A STAGewise ALGORITHM FOR MULTICOMPONENT MULTISTAGE BATCH DISTILLATION CALCULATION

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Key Words: Distillation, Batch Distillation, Simulation Method, Multicomponent, Implicit Euler method

A stagewise algorithm is proposed for the solution of multicomponent multistage batch distillation problems. In order to make the algorithm more precise and flexible, a generalized implicit Euler equation is implemented for numerical integration of the process variables on each stage at succeeding time steps. An overall normalized θ method is also employed to accelerate convergence for each time step. The relative performance of the proposed method compared with the Runge-Kutta method is shown using a numerical example; the CPU time can be decreased by up to 1/300. Comparison of the simulation results with the experiment suggests the adequacy of the proposed method.

Introduction

Recently, chemical industries have become more versatile, pursuing the production of a variety of high value added chemicals. Thus, batch distillation is attracting more attention as a possible separation process which provides high product purity as well as high yield.

Two approaches to model the change in the state inside the batch distillation column with time have been developed; the short-cut approach and the rigorous approach. Since the solution of batch distillation problems has an intrinsically integrational nature, it requires a tremendous amount of calculation for design or optimization purposes. Short-cut approaches are employed in such situations to reduce computation time at the sacrifice of accuracy. They enable us to obtain approximate solutions within a limited time. Rigorous approaches may be used to check the consistency of the solution and to make detailed adjustment if necessary. The role of rigorous approaches becomes more significant whenever a more reliable solution is needed.

The primary concern in development of the rigorous simulation method for batch distillation is to include more practical models, though the increase of calculation load is to be minimized as well. This can be accomplished by employing an integration formula with high accuracy. Distefano(1968) presented a rigorous mathematical model and investigated the applicability of numerical integration methods. Guy(1983) extended Distefano's model by including tray hydraulics. In practice, however, models to be considered will change in each application and sometimes customization may be required. Flexibility is another

factor to be considered when developing algorithms.

In the following, we try to propose an algorithm with high accuracy for rigorous batch distillation calculations and discuss its numerical characteristics through examples.

1. Batch Distillation Model

Figure 1 shows a typical batch distillation column with rectifying stages. The transient balance equations around the stages are the same as those in Distefano(1968) and Guy(1983), provided that the following primary assumptions are included; adiabatic column, negligible vapor holdup, and negligible stage hydraulics.

Total material balance:

$$\frac{dU_j}{dt} = g_j^M \quad (1)$$

$$g_1^M = V_2 - (L_1 + D) \quad (2)$$

$$g_j^M = V_{j+1} + L_{j-1} - V_j - L_j \quad (3)$$

$$g_N^M = L_{N-1} - V_N \quad (4)$$

Component material balance:

$$\frac{d(U_j x_{j,i})}{dt} = g_{j,i}^m \quad (5)$$

$$g_{1,i}^m = V_2 y_{2,i} - (L_1 + D) x_{1,i} \quad (6)$$

$$g_{j,i}^m = V_{j+1} y_{j+1,i} + L_{j-1} x_{j-1,i} - V_j y_{j,i} - L_j x_{j,i} \quad (7)$$

$$g_{N,i}^m = L_{N-1} x_{N-1,i} - V_N y_{N,i} \quad (8)$$

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Fig. 1 Batch distillation column model with rectifying stages

Enthalpy balance:

$$\frac{d(U_j h_j)}{dt} = g_j^h \quad (9)$$

$$g_1^h = V_1 H_1 - (L_1 + D) h_1 - Q_c \quad (10)$$

$$g_j^h = V_{j+1} H_{j+1} + L_{j-1} h_{j-1} - V_j H_j - L_j h_j \quad (11)$$

$$g_N^h = L_{N-1} h_{N-1} - V_N H_N + Q_R \quad (12)$$

Equilibrium relationship:

$$y_{j,i}^* = K_{j,i} x_{j,i} = \gamma_{j,i} \frac{P_i}{P} x_{j,i} \quad (13)$$

Stoichiometric relationships:

$$\sum_{i=1}^c x_{j,i} = 1 \quad (14)$$

$$\sum_{i=1}^c y_{j,i} = 1 \quad (15)$$

We can introduce a plate efficiency in the form of a vaporization efficiency as is explained in Yamada *et al.* (1973). The vapor composition $y_{j,i}$ leaving the plate j is related to $y_{j,i}^*$ in equilibrium with the liquid on the plate j using the vaporization efficiency $E_{j,i}^V$.

$$E_{j,i}^V = \frac{y_{j,i}}{y_{j,i}^*} \quad (16)$$

where $E_{j,i}^V$ is related to the Murphree plate efficiency as follows.

$$E_{j,i}^V = E_{j,i}^{MV} + (1 - E_{j,i}^{MV}) \frac{y_{j+1,i}}{y_{j,i}^*} \quad (17)$$

When ideal stages are assumed $E_{j,i}^{MV} = 1$. Then $E_{j,i}^V = 1$ and $y_{j,i} = y_{j,i}^*$.

We do not discuss plate efficiencies further. The reader may choose a suitable plate efficiency model according to the required precision of calculation.

For enthalpies, h and H , we assume a linear mole-fraction average of pure substances.

$$h = \sum_{i=1}^c x_i h_i^\circ \quad (18)$$

$$H = \sum_{i=1}^c y_i H_i^\circ \quad (19)$$

2. Numerical Integration

The authors have presented a successive relaxation algorithm for steady state multicomponent distillation calculation (Mori *et al.*, 1987). In this attempt to reduce the number of iterative calculations required for convergence, they successfully applied a generalized implicit Euler equation, Eq.(20), in numerical integration.

$$f^{v+1} = f^v + \delta \{ \omega f^{v+1} + (1 - \omega) f^v \} \quad (20)$$

The results also imply the possible application of this equation to the solution of batch distillation problems with higher accuracy.

2.1 Composition and temperature

In the same way as in Mori *et al.* (1987), we can rewrite Eq.(5) into a working form using Eq.(20) with a time increment δ .

$$U_j^{v+1} \bar{x}_{j,i}^{v+1} = U_j^v \bar{x}_{j,i}^v + \delta \{ \omega g_{j,i}^{v+1} + (1 - \omega) g_{j,i}^v \} \quad (21)$$

where a superscript v represents properties at time t and $v+1$ at time $t + \delta$.

By considering the relations in Eqs.(6)~(8), Eq.(21) can be rearranged to give $\bar{x}_{j,i}^{v+1}$'s.

$$\bar{x}_{1,i}^{v+1} = \frac{U_1 \bar{x}_{1,i}^v + \delta \{ \omega V_2^{v+1} y_{2,i}^{v+1} + (1 - \omega) g_{1,i}^v \}}{U_1 + \delta \omega (L_1 + D)} \quad (22)$$

$$\bar{x}_{j,i}^{v+1} = \frac{1}{U_j + \delta \omega (V_j E_{j,i}^{v+1} \bar{K}_{j,i}^{v+1} + L_j)} \{ U_j \bar{x}_{j,i}^v + \delta \{ \omega (V_{j+1}^{v+1} y_{j+1,i}^{v+1} + L_{j-1}^{v+1} \bar{x}_{j-1,i}^{v+1}) + (1 - \omega) g_{j,i}^v \} \} \quad (23)$$

$$\bar{x}_{N,i}^{v+1} = \frac{U_N \bar{x}_{N,i}^v + \delta \{ \omega L_{N-1}^{v+1} \bar{x}_{N-1,i}^{v+1} + (1 - \omega) g_{N,i}^v \}}{U_N + \delta \omega V_N \bar{K}_{N,i}^{v+1}} \quad (24)$$

Combined with a stoichiometric constraint, Eq.(14), we can determine $\bar{T}_j^{v+1}$ and $\bar{x}_{j,i}^{v+1}$ provided that any variables and terms except $\bar{K}_{j,i}^{v+1}$ in the left-hand side of Eqs.(25) and (26) are fixed. $\bar{K}_{j,i}^{v+1}$ is considered to be a function of $\bar{T}_j^{v+1}$ due to a vapor pressure and $\bar{x}_{j,i}^{v+1}$ due to activity coefficients.

$$\sum_{i=1}^c \frac{U_j \bar{x}_{j,i}^v + \delta \{ \omega (V_{j+1}^{v+1} y_{j+1,i}^{v+1} + L_{j-1}^{v+1} \bar{x}_{j-1,i}^{v+1}) + (1 - \omega) g_{j,i}^v \}}{U_j + \delta \omega (V_j E_{j,i}^{v+1} \bar{K}_{j,i}^{v+1} + L_j)} = 1 \quad (25)$$

$$\sum_{i=1}^N \frac{\dot{U}_N \dot{x}_{N,i} + \delta \{ \omega \dot{L}_{N-1} \dot{x}_{N-1,i}^{v+1} + (1-\omega) \dot{g}_{N,i}^{v+1} \}}{\dot{U}_N^{v+1} + \delta \omega \dot{V}_N^{v+1} \dot{K}_{N,i}^{v+1}} = 1 \quad (26)$$

2.2 Flow rates

This part of the model is strongly related to the operation mode or controlling system of the distillation column. For a reasonable selection of process variables to be controlled, we can specify two variables among distillate D , reflux ratio R or reflux rate L_1 , and reboiler heat duty Q_R . These variables that are to be specified may not necessarily be constant with time and may be functions of time. For instance, we describe two combinations of D and Q_R , and R and Q_R in the following.

For constant molar holdup assumption, Eqs.(2)-(4) become

$$g_j^M = 0 \quad (j = 1, \dots, N-1) \quad (27)$$

and

$$g_N^M = -D \quad (28)$$

When we specify the values of the distillate D and the reboiler heat duty Q_R as an operating condition, Eq.(28) holds at any instance. Besides, when we assign the reflux ratio R instead of D , D should vary with time. Applying Eq.(20) to Eq.(1) with the relation of Eq.(28) yields

$$\dot{U}_N^{v+1} - \dot{U}_N^v = -\delta \{ \omega \dot{D}^{v+1} + (1-\omega) \dot{D}^v \} \quad (29)$$

By taking a summation of Eq.(9) from $j = 2$ to N , we obtain

$$\frac{d}{dt} \sum_{j=2}^N U_j h_j = \sum_{j=2}^N g_j^h \quad (30)$$

where

$$\sum_{j=2}^N g_j^h = Q_R - V_2 H_2 + L_1 h_1 \quad (31)$$

Again we can rewrite Eq.(30) as a difference equation using Eq.(20).

$$\sum_{j=2}^N \dot{U}_j^{v+1} h_j^{v+1} - \sum_{j=2}^N \dot{U}_j^v h_j^v = \delta \left\{ \omega \sum_{j=2}^N \dot{g}_j^{v+1} h_j^{v+1} + (1-\omega) \sum_{j=2}^N \dot{g}_j^v h_j^v \right\} \quad (32)$$

From Eqs.(32) and (29) with the relationships, $V_2 = (1+R)D$ and $L_1 = RD$, we can derive the following equation to evaluate the distillate rate $\dot{D}$ at time $t + \delta$.

$$\dot{D}^{v+1} = \frac{1}{\delta \omega \{ (1+R) \dot{H}_2^{v+1} - R \dot{h}_1^{v+1} - \dot{h}_N^{v+1} \}} \left\{ \delta \omega Q_R - \left[\sum_{j=2}^{N-1} \dot{U}_j^{v+1} h_j^{v+1} + \{ \dot{U}_N^{v+1} \dot{h}_N^{v+1} - \sum_{j=2}^N \dot{U}_j^v h_j^v \} \right] + \delta (1-\omega) \sum_{j=2}^N \dot{g}_j^v h_j^v \right\} \quad (33)$$

With the known value of $\dot{D}$, the bottom holdup $\dot{U}_N^{v+1}$ is obtained from Eq.(29). Then, the vapor and liquid flow rates on each stage at time $t + \delta$ are calculated as follows.

$$\dot{V}_N^{v+1} = \frac{Q_R - \dot{D} \dot{h}_{N-1}^{v+1} - \dot{g}_N^{v+1}}{\dot{H}_N^{v+1} - \dot{h}_{N-1}^{v+1}} \quad (34)$$

$$\dot{L}_{N-1}^{v+1} = \dot{V}_N^{v+1} - \dot{D}^{v+1} \quad (35)$$

$$\dot{V}_j^{v+1} = \frac{(\dot{H}_{j+1}^{v+1} - \dot{h}_{j-1}^{v+1}) \dot{V}_{j+1}^{v+1} - (\dot{h}_j^{v+1} - \dot{h}_{j-1}^{v+1}) \dot{L}_j^{v+1} - \dot{g}_j^{v+1}}{\dot{H}_j^{v+1} - \dot{h}_{j-1}^{v+1}} \quad (36)$$

$$\dot{L}_{j-1}^{v+1} = \dot{V}_j^{v+1} - \dot{D}^{v+1} \quad (37)$$

where

$$\dot{g}_j^{v+1} = \frac{\dot{U}_j^{v+1} \dot{h}_j^{v+1} - \dot{U}_j^v h_j^v - \delta (1-\omega) \dot{g}_j^h}{\delta \omega} \quad (38)$$

2.3 Calculation Algorithm

Since the integration formulas described above are implicit, the calculation for succeeding each time increment must be iterative.

For a given column specifications and initial and operating conditions the calculation steps are summarized below.

Step 1 Solve Eqs.(25) and (26) for $\dot{T}_j^{v+1}$ and $\dot{x}_{j,i}^{v+1}$ from the bottom ($j = N$) to the top stage ($j = 2$) with the convergence criterion.

$$\left| \sum_{i=1}^C \dot{x}_{j,i}^{v+1} - 1 \right| \leq \epsilon_T \quad (39)$$

Then, calculate $\dot{x}_{1,i}^{v+1}$ with Eq.(22). When the temperature of the reflux is assigned to its bubble point, execute a bubble point calculation to get $\dot{T}_1^{v+1}$.

After each calculation through the column, vapor compositions $\dot{y}_{j,i}^{v+1}$ are calculated using Eqs.(13) and (16). If the plate efficiency is specified as other than unity, vapor temperature $\dot{T}_j^{v+1}$ is obtained from a dew-point calculation.

Step 2 Evaluate vapor and liquid enthalpies $\dot{H}_j^{v+1}$, $\dot{h}_j^{v+1}$ from the values of $\dot{x}_{j,i}^{v+1}$, $\dot{y}_{j,i}^{v+1}$, $\dot{T}_j^{v+1}$, $\dot{T}_j^{v+1}$ obtained in Step 1.

Step 3 Calculate $\dot{D}$ from Eq.(33) if R and Q_R are specified. Calculate $\dot{U}_N^{v+1}$ from Eq.(29), then $\dot{V}_j^{v+1}$ and $\dot{L}_j^{v+1}$ using Eqs.(34) ~ (38) from $j = N$ to 2.

Step 4 Check the transient component material balance around the distillation process defined by the following equation.

$$\phi = \frac{\sum_{j=1}^N \dot{U}_j \dot{x}_{j,i} - \delta (1-\omega) \dot{D} \dot{x}_{1,i}}{\sum_{j=1}^N \dot{U}_j^{v+1} \dot{x}_{j,i}^{v+1} + \delta \omega \dot{D}^{v+1} \dot{x}_{1,i}^{v+1}} \quad (40)$$

convergence criteria:

$$|\phi_{\max} - 1| < \epsilon_\phi \quad (41)$$

When Eq.(41) is satisfied, forward the calculation to the next time step while holding the calculated values at time $t + \delta$ as the stored values at time t . Otherwise, correct $\dot{x}_{j,i}^{v+1}$ using the overall normalized θ method as

Table 1 Specifications for numerical example

Column:	12 stages (including total condenser and still)
System:	Ethanol (1) / 2-Propanol (2) / Water (3)
Feed:	15 mol
Feed Composition:	0.100 (1) / 0.025 (2) / 0.875 (3)
Total pressure:	760 mmHg
Heat duty:	95.3 W
Reflux temperature:	35 °C
Distillate:	2.58×10^{-4} mol / s
Holdup:	0.5 mol / reflux drum
	0.05 mol / stage
Murphree plate efficiency:	$E_{j,i}^{MV} = 1$
Convergence criteria:	$\varepsilon_T = 10^{-12}$, $\varepsilon_\phi = 10^{-8}$

Fig. 2 Distillation curves of numerical example

follows (Mori *et al*,1994) and return to Step 1.

$$v \dot{x}_{j,i,co}^1 = \theta_j \phi_j^v \dot{x}_{j,i,ca}^1 \quad (42)$$

where

$$\theta_j = \left[\sum_{i=1}^n \phi_i^v \dot{x}_{j,i,ca}^1 \right]^{-1} \quad (43)$$

and ϕ_i is defined in Eq.(40).

3. Numerical Examples and Discussion

The algorithm described above is coded in Fortran 77 and the program is executed on a work station hp712/60 (Hewlett Packard Co.) with double precision. We distinguish the problems as Type I, D and Q_R specified, and Type II, R and Q_R specified. Type I problems may arise from industrial batch distillation columns and Type II problems from laboratory experimental columns. To start the simulation, the column is first brought up to the steady state at total reflux, then distillate withdrawal is started at time $t = 0$. **Table 1** shows the problem specifications (Type I) for separating a ternary mixture. Constant liquid molar holdup is assumed for the condenser and on each tray. The column is operated at atmospheric pressure and pressure drop is neglected. The temperature of the reflux is kept constant

Fig. 3 Time variation of relative errors of water composition in distillate

Fig. 4 Comparison of approximation accuracy of the proposed method

throughout the operation. The physical properties of the pure components are taken from Daubert and Danner (1989) and the activity coefficients for VLE calculation are estimated using ASOG (Tochigi *et al*,1990). In this condition the vapor rate at the bottom V_N is about 2.3×10^{-3} mol/s. The calculation will terminate when the fraction distilled becomes 33.3 % (molar base).

3.1 Weighting factor ω and integration accuracy

Type I problem is solved using the proposed algorithm with a different combination of a time increment δ and a weighting factor ω to examine the integration accuracy. To obtain the reference solution, the same problem is solved using the Runge-Kutta method with successively decreased time increment ($\delta = 3.6 \times 10^{-1} \sim 3.6 \times 10^{-4}$ s). Since the distillation curves coincide within a tolerance of $\pm 10^{-5}$ between the results obtained with $\delta = 3.6 \times 10^{-3}$ and $\delta = 3.6 \times 10^{-4}$, hereafter we employ the latter, shown in **Fig. 2**, as the reference solution. In **Fig. 3** the deviation of the calculated results using the Runge - Kutta method with different time increments is presented as relative errors to the reference solution using the water composition in the distillate. Comparing Fig.2 with Fig.3 shows that the error becomes large where the change in composition is large. This region is also important in that

Table 2 CPU time required for whole calculations

	0.5	0.6	ω 0.7	0.8	0.9	1.0	R-K
1.8×10^2	38 [†]	38	41	44	46	49	n.c.
7.2×10^1	54*	58	60	64	67	71	n.c.
3.6×10^1	68*	74	80	92	90	95	n.c.
1.8×10^1	91*	100	105	112	117	124	n.c.
7.2×10^0	147*	150*	160	167	179	182	n.c.
3.6×10^0	224*	219*	232*	239*	250	261	n.c.
1.8×10^0	n.c.	331*	343*	360*	369*	383*	565
7.2×10^{-1}	n.c.	589*	613*	617*	632*	646*	1138
3.6×10^{-1}	n.c.	932*	953*	1010*	1034*	1052*	2141
1.8×10^{-1}	n.c.	1457*	1488*	1512*	1536*	1560*	4209
7.2×10^{-2}	n.c.	3106*	3085*	3114*	3139*	3204*	9928
3.6×10^{-2}	n.c.	5348	5275	5479	5569	5715	18604*

[†]: CPU time [s]
n.c.: not converged
*: satisfies a condition, maximum error < 3.6×10^{-4} (see Fig. 4)

Fig. 5 Acceleration effect of the normalized θ method

higher accuracy is required for scheduling the operation.

In Fig. 4 the maximum relative errors evaluated in the same manner of Fig. 3 are plotted against the time increment δ with the parameter of the weighting factor ω . The results with $\omega = 0.5$ show higher accuracy compared to other values. They also reveal a trend in which the accuracy first becomes higher and then lower with decreasing time increment. Further investigation revealed this unfavorable behavior is due to amplified error in evaluating slopes $g_{j,i}^m$ and g_j^h at small time increment and can be avoided by using more strict convergence criteria ε_T and ε_ϕ . However, if we accept a level of maximum error up to 3.6×10^{-4} , the necessary time increment can be as large as $\delta = 7.2 \times 10^1$ for $\omega = 0.5$. These results prove that Eq.(20) has enough accuracy for this calculation, as was expected.

3.2 Calculation time

Table 2 shows the CPU time required for the whole calculation with different combinations of time increment δ and weighting factor ω . There are no large differences among the values with the same time increment and different weighting factors. In order to obtain the same accuracy, say a maximum relative error $< 3.6 \times 10^{-4}$, the proposed method ($\delta = 7.2 \times 10^1$, $\omega = 0.5$) requires only 1/300 of the

Table 3 Experiment and calculation conditions

Column:	12stages (including total condenser and still)
System:	Ethanol (1) / 2-Propanol (2) / Water (3)
Feed:	20 mol
Feed Composition:	0.25 (1) / 0.05 (2) / 0.70 (3)
Total pressure:	760 mmHg
Heat duty:	127.7 W (experiment) 133.5 W (calculation)
Reflux temperature:	20 °C
Reflux ratio:	6.9 (time controlled)
Holdup:	0.04 mol / stage
Murphree plate efficiency:	$E_{j,i}^{MV} = 0.75$

Fig. 6 Comparison of experimental and calculated distillate compositions

Runge - Kutta method ($\delta = 3.6 \times 10^{-2}$).

The effect of the overall normalized θ method (Step 4) on reducing the number of iterations for each time step is shown in Fig. 5. This effect is significant at larger time increments compared with a simple direct iteration.

3.3 Comparison with experiment

The experimental and calculation conditions (Type II problem) are shown in Table 3. The 10-stage Oldershaw column used has a 32 mm inner diameter and a 28 mm tray spacing. From preliminary experiments the molar liquid holdup on each plate and the heat duty at reboiler are determined. As for the plate efficiency, although there are many arguments, we assign $E_{j,i}^{MV} = 0.75$ for all plates and components as a rough estimation. The experimental procedure consists of repeating the following three steps ; (i) total reflux operation and vapor rate measurement , (ii) constant reflux operation, and (iii) distillate sampling for analysis. This operation mode is also considered in the simulation.

Figure 6 shows a comparison of the experimental data and the calculated results. There is a slight difference due to the assumption of no heat loss, constant heat duty, constant molar holdup, and constant plate efficiencies. The overall agreement, however, seems to be fairly good.

In order to adapt the proposed algorithm to a variety of situations, the readers may choose other problem specifications and select more realistic models, such as variable

liquid holdup and tray hydraulics. This will be further discussed in detail elsewhere.

Conclusion

We proposed a calculation algorithm for simulating batch distillation process based on a successive stagewise calculation. The results of the numerical examples show a higher accuracy and a lesser CPU time compared with the Runge – Kutta method. In one particular case, with the weighting factor $\omega = 0.5$, the proposed method can take a time increment up to 10^3 greater in value than that of the Runge – Kutta method to yield equivalent accuracy and also the CPU time may decrease by 1/300. A comparison of the simulation with experimental results suggests the adequacy of the proposed method.

Since the proposed algorithm is based on a stagewise calculation, it can be applied easily to a wide variety of situations and configuration of batch distillation processes.

Nomenclature

c	= total number of components	[-]
D	= molar distillate rate	[mol·s ⁻¹]
E^{MV}	= Murphree vapor-phase stage efficiency	[-]
E^V	= vaporization stage efficiency	[-]
f	= function	[-]
g^M	= total material balance	[mol·s ⁻¹]
g^m	= component material balance	[mol·s ⁻¹]
g^h	= heat balance	[J·mol ⁻¹]
H	= vapor molar enthalpy	[J·mol ⁻¹]
h	= liquid molar enthalpy	[J·mol ⁻¹]
K	= vapor-liquid equilibrium ratio	[-]
L	= molar liquid flow rate	[mol·s ⁻¹]
N	= total number of plates in distillation column	[-]
Q_C	= heat load at condenser	[W]
Q_R	= heat load at reboiler	[W]
R	= reflux ratio ($\equiv L_1/D$)	[-]
t	= operation time	[s]
U	= liquid molar hold up	[mol]

V	= molar vapor flow rate	[mol·s ⁻¹]
x	= liquid mole fraction	[-]
y	= vapor mole fraction	[-]
δ	= time increment for numerical integration	[s]
ε	= convergence criterion	[-]
θ	= correction factor	[-]
λ	= heat of vaporization	[J·mol ⁻¹]
v	= indication of operation time t	[-]
ϕ	= objective function	[-]
ω	= weighting factor	[-]
<Subscript>		
ca	= calculated	
co	= corrected	
i	= component	
j	= stage	
$\cdot$	= derivative	
<Superscript>		
$^{\circ}$	= pure component	
$*$	= equilibrium state	

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