TWO-PART MODULAR REDUCED-ORDER MODEL FOR MULTICOMPONENT MULTISTAGE DISTILLATION COLUMNS

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Key Words:

A new, efficient model reduction method for multistage distillation columns is proposed by combining the orthogonal collocation method and the two-part modular concept. To assess the performance of the proposed method, numerical simulation was performed for two distillation examples—the high-purity freon 11–12 binary system and the nonideal ethanol–1-propanol–water ternary system— and the results were compared with those obtained by the methods of existing collocation as well as rigorous equation solving.

It was shown that the proposed method reduces the computing time by about 40% with accuracy comparable to that of the rigorous methods. Furthermore, while the existing collocation method could not properly reproduce the sharp changes of variables in the vicinity of the feed stage, the proposed method could successfully reproduce them as well.

Introduction

With its long history, distillation is a mature and well-established unit operation in the chemical process industries, and various simulation packages have recently become available. The distillation process, however, is usually described by a large number of nonlinear algebraic and/or differential equations, resulting in a long computation time for its solution. Great dimensionality and complexity become more serious if we are concerned with dynamic modeling. Therefore, development of efficient model reduction techniques that can abate modeling complexity while keeping the intended accuracy has been an important research topic.

Various model reduction methods for multistage distillation processes have been reported, including modal analysis,[1] compartmental modeling,[5,7] and others.[11] In most of these works, however, attention has been placed only on obtaining perturbed dynamic models, where knowledge of the steady-state conditions is presumed. Recently, as a different approach, Cho and Joseph[2,3,4] utilized the concept of orthogonal collocation for reduced-order modeling of a distillation process. This method was further refined by Stewart *et al.*[9] and was employed in optimization of a distillation process.[10]

The orthogonal collocation method has a novel feature in that it is applicable to steady-state as well as dynamic models. In addition, it is reported that the reduced-order model through orthogonal collocation shows fairly good accuracy in various distillation examples. The existing collocation approximations, however, consider the whole column as a single domain and take zeros of an orthogonal polynomial defined on the entire domain as the collocation points. Therefore, no distinction is made in the resulting reduced-order models irrespective of feed stage lo-

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cation as long as it is placed between two certain collocation points. Moreover, the existing collocation approximations may not properly reproduce sharp changes in distillation variables near the feed stage since the whole profile of a variable is approximated by a single polynomial which is smooth by its nature.

To overcome these drawbacks of the existing collocation methods, the present work is aimed at devising a new model reduction method for distillation by combining the concept of the orthogonal collocation and the two-part module. In the proposed method, called "*modular polynomial approximation*" (MPA), a distillation column is considered as a combination of two modules separated with respect to the feed stage, and the orthogonal collocation is applied over each module. To assess the performance of the proposed MPA, a simulation study was carried out for the freon 11–12 binary system and the ethanol–1-propanol–water ternary system. The results were compared with those by the existing collocation method as well as those by rigorous methods.

1. Polynomial Approximation of Distillation Model

1.1 Orthogonal collocation for multistage separation model

Here, we briefly review how the concept of the orthogonal collocation can be used for reduced-order modeling of a multistage process.[2] To illustrate the model reduction procedure, we will consider the total mass balance equation of a simple multistage process with no feed or side streams, such as the gas absorption column shown in **Fig. 1**. At the j-th stage, the dynamic interaction of the total mass is represented by

$$\frac{dm_j}{dt}=(L_{j-1}-V_{j-1})-(L_j-V_j), \quad j=1, 2, \cdots, N \tag{1}$$

where m_j denotes holdup in the j-th stage, and L_j and V_j are the liquid- and vapor-phase molar flowrates from and to the j-th stage, respectively. We note that L_j and V_j are defined differently from the usual notation convention where the subscript j denotes the flow from the j-th stage. Since the orthogonal collocation is an approximation method for continuous functions, we introduce a spatial coordinate z as shown in Fig. 1 and regard L, V and m as continuous functions in z rather than discretized variables over the spatial domain. Based on this consideration, we can write Eq. (1) at an arbitrary point in z domain. At z_k, Eq. (1) becomes

$$\frac{dm(z_k)}{dt}=-(L(z_k)-L(z_k-\Delta z))+(V(z_k)-V(z_k-\Delta z)) \tag{2}$$

where Δz denotes the distance between two stages,

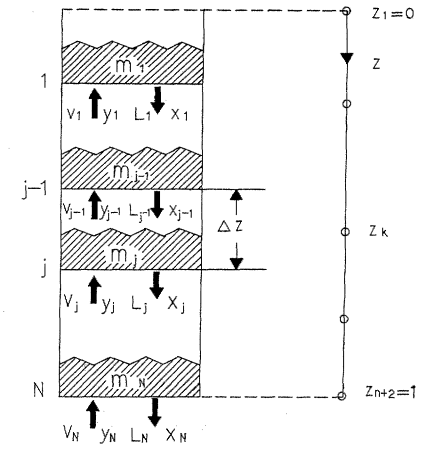


Fig. 1. Schematic diagram of a multistage equilibrium process

which is equal to $1/N$. Since the variables in Eq. (2) are assumed to be continuous in z, high-order polynomials can be tried for approximate representation of the variables. In the orthogonal collocation, coefficients of the trial polynomials are determined such that the residues (equation error) become naught at the so-called collocation points, which consist of boundary points $z=0$, 1 and zeros of an orthogonal polynomial defined over $z\in[0, 1]$. This procedure can be much more simplified if a precollocated polynomial such as the Lagrange interpolation function is employed as the trial polynomial. If we consider $n+2$ collocation points $\{z_k\}$, $k=1, 2, \cdots, n+2$ with $z_1=0$ and $z_{n+2}=1$, the $(n+1)$-th order Lagrange interpolation function $l_k(z)$ which is null at all collocation points except z_k can be employed. In this case, the variables in Eq. (2) are approximated by linear combinations of $l_k(z)$'s. For example, $L(z)$ can be approximated as

$$L(z)=\sum_{k=1}^{n+2} l_k(z)L(z_k) \tag{3}$$

Through the same procedure, V can be approximated by the Lagrange interpolation function. If we substitute these results into Eq. (2) and then make the residues null at the collocation points, the following equation is obtained:

$$\frac{dM(z_j)}{dt}=\sum_{k=1}^{n+2} A_{jk}(V(z_k)-L(z_k)), \quad j=2, \cdots, n+2 \tag{4}$$

where the coefficient A_{jk} is defined as

$$A_{jk}=\frac{l_k(z_j)-l_k(z_j-\Delta z)}{\Delta z} \tag{5}$$

and $M=m\Delta z$. As can be seen from Fig. 1, $z=0$ (or z_1) is located one stage above stage no. 1. At this point, Eq. (2) does not hold since $L(z_1-\Delta z)$ and $V(z_1-\Delta z)$ have no physical meaning. Thus we can write Eq. (4)

only for z_2 to z_{n+2}. The above model reduction procedure can be applied similarly for component as well as enthalpy balance equations. Using the Lagrange interpolation function, we can also treat the equilibrium relationships as will be discussed in the next section.

In this way, we get a reduced-order model of a multistage process. If process variables change smoothly along the z-direction, which is the usual case in practice, sufficiently accurate representation of the variables is possible with low-order polynomials only, even though the real stage number is large, and significant order reduction can be achieved. The variables in the reduced-order model are only fictitious ones and do not usually correspond to any stage variables. Using the interpolation relationship in Eq. (3), however, we can estimate variables at each real stage once we solve Eq. (4) at the assigned collocation points.

1.2 Application to a distillation model

The model reduction technique outlined in the previous section can be similarly applied to a multistage distillation column. Here, we consider a steady-state distillation model with the following assumptions: i) constant pressure, ii) saturated liquid feed, and, iii) total condenser. The mass and enthalpy balance equations can be written as follows for each tray using the notations shown in **Fig. 2**:

Overall mass balance

$$0=(L_{j-1}-V_{j-1})-(L_j-V_j-F) \tag{6}$$

Component mass balance

$$0=(L_{j-1}x^i_{j-1}-V_{j-1}y^i_{j-1})-(L_jx^i_j-V_jy^i_j-Fx^i_F) \tag{7}$$

Enthalpy balance

$$0=(L_{j-1}h_{j-1}-V_{j-1}H_{j-1})-(L_jh_j-V_jH_j-Fh_j) \tag{8}$$

where

$j=0, 1, \cdots, N+1,\ i=1, 2, \cdots, c,$

$F=0$ when $j\neq f,$

$L_{-1}=0,\ V_{-1}=D,\ V_{N+1}=0$

$L_{N+1}=B,\ x^i_{-1}=0,\ y^i_{-1}=x^i_D,\ y^i_{N+1}=0,\ x^i_{N+1}=x^i_B$

In addition to the above equations, information such as constitutive relationships for vapor–liquid equilibria, bubble point and efficiency are needed to complete the description. Among them, the usual choice of efficiency relationship is the Murphree stage efficiency, defined as

$$\eta^i_j=\frac{y^i_{j-1}-y^i_j}{y^{i*}_{j-1}-y^i_j} \tag{9}$$

Direct use of the Murphree efficiency, however, makes the model reduction very complicated. Therefore, the vaporization efficiency E^i_j[6] defined as

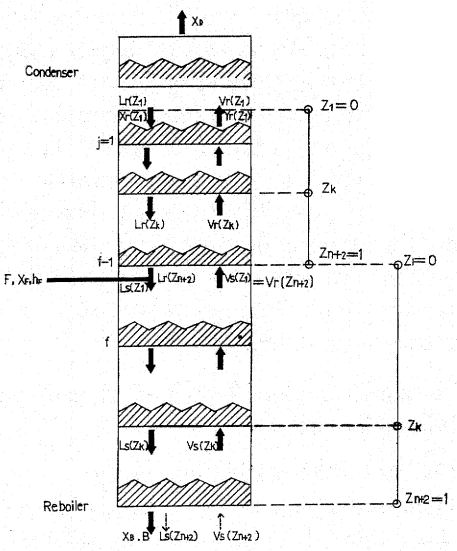


Fig. 2. Schematic diagram of a distillation column

$$y^i_{j-1}=E^i_jK^i_jx^i_j \tag{10}$$

is used in the present work.

The distillation model considered here has a feed stream at the f-th stage and this raises a discontinuity in variables. Therefore, direct application of the orthogonal collocation becomes difficult unless some sort of approximation is introduced for the sudden jump and the discontinuity of distillation variables. To eliminate this difficulty, Cho and Joseph[4] introduced an auxiliary variable W which varies smoothly over the domain. For example, the overall mass balance equation was modified as

$$0=W_{j-1}-W_j \tag{11}$$

where the variable W_j is defined as

$$W_j=\begin{cases} L_j-V_j & \text{for } j=1, \cdots, f-1, f+1, \cdots, N \\ L_j-V_j-F & \text{for } j=f \end{cases} \tag{12}$$

The idea in the previous section is, then, applicable to Eq. (11), which results in the following reduced-order equation:

$$0=\sum_{k=1}^{n1} A_{jk}(L(z_k)-V(z_k))+\sum_{k=n1+1}^{n+2} A_{jk}(L(z_k)-V(z_k)-F) \tag{13}$$

Here $n1$ denotes the number of collocation points above the feed stage. The component mass balance as well as the enthalpy balance equations can also be reduced.

Although successful simulation results were demonstrated for some distillation examples, the method of Cho and Joseph[4] has some inherent disadvantages. As we could expect from the underlying idea of this method, the resulting reduced-order model cannot account for the sharp changes in variables near the feed stage. A more serious problem is that the

resulting reduced-order models have the same form irrespective of feed location as long as it is positioned between two certain collocation points. In the control of high-purity separation, column temperatures near the feed stage are frequently taken as controlled variables because they provide a sensitive indication of the column states while the end-point temperatures do not. For the reduced-order model to be more versatile for dynamic as well as steady-state applications, some improvement should be made to eliminate these disadvantages.

2. Two-part Modular Polynomial Approximation for a Distillation Model

2.1 Reduced-order distillation model

As mentioned previously, the *existing polynomial approximation* (EPA) method for distillation columns has some inherent drawbacks arising from the approximation of the whole distribution of variables in the column by a single polynomial. The MPA we propose has a feature that eliminates the problems of the EPA method.

The underlying idea of MPA is that the column is divided into two separate modules with respect to the feed stage as shown in Fig. 2, and orthogonal collocation is applied to each module. Dimensions of the resulting reduced-order model might be larger than that of the existing one. However, since variables in each module usually have smooth profiles, lower-order polynomials than those in EPA can be successfully adopted. The two-part modular concept was established by Yamada *et al.*[11] as a rigorous steady-state simulation technique, where numerical computation is repeated until the process variables for each module converge at the feed stage. One of the advantages of this approach is that the convergence is less affected by initial estimates of the solutions when compared to other simulation techniniques.

In MPA, the model reduction procedure outlined in section 2 can be applied without modification. Then the following equations are obtained for each module:
Overall mass balance

$$0=\sum_{k=1}^{n+2} A_{jk}(L(z_k)-V(z_k)) \tag{14}$$

Component mass balance

$$0=\sum_{k=1}^{n+2} A_{jk}(L(z_k)x^i(z_k)-V(z_k)y^i(z_k)) \tag{15}$$

Enthalpy balance

$$0=\sum_{k=1}^{n+2} A_{jk}(L(z_k)h(z_k)-V(z_k)H(z_k)) \tag{16}$$

In Eqs. (14)–(16), the number of internal collocation points, n, can be chosen differently for each module.

The constitutive equations become as follows:

Vapor–liquid equilibria

$$y^i(z_j)=\sum_{k=1}^{n+2} l_k(z_j+\Delta z)E^i(z_k)K^i(T(z_k))x^i(z_k) \tag{17}$$

Bubble point relationship

$$\sum_{i=1}^{m} y^i(x^i(z_k),\ T(z_k))=1\,. \tag{18}$$

Equations (14) through (18) hold for $j=2,\ 3,\cdots,\ n+2$.

Boundary conditions are as follows:
For the rectifying section.

$$x^{ri}(z_1)=y^{ri}(z_1)=x_D^i,\ V^r(z_1)=(1+R)D,\ L^r(z_1)=RD \tag{19}$$

At the feed stage,

$$\begin{aligned} &V^s(z_1)=V^r(z_{n+2})\,,\\ &L^s(z_1)=L^r(z_{n+2})+F,\ y^{si}(z_1)=y^{ri}(z_{n+2})\\ &x^{si}(z_1)=(Fx_F^i+L^r(z_{n+2})x^{ri}(z_{n+2}))/L^s(z_1) \end{aligned} \tag{20}$$

For the stripping section,

$$\begin{aligned} &y^{si}(z_{n+2})=0,\ x^{si}(z_{n+2})=(Fx_F-Dx_D^i)/(F+D)\,,\\ &V^s(z_{n+2})=0,\ L^s(z_{n+2})=F-D \end{aligned} \tag{21}$$

The stripping section has no incoming stream from the bottom of the column and therefore a discontinuity in liquid-phase flowrate occurs at the reboiler. This may deteriorate the polynomial approximation of the stripping section and cause numerical instability in the solution. To avoid this problem, we split the bottom product stream into two fictitious incoming and outcoming streams with the same concentration. These fictitious streams are depicted by dashed arrows in Fig. 2. By introducing these streams, the boundary conditions in Eq. (21) are changed to

$$\begin{aligned} &y^{si}(z_{n+2})=x^{si}(z_{n+2})=(Fx_F-Dx_D^i)/(F-D)\,,\\ &L^s(z_{n+2})-V^s(z_{n+2})=F-D \end{aligned} \tag{22}$$

Actually, the constituent equations for each module resemble those for simple multistage countercurrent separation processes such as that in a gas absorption column. In these processes, if the conditions for two incoming streams, one from the top and the other from the bottom of the column, are specified, variables at each stage are uniquely determined with better numerical stability than when the conditions are specified at the column top or bottom. The distillation column is different from the gas absorber in that it has a condenser and a reboiler which recycle streams into the column. However, once we partition the column as shown in Fig. 2, each module can be treated in the same way as in the simple multistage countercurrent separation process.

Although saturated liquid feed and a total con-

denser are assumed in the derivation of the above model, these assumptions can be relaxed and MPA can be applied similarly with only minor modifications. The MPA technique is also applicable to a distillation model with multiple feed and/or side product streams. In this case, however, dimensions of the reduced-order model increase.

2.2 Computation algorithm

In the solution of the model equations it was assumed that the column pressure and the feed conditions such as flowrate, composition and enthalpy are known. Under these assumptions, we took two flowrate conditions as additional constraints. The solution for the whole column was obtained by sequentially solving each module in the rectifying and stripping sections and then returning to the rectifying section until variables from each module coincide at the feed stage. The solution algorithm has two major iteration loops, the outer loop for overall convergence and the inner loop, which is embedded in the outer loop, for each module. Through extensive simulation studies, it was found that the inner loop need not be converged accurately at each outer loop iteration. So only one iteration was performed in the solution of module equations. Details of the computation algorithm when distillate and reflux flowrates are specified are given as follows:

For the rectifying section,

(i) Assume the top composition x_D^i.
(ii) Assume the vapor conditions $V(z_{n+2})$, $y^i(z_{n+2})$.
(iii) Assume initial values of $\{V(z_k)\}$, and $\{T(z_k)\}$, $k=1, \cdots, n+1$.
(iv) Calculate $\{L(z_k)\}$, $k=2, \cdots, n+2$ from the overall mass balance equation (14) with the assumed variables in steps (ii) and (iii), and given $L(z_1)$.
(v) Calculate $\{x^i(z_k)\}$, $k=2, \cdots, n+2$ from the component mass balance equation (15) combined with the equilibrium relationship (17).
(vi) Update $\{T(z_k)\}$, $k=1, \cdots, n+1$ from the bubble point relationship (18).
(vii) Calculate $\{y^i(z_k)\}$, $k=1, \cdots, n+1$ from the equilibrium relationship (17).
(viii) Update $\{V(z_k)\}$, $k=2, \cdots, n+1$ from the enthalpy balance equation (16).

For the stripping section,

(ix) Using the boundary conditions in Eq. (20), calculate $L(z_1)$ and $x^i(z_1)$ for the stripping section.
(x) Calculate $y^i(z_{n+2})$ from the overall mass balance in Eq. (22).
(xi) Assume $V(z_{n+2})$.
(xii) Follow the same procedures as in (iii) through (viii).
(xiii) Update x_D^i using the θ-method[6] until $|\theta-1|<0.0001$.
(xiv) Return to step (iii).

Table 1. Operating conditions for simulated systems

	Example 1	Example 2
No. of components	2	3
No. of stages	25	20
Feed stage	13	10
Feed conditions		
Composition		
	Freon-11 0.54	Ethanol 0.20
	Freon-12 0.43	1-Propanol 0.30
		Water 0.50
Temperature (K)	307.2	356.7
Flowrate (mol/hr)	11514.0	100.0
Top product flowrate (mol/hr)	4940.0	50.0
Reflux ratio	4.0	2.0
Vaporization efficiency	1.0	0.89
Operating pressure (KPa)	6.078×10^2	1.013×10^2

3. Simulation Studies

To evaluate the performance of the proposed MPA, numerical simulations have been made for two distillation examples: the freon 11–12 binary system and the ethanol–1-propanol–water ternary system. Details of the simulating condition for both systems are given in **Table 1**. While the freon 11–12 system is relatively ideal with a large boiling point difference, it requires high-purity separation. On the other hand, the ethanol–1-propanol–water system has a high degree of nonideality and requires tedious phase-equilibrium calculation. For both systems, the simulation results obtained by MPA are compared with those by rigorous methods (the equation-solving method[6] for the binary and the Newton–Raphson method[8] for the ternary systems) as well as those by EPA.

The necessary computer programs were written in Fortran-77 and executed in IBM-PC-XT.

3.1 Freon 11–12 binary system

Distributions of liquid-phase composition of freon 11 obtained by MPA, EPA, and equation-solving methods are shown in **Fig. 3**. The result by MPA is obtained with two internal collocation points for both rectifying and stripping sections. In this case, the resulting reduced-order model is composed of equations at five collocation points, two sets of two internal points and one at the module boundary. To compare MPA with EPA on the same basis, five internal collocation points were used in the simulation by EPA. From Fig. 3, we can see that the concentration profile by MPA follows the rigorous result more closely than that by EPA over the whole region. At the feed stage in particular, MPA gives a nearly exact result while EPA shows large deviation from the rigorous one. This is anticipated since MPA assures

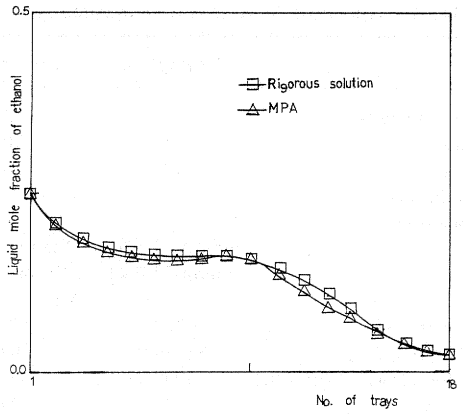


Fig. 3. Converged distributions of liquid-phase mole fraction for the binary system

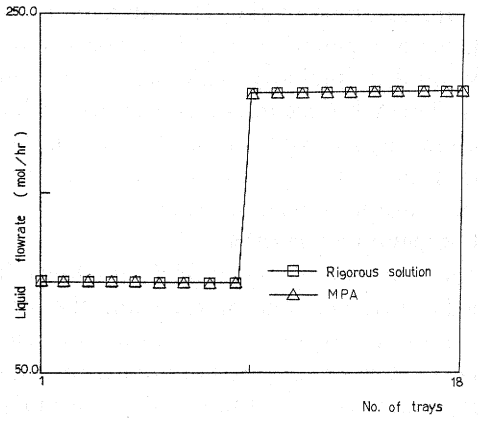


Fig. 4. Converged distributions of liquid-phase molar flowrates for the binary system

mass balance between each collocation point and feed stage (Of course, the feed stage is one of the collocation points).

Figure 4 shows the distributions of liquid-phase flowrate under the same simulating conditions as in Fig. 3. Compared to the result by EPA, we can see that significant improvement can be achieved when using MPA. A sudden jump in flowrate at the feed stage is completely reproduced in MPA, whereas only a smooth transition is made in EPA.

The required computation times for the three methods are compared in **Table 2**. As shown in this table, computation loads for MPA and EPA are almost the same, about half that by the equation-solving method.

3.2 Ethanol–1-propanol–water ternary system

In **Figs. 5–6**, simulation results for the ethanol–1-propanol–water ternary system are summarized and the results by MPA are compared with those by the rigorous Newton–Raphson method. As we can see from the figures, the MPA solutions show very close agreement with the rigorous solutions. In the simulation with MPA, two internal collocation points were used for both rectifying and stripping sections as in the previous example.

Table 2. Comparison of CPU time required for the different algorithms (binary system)

Algorithm	CPU time (sec)
5-pt. EPA	9.7
MPA	10.3
Equation solving	17.5

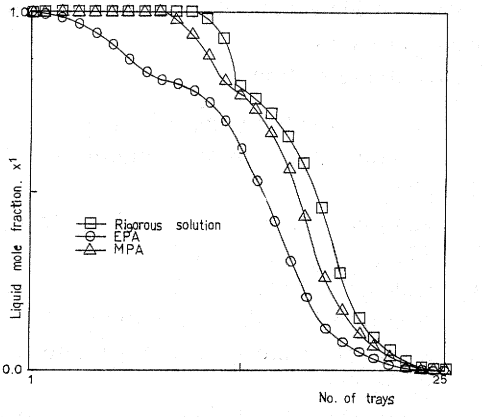


Fig. 5. Converged distributions of liquid-phase mole fraction for the ternary system

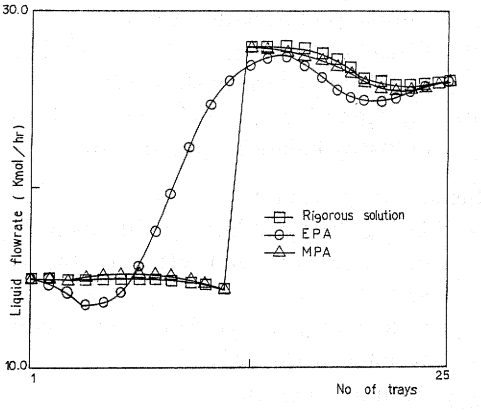


Fig. 6. Converged distributions of liquid-phase molar flowrates for the ternary system

Conclusions

Through this work, a new model reduction method, called MPA, for the multistage distillation process has been proposed by extending the advantages of EPA, which is based on orthogonal collocation. Through the implementation of MPA to simulate binary and ternary mixture distillation examples, the following conclusion can be drawn:

By adopting the modular concept, the congenital problem of EPA that lumped flowrate discontinuities at the feed stage in a polynomial is nicely solved. As a result, retaining similar computational burden, the MPA shows significant improvement in accuracy over the EPA.

With only about one-fifth order of the rigorous model, the reduced-order model is proved to have an accuracy comparable to that of the rigorous one. This implies that the proposed MPA can be used as a reliable time-saving distillation simulator.

The MPA method can be of course utilized for reduced-order dynamic modeling of distillation processes. Extention of MPA applications to on-line identification and control of distillation processes are being under study in our research group.

Acknowledgement

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Nomenclature

A	= orthogonal collocation matrix	
c	= number of components	
D	= top product flowrate	[mol/s]
E	= vaporization efficiency	
F	= feed flowrate	[mol/s]
f	= feed stage	
H	= vapor-phase molar enthalpy	[J/mol]
h	= liquid-phase molar enthalpy	[J/mol]
K	= vapor–liquid equilibrium distribution constant	
L	= liquid-phase flowrate inside the column	[mol/s]
l	= Lagrange interpolation function	
m	= liquid holdup	[mol]
N	= number of stages	
R	= reflux ratio	
T	= temperature	[K]
V	= vapor-phase flowrate inside the column	[mol/s]
W	= transformation variable defined in Eqs. (11) and (12)	
x	= liquid-phase mole fraction	
y	= vapor-phase mole fraction	
z	= spatial coordinate for collocation	
η	= Murphree stage efficiency	

〈Superscripts〉

i	= i-th component
r	= rectifying section
s	= stripping section
*	= saturated state

〈Subscripts〉

B	= bottom flow
D	= distillate
F	= feed stage
j	= j-th stage or j-th collocation point
k	= k-th collocation point

〈Abbreviations〉

EPA	= existing polynomial approximation
MPA	= modular polynomial approximation

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