Study on Jocabi Iteration and Matrix Dissociation in Batch Distillation Simulation

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Abstract. A new method including dissociation of the complicated partial differential matrix and iterative computation of Jocabi matrix was used to solve a system of linear equations and further was used to investigate batch distillation simulation preventing the analog distortion problem. Results simulated showed that distillation curves on separation system with ethanol, n-propanol and n-butanol could have reflected actual concentration distribution of each component and indirectly indicated that new logical operation with assignment operator of partial differential matrix could effectively have been put into practice avoiding computational divergence in numerical calculation and keeping stability of the simulation system.

Introduction

Batch distillation is a unit operation widely used in the fields such as fine chemical industry and pharmaceutical industry [1, 2, and 3] because it can separate multi-component liquid mixtures with different separation requirements by using a single distillation column and can allow a wide range of variation for different feed ingredient, which is especially suitable for the occasions where the processing capacity is smaller and the separation task is often changed. In current experimental investigations operational control of distillation column, scale-up of distillation column and operational calculation of distillation column had become hot spots [4, 5, 6 and 7]. Moreover, process simulation of batch distillation as an important mean also had played important roles for designing future new column and for forecasting operational state whether batch physical distillation or batch reactive distillation [8, 9, 10, 11 and12]. However, concentration corrections for each column plate still are an unsolved problem to ensure that the simulation results can be convergent at each time step although simple correction had been made [13]. Thus, a new equation set regarding concentration correction will be proposed and a new approach will also be used to search for the solution of the mathematical model in this work.

Mathematical Model Establishment

Assume that there were m components being separated in a batch distillation column, thus overall material balance equation for any i component in m components could have been written as
\[
\left[ t \right] \left( d_{i} \right)_{\tau} = \sum_{j=0}^{m} \left[ \left( U_{i,j}^{\tau} \right)_{\tau} - \left( U_{i,j}^{\tau} \right)_{\tau} \right].
\]

(1)

Where \( \tau, (d_{i})_{\tau} \) and \( (U_{i,j})_{\tau} \) were a distillation time, an actual value of distillation rate of any \( i \) component between \( \tau \) time and \( \tau + 1 \) time and an actual storage value for any \( i \) component in any \( j \) column plate between \( \tau \) time and \( \tau + 1 \) time, respectively.

Using implicit integration the equation (1) could have been changed to become

\[
- \frac{1}{\mu} \left( d_{i} \right)_{\tau} + \left( \frac{1}{\mu + \Delta \tau} \sum_{j=0}^{m} \left( U_{i,j}^{\tau} \right)_{\tau} \right) = \left( d_{i}^{\tau} \right)_{\tau} + \left( \frac{1}{\mu + \Delta \tau} \sum_{j=0}^{m} \left( U_{i,j}^{\tau} \right)_{\tau} \right).
\]

where \( \mu \) was an implicit integral constant used.

In order to be sure that overall component concentration in any \( j \) column plate was normalized within each time step \( \Delta \tau \), thus concentration correction must have been done before the next time data were performed.

Herein a set of weighting factors \( \theta_{1}, \theta_{2}, \ldots, \theta_{m}, (\theta_{j} > 0) \), were assumed to make

\[
\left( \frac{U_{i,j}}{d_{i}} \right)_{\tau} = \theta \left( \frac{U_{i,j}}{d_{i}} \right)_{\tau} \quad (i=1, 2, 3, \ldots, m \text{ and } j=1, 2, 3, \ldots, N+1).
\]

(3)

where \( \theta \) \left( \frac{U_{i,j}}{d_{i}} \right) \) and \( \left( \frac{U_{i,j}}{d_{i}} \right) \) were a weight factor for any \( j \) column plate, a ratio between calculated \( U_{i,j} \) and calculated \( d_{i} \) and a ratio between actual \( U_{i,j} \) and actual \( d_{i} \), respectively.

Furthermore, the equation (2) became

\[
- \frac{1}{\mu} \left( d_{i} \right)_{\tau} + \left( \frac{1}{\mu + \Delta \tau} \sum_{j=0}^{m} \left( U_{i,j}^{\tau} \right)_{\tau} \right) = \left( d_{i}^{\tau} \right)_{\tau} + \left( \frac{1}{\mu + \Delta \tau} \sum_{j=0}^{m} \left( U_{i,j}^{\tau} \right)_{\tau} \right) \lambda_{j} + \sum_{j=0}^{m} \theta \left( \frac{U_{i,j}}{d_{i}} \right)_{\tau} + \theta_{j} \left( \frac{U_{i,j}}{d_{i}} \right)_{\tau}.
\]

(4)

where \( K \) and \( \lambda_{j} \) were liquid vapor ratio and a ratio between liquid holdup at condenser of column top and vapor velocity, respectively.

Thus, an actual distillation rate of \( i \) component at condenser of column top and at \( \tau + 1 \) time became

\[
\left( d_{i}^{\tau + 1} \right)_{\tau} = \frac{- \frac{1}{\mu} \left( d_{i} \right)_{\tau} + \left( \frac{1}{\mu + \Delta \tau} \sum_{j=0}^{m} \left( U_{i,j}^{\tau} \right)_{\tau} \right) + \lambda_{j} \sum_{j=0}^{m} \theta \left( \frac{U_{i,j}}{d_{i}} \right)_{\tau} + \theta_{j} \left( \frac{U_{i,j}}{d_{i}} \right)_{\tau}}{1 + \left( \frac{1}{\mu + \Delta \tau} \sum_{j=0}^{m} \left( U_{i,j}^{\tau} \right)_{\tau} \right) \lambda_{j} + \sum_{j=0}^{m} \theta \left( \frac{U_{i,j}}{d_{i}} \right)_{\tau} + \theta_{j} \left( \frac{U_{i,j}}{d_{i}} \right)_{\tau}}.
\]

(5)

The equation (5) showed that actual distillation rates of the components at condenser of column top and at \( \tau + 1 \) time were merely functions regarding weight factors \( \theta_{1}, \theta_{2}, \ldots, \theta_{m} \), while each term in the equation (5) could have been calculated from given conditions or other values drawn from Thomas Algorithm.

These weighting factors must have ensured that following equation set \( g' \) always had been true synchronously at \( \tau + 1 \) time, that was

\[
g_{1}(\theta_{1}, \theta_{2}, \ldots, \theta_{m}) = \sum_{j=0}^{m} \left( d_{i}^{\tau + 1} \right)_{\tau} - D = 0
\]

\[
g_{2}(\theta_{1}, \theta_{2}, \ldots, \theta_{m}) = \sum_{j=0}^{m} \theta \left( \frac{U_{i,j}}{d_{i}} \right)_{\tau} \left( d_{i}^{\tau + 1} \right)_{\tau} - H_{1} = 0
\]

\[
\vdots
\]

\[
g_{m}(\theta_{1}, \theta_{2}, \ldots, \theta_{m}) = \sum_{j=0}^{m} \theta \left( \frac{U_{i,j}}{d_{i}} \right)_{\tau} \left( d_{i}^{\tau + 1} \right)_{\tau} - H_{m} = 0
\]

(6)

where \( D \) and \( H_{j} \) were constant distillation rate assumed at column top and liquid holdup at column
plate except for condenser of column top.

Moreover, in order to make calculation easier above the equation set \( g \) could have been simply become following equation set \( g \) without dimension:

\[
\begin{align*}
\frac{g_1(\theta, \theta_2, \ldots, \theta_{N+1})}{D} &= \frac{1}{n} \sum_{i=1}^{n} \left[ d_{i1} \right] - 1 = 0 \\
\frac{g_j(\theta, \theta_2, \ldots, \theta_{N+1})}{H_j} &= \frac{1}{\sum_{i=1}^{n} \theta_j \left[ U_{ij} \right]} \left[ d_{ij} \right] - 1 = 0 \\
\frac{g_{N+1}(\theta, \theta_2, \ldots, \theta_{N+1})}{H_{N+1}} &= \frac{1}{\sum_{i=1}^{n} \theta_j \left[ U_{N+1 i} \right]} \left[ d_{N+1 i} \right] - 1 = 0
\end{align*}
\]  

(7)

Model Solution

Observing the first equation of equation set (7) we knew that distillation rate had been independent to those weight factors whether \( \tau \) time or \( \tau+1 \) time. Thus, below N+1 equations of equation (7) with weight factors \( \theta_{j1, 2, 3, \ldots, n+1} \) could have been used to calculate weight factors. These equations used could have been written as following matrix format

\[
AX = G.
\]

(8)

Where matrix A, matrix X and matrix G could have been written as follows:

\[
A = \begin{bmatrix}
\frac{\partial g_1}{\partial \theta_1} & \ldots & \frac{\partial g_1}{\partial \theta_{N+1}} \\
\vdots & \ddots & \vdots \\
\frac{\partial g_{N+1}}{\partial \theta_1} & \ldots & \frac{\partial g_{N+1}}{\partial \theta_{N+1}}
\end{bmatrix}
\]

(9)

\[
X = \begin{bmatrix}
\Delta \theta_1 \\
\vdots \\
\Delta \theta_j \\
\vdots \\
\Delta \theta_{N+1}
\end{bmatrix}
\]

(10)

and

\[
G = \begin{bmatrix}
-g_1 \\
\vdots \\
-g_j \\
\vdots \\
-g_{N+1}
\end{bmatrix}
\]

(11)

In order to make matrix G with I line have become a zero matrix with I line by computer operation in precision range, mathematical processing must have been done for matrix A with I line and J row and for matrix X with I line and one row, where \( i = 1, 2, 3, \ldots, N+1 \) and \( j = 1, 2, 3, \ldots, N+1 \).
On the one hand, after superscripts of \( \left( \frac{U^{(\tau)}}{d^{(\tau)}} \right) \) and of \( (d^{(\tau)}) \), at \( \tau + 1 \) time were neglected simultaneously each element of matrix A could have processed in terms of every line.

Thus, for the first line, following element expressions could have been written:

\[
\begin{align*}
\frac{\partial \xi_i}{\partial \theta_j} &= \frac{1}{H_i} \left[ \sum_{m=1}^{n} \left( \frac{U_{j,m}}{d_{i,m}} \right) (d_{i,m}) + \theta_i \sum_{m=1}^{n} \left( \frac{U_{j,m}}{d_{i,m}} \right) \frac{\partial}{\partial \theta_j} (d_{i,m}) \right] \\
\frac{\partial \xi_i}{\partial \theta_k} &= \frac{1}{H_i} \left[ \sum_{m=1}^{n} \left( \frac{U_{j,m}}{d_{i,m}} \right) \frac{\partial}{\partial \theta_k} (d_{i,m}) \right] \\
\frac{\partial \xi_i}{\partial \theta_l} &= \frac{1}{H_i} \left[ \sum_{m=1}^{n} \left( \frac{U_{j,m}}{d_{i,m}} \right) \frac{\partial}{\partial \theta_l} (d_{i,m}) \right] \\
\frac{\partial \xi_i}{\partial \theta_m} &= \frac{1}{H_i} \left[ \sum_{m=1}^{n} \left( \frac{U_{j,m}}{d_{i,m}} \right) \frac{\partial}{\partial \theta_m} (d_{i,m}) \right]
\end{align*}
\]

(12)

For the line \( I (I = 1, 2, 3 \cdots N + 1) \), following element treatment could have been done:

\[
\begin{align*}
\frac{\partial \xi_i}{\partial \theta_j} &= \frac{\theta_i}{H_i} \sum_{m=1}^{n} \left( \frac{U_{j,m}}{d_{i,m}} \right) \frac{\partial}{\partial \theta_j} (d_{i,m}) \\
\frac{\partial \xi_i}{\partial \theta_k} &= \frac{\theta_i}{H_i} \sum_{m=1}^{n} \left( \frac{U_{j,m}}{d_{i,m}} \right) \frac{\partial}{\partial \theta_k} (d_{i,m}) \\
\frac{\partial \xi_i}{\partial \theta_l} &= \frac{\theta_i}{H_i} \sum_{m=1}^{n} \left( \frac{U_{j,m}}{d_{i,m}} \right) \frac{\partial}{\partial \theta_l} (d_{i,m}) \\
\frac{\partial \xi_i}{\partial \theta_m} &= \frac{\theta_i}{H_i} \sum_{m=1}^{n} \left( \frac{U_{j,m}}{d_{i,m}} \right) \frac{\partial}{\partial \theta_m} (d_{i,m}) \\
\frac{\partial \xi_i}{\partial \theta_n} &= \frac{\theta_i}{H_i} \sum_{m=1}^{n} \left( \frac{U_{j,m}}{d_{i,m}} \right) \frac{\partial}{\partial \theta_n} (d_{i,m}) \\
\frac{\partial \xi_i}{\partial \theta_{n+1}} &= \frac{\theta_i}{H_i} \sum_{m=1}^{n} \left( \frac{U_{j,m}}{d_{i,m}} \right) \frac{\partial}{\partial \theta_{n+1}} (d_{i,m})
\end{align*}
\]

(13)

For the line \( N+1 \), following element format could have been drawn:

\[
\begin{align*}
\frac{\partial \xi_i}{\partial \theta_j} &= \frac{\theta_i}{H_i} \sum_{m=1}^{n} \left( \frac{U_{j,m}}{d_{i,m}} \right) \frac{\partial}{\partial \theta_j} (d_{i,m}) \\
\frac{\partial \xi_i}{\partial \theta_k} &= \frac{\theta_i}{H_i} \sum_{m=1}^{n} \left( \frac{U_{j,m}}{d_{i,m}} \right) \frac{\partial}{\partial \theta_k} (d_{i,m}) \\
\frac{\partial \xi_i}{\partial \theta_l} &= \frac{\theta_i}{H_i} \sum_{m=1}^{n} \left( \frac{U_{j,m}}{d_{i,m}} \right) \frac{\partial}{\partial \theta_l} (d_{i,m}) \\
\frac{\partial \xi_i}{\partial \theta_m} &= \frac{\theta_i}{H_i} \sum_{m=1}^{n} \left( \frac{U_{j,m}}{d_{i,m}} \right) \frac{\partial}{\partial \theta_m} (d_{i,m}) \\
\frac{\partial \xi_i}{\partial \theta_{n+1}} &= \frac{\theta_i}{H_i} \sum_{m=1}^{n} \left( \frac{U_{j,m}}{d_{i,m}} \right) \frac{\partial}{\partial \theta_{n+1}} (d_{i,m}) \\
\frac{\partial \xi_i}{\partial \theta_{n+2}} &= \frac{1}{H_i} \sum_{m=1}^{n} \left( \frac{U_{j,m}}{d_{i,m}} \right) (d_{i,m}) + \theta_i \sum_{m=1}^{n} \left( \frac{U_{j,m}}{d_{i,m}} \right) \frac{\partial}{\partial \theta_{n+1}} (d_{i,m})
\end{align*}
\]

(14)

where
and where \( i = 1, 2, 3 \ldots, m \) and \( j = 1, 2, 3 \ldots, N + 1 \).

In order to facilitate computer operation, the above matrix \( A \) was split into a sum of matrix \( B \) and matrix \( C \)\[^{[14]} \]. That was

\[
B = \begin{bmatrix}
B_{11} & \cdots & 0 & \cdots & 0 \\
\vdots & \ddots & \vdots & \ddots & \vdots \\
0 & \cdots & B_{j,j} & \cdots & 0 \\
\vdots & \ddots & \vdots & \ddots & \vdots \\
0 & \cdots & 0 & \cdots & B_{N,N,j}
\end{bmatrix}
\]

(16)

and

\[
C = \begin{bmatrix}
C_{11} & \cdots & C_{1,j} & \cdots & C_{1,N}
\vdots & \ddots & \vdots & \ddots & \vdots \\
\vdots & \ddots & \vdots & \ddots & \vdots \\
C_{N,1} & \cdots & C_{N,j} & \cdots & C_{N,N}
\end{bmatrix}.
\]

(17)

Where

\[
B_{j,i} = \frac{1}{H_i} \sum_{\tau=1}^{m} \left[ \frac{u_{\tau}}{d_i} \right] (d_{\tau})_i
\]

(18)

and

\[
C_{i,j} = \frac{\theta_i}{H_i} \sum_{\tau=1}^{m} \left[ \frac{u_{\tau}}{d_i} \right] \frac{\partial}{\partial \theta_j} (d_{\tau})_i.
\]

(19)

and where \( i = 1, 2, 3 \ldots, m \), \( j = 1, 2, 3 \ldots, N + 1 \), \( \tau = 1, 2, 3 \ldots, N + 1 \) and \( J = 1, 2, 3 \ldots, N + 1 \).

On the other hand, each element of matrix \( X \) could have written as

\[
\Delta \theta_j = \theta_j^{+1} - \theta_j,
\]

(20)

where \( k \) is iterations number of times.

Using iterative computation of Jacobi matrix solution of above equation set (8), matrix \( X \), could have been drawn after number of \( k \) times for the iterations were performed by computer. Furthermore, after the calculation accuracy meted the requirement weight factors value \( \theta_j \) also could have been calculated from following equation

\[
\theta_j^{+1} = \theta_j + \Delta \theta_j,
\]

(21)

Therefore, an actual distillation rate \( (d_{\tau})_i \) at \( \tau + 1 \) time for each component separated could further have been computed using weight factor \( \theta_j^{+1} \).

However, an actual concentration of the component at column top often was used in simulation, thus herein calculation equations of the actual concentration at column top, any \( j \) plate and at \( \tau + 1 \) time were also given. Expressions were

\[
x_{j,0} = \frac{(d_{\tau})_j}{\sum_{i=1}^{m} (d_{\tau})_i}
\]

(22)

and
\[
\sum_{i=1}^{m} \frac{U_{i,j}}{d_i} (d_i)_{w_i} = \sum_{i=1}^{N+1} \frac{U_{i,j}}{d_i} (d_i)_{w_i}
\]

(23)

Where \(x_{i,0}\) and \(x_{i,j}\) respectively were concentration of i component at column top condenser and concentration of i component at any j plate, and where \(i=1,2,3\ldots m\) and \(i=1,2,3\ldots N+1\).

**Results and Discussion**

After conventional Thomas matrix operation was applied to solve every component concentration in multi-component mixture at column top and at next time abovementioned multi-stage revision were performed to make sure that the sum of concentrations had always become integer one whether this time or next time avoiding error accumulation and keeping computational convergence. Calculation programs including abovementioned computational sub-programs were used to simulate batch distillation process among ethanol, n-propanol and n-butanol. Schematic diagram of distillation product composition at the column top with distillation time under the conditions given were plotted in Figure 1. As seen in Figure 1 formed by simulation, ethanol was first distilled as a light component to become a product at the column top and then n-propanol was distilled as an intermediate component to become the second product in terms of product purity required. Finally, the heavy component was distilled from the column top. Thus, identification of distillation time for different products could have been made from these curves simulated.

![Figure 1](https://example.com/figure1.png)

Figure 1. Schematic diagram of routine operation simulation between component concentrations of column top and distillation time.

Afterwards, under the simulated conditions experimental study on the products distilled and collected at the column top were done to verify the accuracy of the simulation. Using same time step products collected at the column top were tested by gas phase chromatography and three kinds of component concentration data formed could have met results simulated. In other words, experimental results showed that the batch distillation simulation among ethanol, n-propanol and n-butanol had been reasonable.

In conclusion, Jocabi matrix could have been succeeded in solving a problem of weight factors for any j plate to prevent computational divergence in numerical calculation and in ensuring effectiveness of the batch distillation simulation.
Conclusions

Through the application of Jocabi iteration and matrix splitting in batch distillation simulation for three components’ system, following conclusions could have been drawn:

1) Matrix splitting could have succeeded in solving the problem of assignment operator for a matrix with a complicated partial differential element.
2) Weight factors assumed could have corrected calculated distillation rate value of component at column top from Thomas matrix calculation.
3) Weight factors of each plate could have achieved by using Jocabi iteration in computer and furthermore obtained results could have been used to calculate an actual concentration of every component at each plate and at next step time.
4) Concentration distribution of components separated in simulation curves plotted could have been validated by experimental analysis and indirectly could have proved that new logical operation with assignment operator of partial differential matrix could effectively have solved the divergence problem of numerical calculation.
5) Mathematical models formed and computational programs derived would have had a possibility to become a basis of operational calculation of batch distillation such as output value per hour with a reflux ratio or with a theoretical plate number.

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Nomenclature

A  Matrix (-)
B  Matrix (-)
C  Matrix (-)
D  Actual value of total distillation rate at column top (mol s\(^{-1}\))
d  Actual value of a component distillation rate at column top (mol s\(^{-1}\))
G  Matrix (-)
H  Liquid holdup (-)
g  Equation set (-)
g  Equation set (mol)
I  Line number of a matrix (-)
J  Row number of a matrix (-)
K  Liquid vapor ratio (-)
k  Number of times for iterations (-)
m  Total component number (-)
N  Total theoretical plate number (-)
t  Distillation time (s)
U  Actual storage value of material (mol)
X  Matrix (-)
x  Concentration of a component (mol mol\(^{-1}\))
λ  Ratio between liquid holdup at condenser of column top and vapor velocity (s)
µ  Implicit integral constant (-)
θ  Weight factor (-)
Δ  Change value (-)

Subscript

c a  Calculated value
co  Actual value
i  Number of components
j  Number of the theoretical plate

**Superscript**
0  Number zero of the theoretical plate or initial value
τ  Time series number

**References**


