/dt = V_r(y_1 - x_1). \tag{1}$$

For each tray

$$H_m dx_j/dt = V_m(y_j - y_{j-1}) + L_m(x_{j-1} - x_j) + qF_1x_f + (1-q)F_2x_f$$
$$j = 2, 3, \cdots, NT-1 \tag{2}$$

where

$$F_1 = \begin{cases} F & \text{for } j = NF \\ 0 & \text{otherwise} \end{cases}$$

$$F_2 = \begin{cases} F & \text{for } j = NF-1 \\ 0 & \text{otherwise.} \end{cases}$$

For the reboiler

$$H_b dx_{NT}/dt = L_s x_{NT-1} - V_s y_{NT-1} - Bx_{NT}. \tag{3}$$

Vapor-liquid equilibria

$$y_j=\alpha_m x_{j+1}/[1+(\alpha_m-1)x_{j+1}],\ j=1,\ 2,\ \cdots,\ NT-1 \quad (4)$$

where m = r for the rectifying section, s for the stripping section

and

$$L_s=L_r+qF \quad (5)$$

$$V_s=V_r-(1-q)F. \quad (6)$$

REDUCED-ORDER MODELING BY COLLOCATION METHOD

Although the distillation model expressed in Eqs. (1) to (6) is a simplified one, it has a large dimensionality equal to the total number of plates including the condenser and reboiler. To reduce the order of the model, the MPA concept by Kim et al. [10] is adopted, where independent collocation is performed for each of the rectifying and stripping sections while preserving the mass balance between the two sections. One more refinement performed in this work is the introduction of the cubic spline as a trial function which is smoother and more flexible than the Lagrange interpolation function. It is motivated by the fact that the concentration profiles in a column are usually very smooth irrespective of the number of plates. Although the polynomials are also smooth in nature, the degree should be at least cubic to represent various conceivable shapes of concentration profiles.

In Fig. 2, the coordinates and notations used in the reduced-order modeling by the MPA are depicted. For each section of the column a continuous spatial coordinate, $z \in [0, 1]$ is assigned, and all the variables are assumed to be continuous in z instead of discretized ones. Since these variables should obey the mass balances at any spatial point z, the Eqs. (1) to (4) should be rewritten at some preassigned collocation points. To make the order of the resulting model as low as possible, in this work, the reboiler is treated as one of the stripping stages. Unlike ordinary stages, however, the reboiler has no inflow from below, resulting in a different mass balance equation rendering the collocation difficult to be applied. To overcome this difficulty, bottom product flow is considered to be split into two streams, of which the flow rates are V_s (inflow) and L_s (outflow), respectively, around the flow splitter, as shown in Fig. 2. Consequently, the mass balance equation of the reboiler becomes the same as that of the stripping stages except that H_b is used instead of H_s.

Now, the model equations rewritten at the collocation points are as follows:

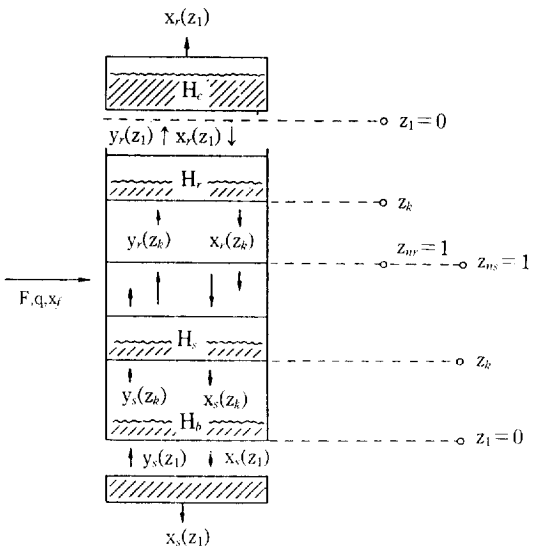

Fig. 2. Distillation column for reduced-order modeling.

For the condenser

$$H_c dx_r(z_1)/dt=V_r[y_r(z_1)-x_r(z_1)]. \quad (7)$$

For the collocation point z_k in the rectifying section

$$H_r dx_r(z_k)/dt=V_r[y_r(z_k)-y_r(z_k-\Delta z_r)]-L_r[x_r(z_k)-x_r(z_k-\Delta z_r)],\ k=2,\ 3,\ \cdots,\ nr. \quad (8)$$

For the collocation point z_k in the stripping section

$$H_s dx_s(z_k)/dt=V_s[y_s(z_k)-y_s(z_k+\Delta z_s)]-L_s[x_s(z_k)-x_s(z_k+\Delta z_s)],\ k=1,\ 2,\ \cdots,\ ns-1 \quad (9)$$

when $k=1$, $H_s=H_b$.

Equilibrium relationships

$$y_r(z_k-\Delta z_r)=\alpha_r x_r(z_k)/[1+(\alpha_r-1)x_r(z_k)],\quad k=2,\ 3,\ \cdots,\ nr \quad (10)$$

$$y_s(z_k)=\alpha_s x_s(z_k-\Delta z_s)/[1+(\alpha_s-1)x_s(z_k-\Delta z_s)],\quad k=2,\ 3,\ \cdots,\ ns. \quad (11)$$

In the above equations, Δz denotes the stage height in the z coordinate, which is equal to $1/(NF-2)$ for the rectifying and $1/(NT-NF+1)$ for the stripping sections, respectively.

The boundary conditions for Eqs. (7) to (9) are as follows:

At z_1 in the stripping section

$$y_s(z_1)=x_s(z_1). \quad (12)$$

At the feed stage

$$L_s x_s(z_{ns}) = L_r x_r(z_{nr}) + qFx_f \tag{13}$$

$$V_s y_s(z_{ns}) = V_r y_r(z_{nr}) - (1-q)Fx_f. \tag{14}$$

Now an interpolation function $S_j(z)$ is introduced such that

$$x(z) = \sum_{j=1}^{n} S_j(z)x(z_j) \tag{15}$$

and $x(z_k-\Delta z)$ and $x(z_k+\Delta z)$ approximated as

$$x(z_k-\Delta z) = \sum_{j=1}^{n} S_j(z_k-\Delta z)x(z_j),$$

$$x(z_k+\Delta z) = \sum_{j=1}^{n} S_j(z_k+\Delta z)x(z_j). \tag{16}$$

Similarly, $y(z_k-\Delta z)$ and $y(z_k+\Delta z)$ can be approximated using the interpolation function. To simplify the notations, the followings are defined.

$$a_i(z) = S_i(z-\Delta z)$$

$$b_i(z) = S_i(z+\Delta z)$$

$$c_i(z) = S_i(z) - S_i(z-\Delta z)$$

$$d_i(z) = S_i(z) - S_i(z+\Delta z). \tag{17}$$

Then Eqs. (8) and (9) can be rearranged as follows: At z_k in the rectifying section,

$$H_r \frac{dx_r(z_k)}{dt} = \sum_{j=1}^{nr} c_j(z_k)[V_r y_r(z_j) - L_r x_r(z_j)],$$

$$k = 2, \cdots, nr. \tag{18}$$

At z_k in the stripping section,

$$H_s \frac{dx_s(z_k)}{dt} = \sum_{j=1}^{ns} d_j(z_k)[V_s y_s(z_j) - L_s x_s(z_j)],$$

$$k = 1, \cdots, ns-1 \tag{19}$$

$H_s = H_b$ when $k = 1$.

Substituting the boundary conditions (12) through (14) into Eqs. (7), (18) and (19) and then rearranging the resulting equations yield the following vector differential equastions.

$$d\mathbf{x}/dt = -\mathbf{K}_1\mathbf{x} + \mathbf{K}_2\mathbf{y} - \mathbf{f}_1 x_f \tag{20}$$

where

$$\mathbf{K}_1 = \begin{bmatrix} V_r/H_r & 0 & \cdots & 0 & & & \\ \frac{L_r}{H_r}\begin{bmatrix} c_1(z_2) & \cdots & c_{nr}(z_2) \\ \vdots & & \vdots \\ c_1(z_{nr}) & \cdots & c_{nr}(z_{nr}) \end{bmatrix} & & & & \mathbf{0} & \\ & \frac{L_r}{H_s} d_{ns}(z_{ns-1}) & & \frac{L_s}{H_s}\begin{bmatrix} d_{ns-1}(z_{ns-1}) & \cdots & \left(1-\frac{V_s}{L_s}\right)d_1(z_{ns-1}) \\ d_{ns-1}(z_2) & \cdots & \left(1-\frac{V_s}{L_s}\right)d_1(z_2) \end{bmatrix} \\ \mathbf{0} & \frac{L_r}{H_s} d_{ns}(z_2) & & & \\ & \frac{L_r}{H_r} d_{ns}(z_1) & & \frac{L_s}{H_b}\begin{bmatrix} d_{ns-1}(z_1) & \cdots & \left(1-\frac{V_s}{L_s}\right)d_1(z_1) \end{bmatrix} \end{bmatrix}$$

$$(nr+ns-1)\times(nr+ns-1)$$

$$\mathbf{K}_2 = \begin{bmatrix} \begin{bmatrix} H_r/H_r & 0 & \cdots & 0 \\ c_1(z_2) & & \cdots & c_{nr}(z_2) \\ c_1(z_{nr}) & & \cdots & c_{nr}(z_{nr}) \end{bmatrix} & & & \mathbf{0} \\ \frac{V_r}{H_r} & & & \\ & \frac{V_r}{H_s} d_{ns}(z_{ns-1}) & & \frac{V_s}{H_s}\begin{bmatrix} d_{ns-1}(z_{ns-1}) & \cdots & d_2(z_{ns-1}) \\ d_{ns-1}(z_2) & \cdots & d_2(z_2) \end{bmatrix} \\ \mathbf{0} & \frac{V_r}{H_s} d_{ns}(z_2) & & \\ & \frac{V_r}{H_r} d_{ns}(z_1) & & \frac{V_s}{H_b}\begin{bmatrix} d_{ns-1}(z_1) & \cdots & d_2(z_1) \end{bmatrix} \end{bmatrix}$$

$$(nr+ns-1)\times(nr+ns-2)$$

$$\mathbf{x}=[x_r(z_1)\cdots x_r(z_{nr})\ \ x_s(z_{ns-1})\cdots x_s(z_1)]^T,\quad (nr+ns-1)\times 1$$
$$\mathbf{y}=[y_r(z_1)\cdots y_r(z_{nr})\ \ y_s(z_{ns-1})\cdots y_s(z_2)]^T,\quad (nr+ns-2)\times 1$$
$$\mathbf{f}_1=[0\ \cdots\ 0\quad \frac{F}{H_s}d_{ns}(z_{ns-1})\cdots\quad \frac{F}{H_b}d_{ns}(z_1)]^T,\quad (nr+ns-1)\times 1. \tag{21}$$

Similarly, the equilibrium relationships expressed by Eqs. (10) and (11) are rearranged using the interpolation functions as follows:

$$\mathbf{Ey}=\mathbf{g}+\mathbf{f}_2x_f \tag{22}$$

where

$$\mathbf{E}=\begin{bmatrix} a_1(z_2)\cdots a_{nr}(z_2) & \\ \vdots\quad\ \vdots & \mathbf{0} \\ a_1(z_{nr})\cdots a_{nr}(z_{nr}) & \\ 0\cdots 0\ \ V_r/V_s & \\ \mathbf{0} & \mathbf{I} \end{bmatrix}$$
$$(nr+ns-2)\times(nr+ns-2)$$

$$\mathbf{g}=[\frac{\alpha_r x_r(z_2)}{1+(\alpha_r-1)x_r(z_2)}\cdots\frac{\alpha_r x_r(z_{nr})}{1+(\alpha_r-1)x_r(z_{nr})},$$
$$\frac{\alpha_s x_s(z_{ns}-\Delta z_s)}{1+(\alpha_s-1)x_s(z_{ns}-\Delta z_s)}\cdots\frac{\alpha_s x_s(z_2-\Delta z_s)}{1+(\alpha_s-1)x_s(z_2-\Delta z_s)}]^T$$
$$(nr+ns-2)\times 1$$

$$\mathbf{f}_2=\underbrace{[0\ \cdots\ 0}_{nr-1}\ \underbrace{(1-q)F/V_s 0\cdots 0]}_{ns-1}{}^T \tag{23}$$
$$(nr+ns-2)$$

where $x_s(z_k-\Delta z_s)$ is substituted by the expression in Eq. (16).

The vector $\mathbf{y}$ in Eq. (20) can be eliminated using Eq. (22) and the resulting reduced-order model is represented by a nonlinear vector differential equation with respect to $\mathbf{x}$ only.

$$d\mathbf{x}/dt=-\mathbf{K}_1\mathbf{x}+\mathbf{K}_2\mathbf{E}^{-1}[\mathbf{g}+\mathbf{f}_2x_f]-\mathbf{f}_1x_f \tag{24}$$

Through this reduction, order of the underlying distillation model is reduced from NT to nr+ns−1, producing a reduced-order model parameterized by α_r, α_s, H_r, and H_s which are imbedded in the vectors $\mathbf{g}$ and $\mathbf{f}_1$ and the matrices $\mathbf{K}_1$ and $\mathbf{K}_2$.

CONSTRUCTION OF CUBIC SPLINE INTERPOLATION FUNCTION

The reduced-order model in Eq. (24) is valid for any type of interpolation function. Accuracy of the model, however, may be significantly affected by a specific type of the interpolation function used. In this section, the construction procedure of the cubic spline interpolation function used in the present work is briefly described.

The cubic spline function is a piecewise cubic polynomial in which not only the function itself and the slope but also the second derivative are continuous [12]. To show how the cubic spline interpolation function is constructed, a domain, over which a function u(z) to be approximated is defined, with n collocation points is considered first as in Fig. 3. The piecewise cubic polynomial $\bar{u}_i(z)$ defined over a subdomain $[z_i, z_{i+1}]$ should satisfy the following conditions:

$$\bar{u}_{i-1}(z_i)=\bar{u}_i(z_i),\ i=2,3,\cdots,n-1$$
$$\bar{u}_{i-1}^{(1)}(z_i)=\bar{u}_i^{(1)}(z_i),\ i=2,3,\cdots,n-1$$
$$\bar{u}_{i-1}^{(2)}(z_i)=\bar{u}_i^{(2)}(z_i),\ i=2,3,\cdots,n-1$$
$$\bar{u}_i(z_i)=u(z_i),\ i=1,2,\cdots,n \tag{25}$$

where the superscript (j) denotes the j-th derivative. If we define M_i as the second derivative of u at the collocation point z_i, the cubic polynomial over each subdomain is obtained as follows [12]:

$$\bar{u}_i(z)=\beta_{1i}(z)M_i+\beta_{2i}(z)M_{i+1}+\beta_{3i}(z)u(z_i)+\beta_{4i}(z)u(z_{i+1}) \tag{26}$$

where $\beta_{1i}(z)=\frac{1}{6}[\frac{(z_{i+1}-z)^3}{h_i}-h_i(z_{i+1}-z)]$

$$\beta_{2i}(z)=\frac{1}{6}[\frac{(z-z_i)^3}{h_i}-h_i(z-z_i)]$$
$$\beta_{3i}(z)=\frac{(z_{i+1}-z)}{h_i},\quad \beta_{4i}(z)=\frac{(z-z_i)}{h_i}$$

and $h_i=z_{i+1}-z_i$.

Here M_i's are determined by solving

$$h_iM_i+2(h_i+h_{i+1})M_{i+1}+h_{i+1}M_{i+2}=$$
$$\frac{6}{h_ih_{i+1}}[h_iu(z_{i+2})-(h_i+h_{i+1})u$$
$$(z_{i+1})+h_{i+1}u(z_i)],\ i=1,2,\cdots,n-2. \tag{27}$$

Since the total number of equations in Eq. (27) is n−2 while the number of variables M_i is n, two supplementary spline conditions are needed. Usually any pair of the following end conditions are used as the supplementary conditions.

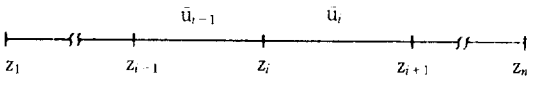

Fig. 3. Coordinate for cubic spline functions.

$$\text{At } z=z_1,\ M_1=0 \text{ or } \bar{u}_1^{(1)}(z_1)=0$$

$$\text{At } z=z_n,\ M_n=0 \text{ or } \bar{u}_n^{(1)}(z_n)=0. \tag{28}$$

In Eq. (28), $\bar{u}^{(1)}=0$ constrains the interpolation function to have zero slope while $M=0$ allows any slope except that the point concerned is an inflection point. Now the following four cases are paired off from Eq. (28) as the candidates for the supplementary end conditions.

$$\text{Condition 1}: \bar{u}_1^{(1)}(z_1)=M_n=0$$

$$\text{Condition 2}: M_1=M_n=0$$

$$\text{Condition 3}: M_1=\bar{u}_n^{(1)}(z_n)=0$$

$$\text{Condition 4}: \bar{u}_1^{(1)}(z_1)=\bar{u}_n^{(1)}(z_n)=0. \tag{29}$$

Now, in order to formulate the interpolation function from the cubic splines, M_i in Eq. (26) is first eliminated using Eq. (27) together with appropriate supplementary conditions. Then the resulting equation will look like.

$$\bar{\mathbf{u}}(z)=\mathbf{B}(z)\ \mathbf{u} \tag{30}$$

where

$$\mathbf{u}^t=[u(z_1),\ u(z_2),\cdots,\ u(z_n)]$$

$$\bar{\mathbf{u}}^t(z)=[\bar{u}_1(z),\ \bar{u}_2(z),\cdots,\bar{u}_{n-1}(z)]$$

The matrix **B** can be easily obtained by treating Eqs. (26) and (27). To have an interpolation function as in the form of Eq. (15), the following piecewise continuous function is introduced:

$$\mathbf{v}^t(z)=[v_i(z)] \tag{31}$$

where,

$$v_i(z)=\begin{cases}1 \text{ for } z\in[z_i,\ z_{i-1}]\\ 0 \text{ otherwise}\end{cases}$$

Then we have

$$\bar{u}(z)=\mathbf{v}^t\mathbf{B}(z)\mathbf{u},\ z\in[0,\ 1] \tag{32}$$

Therefore,

$$[S_1(z)\ S_2(z)\cdots S_n(z)]=\mathbf{v}^t\mathbf{B}(z) \tag{33}$$

NUMERICAL STUDY

In this section, steady-state and also dynamic performances of the proposed model are demonstrated through numerical simulation. Simulation results with the rigorous stage-by-stage model as well as the reduced-order model with the Lagrange interpolation function are also povided for comparison.

Table 1. Lists of column dimensions and simulation conditions

Total no. of stages	NT=15
Feed stage	NF=8
Plate	sieve, 3″ ID, 6″ height
Normal holdups	H_c=20 mol, H_r=3 mol, H_s=4 mol, H_b=80 mol
Feed flowrate	216.0 mol/hr
Feed conditions	q=1, x_f=0.5
Relative volatility	α_r=1.68 or 2.0, α_s=2.4 or 3.0
Top product flowrate	108.0 mol/hr
Reflux ratio	2
Collocation points	nr=3, ns=3

Table 1 shows physical dimensions and nominal operating conditions of the distillation model assumed in the numerical study. These values are taken from an experimental setup in the authors' laboratory. To make the order of the resulting model as low as possible, three collocation points which mean one internal collocation point are assumed in each section of the column.

1. Steady-state simulation

The steady-state equations of reduced-order models can be readily obtained from Eq. (24) by setting d/dt=0. To solve them, a sequential method [13] is used. Results of steady-state simulations are summarized from Figs. 4 to 6 for two different relative volatility cases.

In Figs. 4 to 6, we can see that closer approximation to the underlying rigorous model can be obtained as a whole with the cubic splines unless oddly chosen end conditions are imposed. It is thought to come from the flexibility of the cubic splines which is piecewise cubic, whereas the Lagrange interpolation function with one internal collocation point is only quadratic, which cannot suitably represent the S-shaped concentration profiles especially in the stripping section.

In Figs. 4 and 5, effects of the spline end conditions and the location of collocation point in the stripping section are shown for the case of $\alpha_r=2.0$ and $\alpha_s=3.0$. As can be seen in Fig. 4, end condition 1 in Eq. (29) for both sections [spline condition (1, 1)] is found to fit the rigorous model most accurately. It is because the concentration profiles around column ends are rather flat by higher values of relative volatilities. For the internal collocation point, as shown in Fig. 5, the loca-

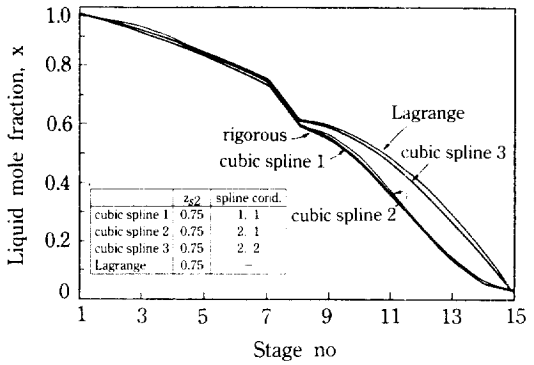

Fig. 4. Effect of supplementary spline conditions on steady-state concentration profiles [$\alpha_r=2.0$, $\alpha_s=3.0$, $z_r=(0.0, 0.5, 1.0)$].

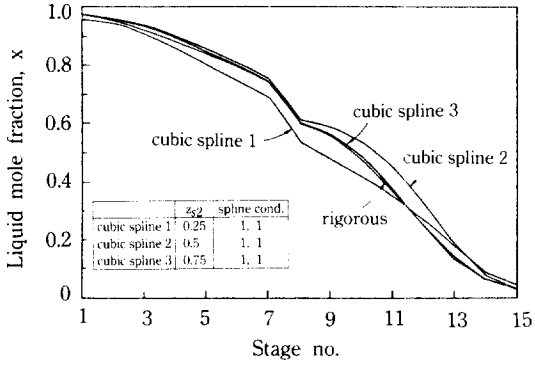

Fig. 5. Effect of internal collocation point on steady-state concentration profiles [$\alpha_r=2.0$, $\alpha_s=3.0$, $z_r=(0.0, 0.5, 1.0)$].

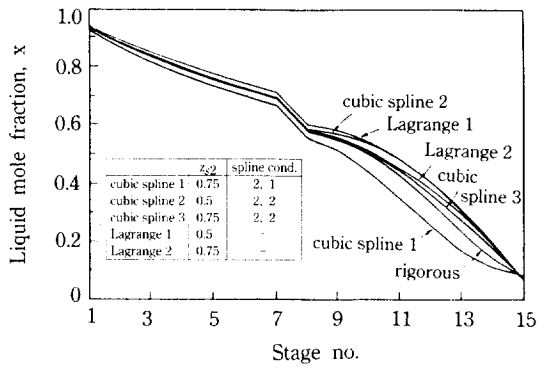

Fig. 6. Steady-state concentration profiles of the reduced-order models [$\alpha_r=1.68$, $\alpha_s=2.4$, $z_r=(0.0, 0.5, 1.0)$].

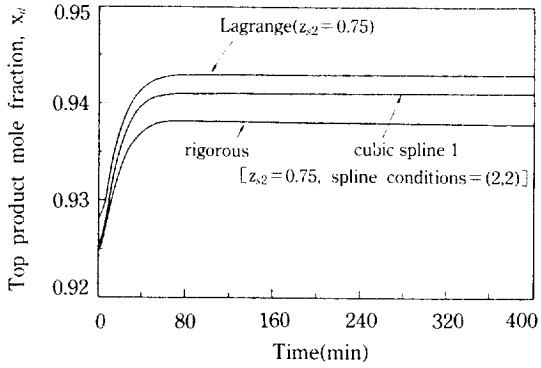

Fig. 7. Dynamic responses of top product mole fraction to 10% step increase of vapor flow rate ($\alpha_r=1.68$, $\alpha_s=2.4$).

tion near the feed plate, say $z_{s2}=0.75$, produces better approximation than $z_{s2}=0.5$ or 0.25. Effects of the location of collocation point in the rectifying section have also been investigated. In this case, however, any noticeable consequences could not have been observed. Figure 6 shows the simulation results for $\alpha_r=1.68$ and $\alpha_s=2.4$. With spline end condition 2 for both sections [spline condition (2, 2)] and $z_{s2}=0.75$, the reduced-order model approximates the underlying distillation model most closely.

As is shown above, the spline end conditions and location of the internal collocation point have crucial effects on the model performance. Between them, the spline end condition can be rather easily determined once the concentration profile in the column concerned is available. For example, if the profile is flat at a column end, say $z=z_1$, but has a slope at the feed stage, say $z=z_n$, then the condition 1 in Eq. (29) should be preferably chosen for the corresponding column section. If the profile has slopes at z_1 as well as z_n, the condition 2 will fit the profile. We can obviously see that the results in Figs. 4 to 6 comply with this consideration.

Finding an optimum location of the internal collocation point, however, seems to be rather tricky. Through further numerical studies, we have found that the optimun location is strongly dependent upon the spline end condition chosen as well as the overall profile shape. When the spline end condition has zero first-order and second-order derivatives at each respective end such as in condition 1 or 3, the optimum location always lies at a point biased to the end where the second-order derivative is zero. For example, when the condition 1 is chosen, the optimum location lies in (0.5, 1.0), more probably near 0.75, which is exemplified in Fig. 5. In case that the spline end condition adopted has zero second-order derivatives at both ends and the overall shape of the profile is rather

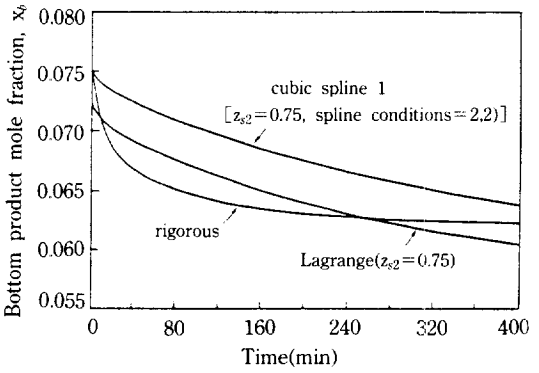

Fig. 8. Dynamic responses of bottom product mole fraction to 10% step increase of vapor flow rate (α_r= 1.68, α_s=2.4).

linear, approximation result appears to be less sensitive to the location of the collocation point. In the same case but the profile is curved, the optimum point usually lies in the half region for the low slope end point.

One thing we should remember is that the prime objective of the proposed reduced-order model is to use it for real-time applications instead of off-line column design. Therefore, it can be presumed that a typical concentration profile of the column is available in advance. Based on this a prior information and the above mentioned guides, the spline end conditions and location of the collocation point which fit the column best might be determined.

2. Dynamic simulation

Dynamic simulation of the reduced-order model has been carried out by directly solving Eq. (24) using an ordinary differential equation package. Figures 7 and 8 show transient responses of end products when the vapor flow rate is increased by 10% stepwise from its steady-state value. As far as the response dynamics is concerned, we can see that the two reduced-order model produce almost the same reaction curves. Comparing with the rigorous model, however, both the reduced-order models yield more sluggish responses, especially in the stripping section. As was mentioned in part III, the reboiler was treated as one of the stripping stage in the course of collocation. Consequently, when one internal collocation point is considered, the stripping section is lumped with two differential equations, one at the internal collocation point and the other at the reboiler, while H_b instead of H_s is used for the equation at the reboiler. But since H_b is about twenty times larger than H_s, effective tray holdup in the stripping section appears larger than that of the underlying distillation model, resulting in longer time constant. This dynamic discrepancy, however, can be rectified to an extent if we tune H_b to a smaller value.

CONCLUSIONS AND FURTHER COMMENTS

A generic and compact form of reduced-order distillation model has been developed using the collocation method combined with the MPA concept by Kim et al.[10]. To further improve accuracy of the reduced-order model even with the lowest order, the cubic spline interpolation function has been utilized. Through steady-state and dynamic tests of the proposed distillation model, the following conclusions could be drawn.

1. The proposed model was found to be superior to the existing one with the Lagrange interpolation function when they have the same order.

2. The proposed model with order 5 can represent the 13-stage distillation column with sufficient accuracy. Such accuracy comes from the flexibility of the spline functions and is expected for a column with more stages and/or higher relative volatilities. On the other hand, the same order reduced model with the Lagrange interpolation function cannot be expected to adequately represent the higher degree separation column due to the quadratic nature of the interpolation function.

The proposed reduced-order distillation model has been constructed based on a physical model with some idealized assumptions. In spite of an improved model-reducing technique, therefore, some kind of model tuning is needed for the proposed model to play as a practical simulator. For model tuning in real time environment, recursive parameter estimation techniques is considered to be useful, since the proposed model is parameterized by α_r, α_s, H_r and H_s where the first two determine the separation degree while the other two govern the column dynamics.

Using the proposed reduced-order model, nonlinear model predictive control and on-line optimization studies combined with recursive identification by a nonlinear filtering algorithm is now under way. Experimental verification in a pilot scale distillation column will be done in due course.

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NOMENCLATURE

a(z), b(z), c(z) and d(z) : derived functions from inter-

polation functions, defined in Eq. (17)
E : matrix defined in (23)
$\mathbf{f}_1, \mathbf{f}_2$: vectors defined in (21) and (23), respectively
F : feed flow rate [mol/s]
g : vector defined in (23)
h : distance between two adjacent collocation points, defined in (26)
H : liquid holdup [mol]
$\mathbf{K}_1$, $\mathbf{K}_2$: matrices defined in (21)
L : liquid flow rate [mol/s]
M : second derivative of spline function
nr : number of collocation points in the rectifying section
ns : number of collocation points in the stripping section
NF : feed stage number from the condenser
NT : total number of stages including the condenser and the reboiler
q : 1-(fraction of the feed vaporized)
S(z) : interpolation function
t : time [sec]
u(z) : any continuous function defined on [0, 1]
$\bar{u}(z)$: cubic spline interpolation function
u, $\ddot{\mathbf{u}}$: vectors defined in (30)
V : vapor flow rate [mol/s]
v(z) : a discontinuous function defined in (31)
v : vector defined in (31)
x : liquid phase mole fraction
x : vector of which components are liquid phase mole fractions at collocation points
y : vapor phase mole fraction
y : vector of which components are vapor phase mole fractions at collocation points
z : spatial coordinate for collocation

Greek Letters

α : relative volatility
β : defined in (26)

Subscripts

b : reboiler
c : condenser
f : feed
r : rectifying section
s : stripping section

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