CHAPTER IV

TRIDIAGONAL MATRIX FOR DISTILLATION

Product distribution for multicomponent distillation in complex columns can be computed by this tridiagonal matrix algorithm. Method is simple, fast and numerically stable.

A new iterative is developed for solving problems of multicomponent distillation in complex columns. This method employs the tridiagonal matrix algorithm for the solution of the linearized material balance equations, and uses Newton's method for the convergence of column temperature profile. The material balance is solved simultaneously for each component, and therefore no matching is required. Both distributed and non-distributed components are handled with equal ease. The computational procedure is simple, fast, and numerically stable, and can be readily adapted to digital computers of moderate size.

4.1 MATHEMATICAL MODEL

For the convenience of deriving the general working equations, a hypothetical system as shown in Figure 4.1 is considered as the model column. This column has n equilibrium stages including a condenser (partial, total or compound condenser) and a reboiler. The stages (trays or plates) are numbered from top to bottom with the condenser as the first stage and the reboiler as the nth stage. It is assumed that one feed stream F_j, one vapour side stream W_j, one liquid side stream U_j, and one intercooler or interheater Q_j exist at each stage except for the condenser

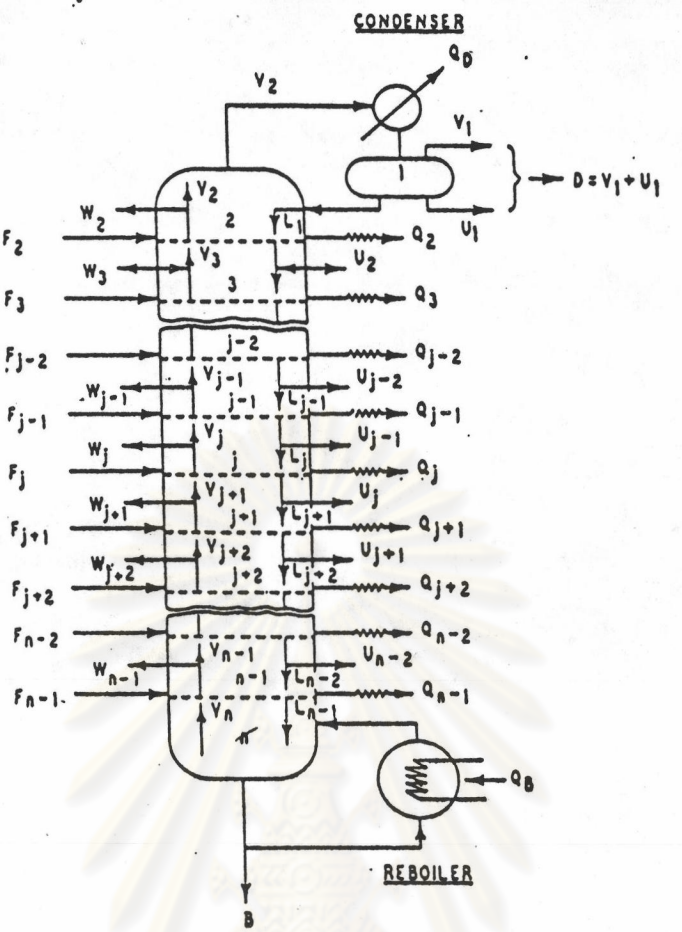

Figure 4.1. A material balance is solved simultaneously for each component.

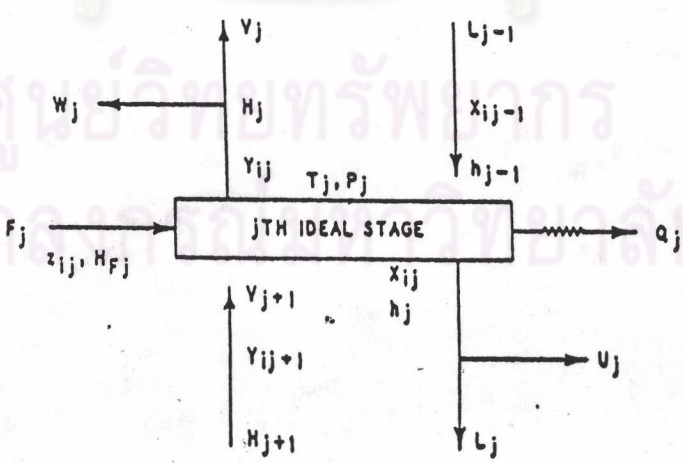

Figure 4.2. An ideal equilibrium stage is represented by Equation(4-1)to(4-4)

and the reboiler. This model column can be reduced to any simpler one by setting the undesired quantities to zero. Thus for a conventional column all the quantities of the external streams except F_j, Q_D, Q_B, D and B are zero.

Each stage in the model column is assumed to be an equilibrium stage, that is, the vapor stream leaving the stage is in equilibrium with the liquid stream leaving the same stage. Figure 4.2 shows such an ideal equilibrium stage.

The MESH Equations. There are generally four sets of equations which must be satisfied in a rigorous equilibrium stage calculation. They are the material balance equation(M), the equilibrium equation(E), the summation equation(S) of mole fractions, and the heat balance equation(H). These four sets of equations are designated as MESH equations in this article.

Depending on what variables are chosen and how the material and heat balances are written, there are different way to express the MESH equations. In this work, the material and heat balances are written around each stage and the independent variables are the mole fractions of liquid $x_{i,j}$, the vapor rate profile V_j, and the temperature profile T_j.

Referring to Figures 4.1 and 4.2, the MESH equations for the model column are readily derived as follows:

M-Equation

$$M_{ij}\left(x_{ij},V_j,T_j\right) = L_{j-1}x_{i,j-1} - \left(V_j + W_j\right)y_{ij} - \left(L_j + U_j\right)x_{ij} + V_{j+1}y_{i,j+1} + F_j z_{ij} = 0 \quad (4\text{-}1)$$

E-Equation

$$E_j\left(x_{ij},V_j,T_j\right) = y_{ij} - K_{ij}x_{ij} = 0 \quad (4\text{-}2)$$

S-Equation

$$S_j\left(x_{ij},V_j,T_j\right) = \sum_{i=1}^{m} y_{ij} - 1.0 = 0 \qquad (4\text{-}3)$$

or

$$S_j\left(x_{ij},V_j,T_j\right) = \sum_{i=1}^{m} x_{ij} - 1.0 = 0 \qquad (4\text{-}3a)$$

H-Equation

$$H_j\left(x_{ij},V_j,T_j\right) = L_{j-1}h_{j-1} - \left(V_j + W_j\right)H_j - \left(L_j + U_j\right)h_j + V_{j+1}H_{j+1} + F_jH_{F_j} - Q_j = 0 \qquad (4\text{-}4)$$

Equation (4-1) and (4-2) are now combined and the L's are expressed as functions of V's by an overall material balance of all stages from the condenser through the j th stage.

$$L_j = V_{j+1} + \sum_{k=2}^{j}\left(F_k - W_k - U_k\right) - D \quad , 2 \le j \le n-1 \qquad (4\text{-}5)$$

where,

$$D = V_1 + U_1 \qquad (4\text{-}6)$$

The *M*-equation is then reduced to a tridiagonal matrix from,

$$B_1x_{i1} + C_1x_{i2} = D_1 \qquad (4\text{-}7)$$

$$A_jx_{i,j-1} + B_jx_{ij} + C_jx_{i,j+1} = D_j \quad , 2 \le j \le n-1 \qquad (4\text{-}8)$$

$$A_n x_{i,n-1} + B_n x_{in} = D_n \tag{4-9}$$

or in matrix notation as,

$$\begin{bmatrix} B_1 & C_1 & & & \\ A_2 & B_2 & C_2 & & \\ & A_j & B_j & C_j & \\ & & A_{n-1} & B_{n-1} & C_{n-1} \\ & & & A_n & B_n \end{bmatrix} \begin{bmatrix} x_{i1} \\ x_{i2} \\ x_{ij} \\ x_{i,n-1} \\ x_{in} \end{bmatrix} = \begin{bmatrix} D_1 \\ D_2 \\ D_j \\ D_{n-1} \\ D_n \end{bmatrix} \tag{4-10}$$

or simply,

$$[A_{Bc}]\{x_{ij}\} = \{D_j\}, \qquad 2 \le j \le m \tag{4-10a}$$

where,

$$B_1 = -(V_1 K_{i1} + U_1)\ ;\ C_1 = V_2 K_{i2}\ ; D_1 = 0 \tag{4-11}$$

$$A_j = L_{j-1} = V_j + \sum_{k=2}^{j-1}(F_k - W_k - U_k) - D \quad , \quad 2 \le j \le n-1 \tag{4-12a}$$

$$\begin{aligned} B_j &= -\left[(V_j + W_j) K_{ij} + (L_j + U_j)\right] \\ &= -\left[(V_j + W_j) K_{ij} + V_{j+1} + \sum_{k=2}^{j}(F_k - W_k - U_k) - D + U_j\right], 2 \le j \le n-1 \end{aligned} \tag{4-12b}$$

$$C_j = V_{j+1} K_{i,j+1} \quad , \quad 2 \le j \le n-1 \tag{4-12c}$$

and

$$A_n = V_n + B;\ B_n = -(V_n K_{in} + B)\ ; D_n = 0 \tag{4-13}$$

With the above manipulation of the M and E equation and further manipulations of the S and H equations,the MESH equation for multicomponent separation at constant pressure in a complex column become,

$$M_{ij}\left(x_{ij},V_j,T_j\right)=\left[A_{Bc}\right]\left\{x_{ij}\right\}-\left\{D_j\right\}=0 \quad ; \quad 1\le i\le m \quad \text{and} \quad 1\le j\le n \tag{4-14}$$

$$S_j\left(x_{ij},T_j\right)=\sum_{i=1}^{m}K_{ij}x_{ij}-1.0=0 \quad , \quad 1\le j\le n \tag{4-15}$$

$$\begin{aligned}H_j\left(x_{ij},V_j,T_j\right)=&\left(H_{j+1}-h_j\right)V_{j+1}-\left(H_j-h_j\right)\left(V_j+W_j\right)\\&-\left(h_j-h_{j-1}\right)L_{j-1}+F_j\left(H_{F_j}-h_j\right)-Q=0 \quad , \quad 1\le j\le n\end{aligned} \tag{4-16}$$

There are n(m+2) independent variables in these n(m+2) equations and therefore this system of equations is consistent. The problem now is to find a set of values of x_{ij}, V_j and T_j to satisfy these MESH equations. Because of their non-linear nature, a direct simultaneous solution is very difficult if not impossible. Consequently, the solution is generally obtained by using some iterative approaches. A simple and fast iterative procedure is presented in the following sections.

4.2 THE TRIDIAGONAL MATRIX METHOD

When the flow rates and compositions of feed streams are given, and the amounts of all the product streams are specified, F_j, z_{ij}, W_j, U_j, D and B are all constants. If an initial set of V_j and T_j is assumed, $\left[A_{Bc}\right]$ and $\{D\}$ are also constant, provided that the equilibrium ratios, K_{ij}'s, can be expressed as functions of T_j's. Then the M-equation, Equation (4-14), is a linear system. By taking advantage of the tridiagonal form of the matrix $\left[A_{Bc}\right]$ and by grouping the vector $\{D\}$ with $\left[A_{Bc}\right]$ as,

$$\begin{bmatrix} B_1 & C_1 & & & & D_1 \\ A_2 & B_2 & C_2 & & & D_2 \\ & A_j & B_j & C_j & & D_j \\ & & A_{n-1} & B_{n-1} & C_{n-1} & D_{n-1} \\ & & & A_n & B_n & D_n \end{bmatrix} , \quad 1 \le i \le m \tag{4-17}$$

the solution of Equation (4-14) and $[x_{ij}]$ can be easily obtained by use of a simple algorithm derived from the Gauss elimination method. In this algorithm, two auxiliary quantities, p_j and q_j are calculated by first evaluating p_j and q_j and advancing forward with j increasing, that is,

$$p_1 = C_1/B_1 ; q_1 = D_1/B_1 \tag{4-18a}$$

$$p_j = C_j/(B_j - A_j p_{j-1}) , \; 2 \le j \le n-1 \tag{4-18b}$$

$$q_j = (D_j - A_j q_{j-1})/(B_j - A_j p_{j-1}) , \; 2 \le j \le n \tag{4-18c}$$

Then, values of x_{ij}'s are calculated by first evaluating x_{in} and receding backward with j decreasing until x_{i1} is reached. Thus,

$$x_{in} = q_n \tag{4-19a}$$

$$x_{ij} = q_j - p_j x_{i,j+1} , \; 1 \le j \le n-1 \tag{4-19b}$$

When the x's obtained from the above algorithm are substituted into the S-equation, Equation (4-15) and if K_{ij}'s could be expressed as function of T_j such as

$$K_{ij} = a_{1i} + a_{2i} T_j + a_{3i} T_j^2 + a_{4i} T_j^3 \quad , \quad 1 \le i \le m \tag{4-20}$$

the S-equation is a function of T only, that is,

$$S_j(T_j) = \sum_{i=1}^{m} \left(\sum_{k=1}^{4} a_{ki} T_j^{k-1} \right) x_{ij} - 1.0 = 0 \quad , \quad 1 \le i \le n \tag{4-21}$$

For the solution of this equation, most of the previous investigators employed the Newton-Raphson iterative method. Others used the method of false position.

Muller's method is, in a sense, a generalization of the method of false position. As shown in Figure 4.3, a quadratic curve $g_1(T_j) = 0$, is drawn through three points, (T_{j1}, S_{j1}), (T_{j2}, S_{j2}) and (T_{j3}, S_{j3}), on the curve of $S_j(T_j) = 0$. The root , T_{j4} of this quadratic equation is taken as the first approximation of the root of $S_j(T_j) = 0$. For a more acculate root, $S_{j4} = S_j(T_{j4})$ is evaluated. The point (T_{j3}, S_{j3}) is then replaced by (T_{j4}, S_{j4}). The process is replaced until

$$S_{ik} = S_j(T_{ik}) \leq \varepsilon$$

where, ε is a predescribed tolerance.

The iterative formula of Muller's method can be derived in various forms. For a general equation, $S_j(T_j) = f(z) = 0$, the formula which is easily adaptable to digital computers is given as follow: Start with the initial values of z_1, z_2, and z_3 sequance of iterants, z_4, z_5,...., z_k, are obtained from

$$z_k = z_{k-1} + (z_{k-1} - z_{k-2})\, d_k \ , \ k \geq 4 \qquad (4\text{-}22)$$

where,

$$d_k = \frac{-2f(z_{k-1})(1+d_{k-1})}{b \pm \sqrt{b^2 - 4f(z_{k-1})\, d_{k-1}(1+d_{k-1})\, c}} \ , \ k \geq 4 \qquad (4\text{-}22a)$$

$$d_3 = (z_3 - z_2)/(z_2 - z_1) \qquad (4\text{-}22b)$$

$$b = f(z_{k-3})d_{k-1}^2 - f(z_{k-2})(1+d_{k-1})^2 + f(z_{k-1})(1+2d_{k-1}) \qquad (4\text{-}22c)$$

$$c = f(z_{k-3})\, d_{k-1} - f(z_{k-2})(1+d_{k-1}) + f(z_{k-1}) \qquad (4\text{-}22d)$$

When x_{ij}'s are obtained from the M-equation and new T_j's are calculated from the S-equation by Muller's method, new values of V_j can be calculated directly from the H-equation, Equation (4-16). The enthalpies of the internal vapor and liquid streams can be calculated by use of either the ideal solution approach or Yen's generalized equations. Enthalpies of feed streams and given or specified.

In the ideal solution approach the enthalpies of the internal streams are calculated by:

$$H_j = \sum_{i=1}^{m} y_{ij}\left(b_{1i} + b_{2i}T_j + b_{3i}T_j^2 + b_{4i}T_j^3\right) \quad , \quad 1 \le j \le n \tag{4-23}$$

$$h_j = \sum_{i=1}^{m} x_{ij}\left(c_{1i} + c_{2i}T_j + c_{3i}T_j^2 + c_{4i}T_j^3\right) \quad , \quad 1 \le j \le n \tag{4-24}$$

Computational Procedure:

Step 1. Assume an initial vapor rate profile $\left(V_j\right)_0$ by means of constant molal overflow and a linear temperature profile $\left(T_j\right)_0$.

Step 2. Calculate K_{ij} by use of Equation (4-20) or the Chao-Seader correlation, and then calculate the elements of the matrix$\left[A_{Bc}\right]$, using Equation (4-11), (4-12), and (4-13).

Step 3. Solve the M-equation, Equation (4-14), for x_{ij}'s, using the tridiagonal matrix algorithm, Equation (4-18) and (4-19).

Step 4. Substitute the calculated x_{ij}'s and K_{ij} into Equation (4-21) or Equation (4-15) and solve the latter by Muller's iterative formula, Equations (4-22), for new values of $\left(T_j\right)_k$.

Step 5. Calculate the enthalpies of the internal vapor and liquid streams by Equations (4-23) and (4-24) respectively or by use of Yen's generalized equations.

Step 6. Solve Equation (4-16) for a new set of $(V_j)_k$.

Step 7. Repeat steps (2) through (6) until $\left((T_j)_k - (T_j)_{k-1}\right)^2 \leq \varepsilon_T$. where, ε_T is a predescribed tolerance.

The block diagram of such a computational routine is shown in Figure 4.4.

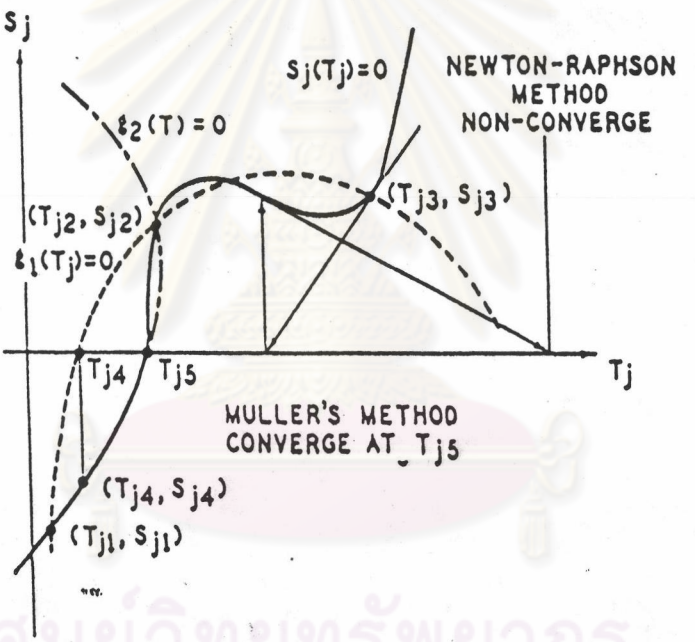

Figure 4.3 How Muller's method compare graphically with Newton-Raphson.

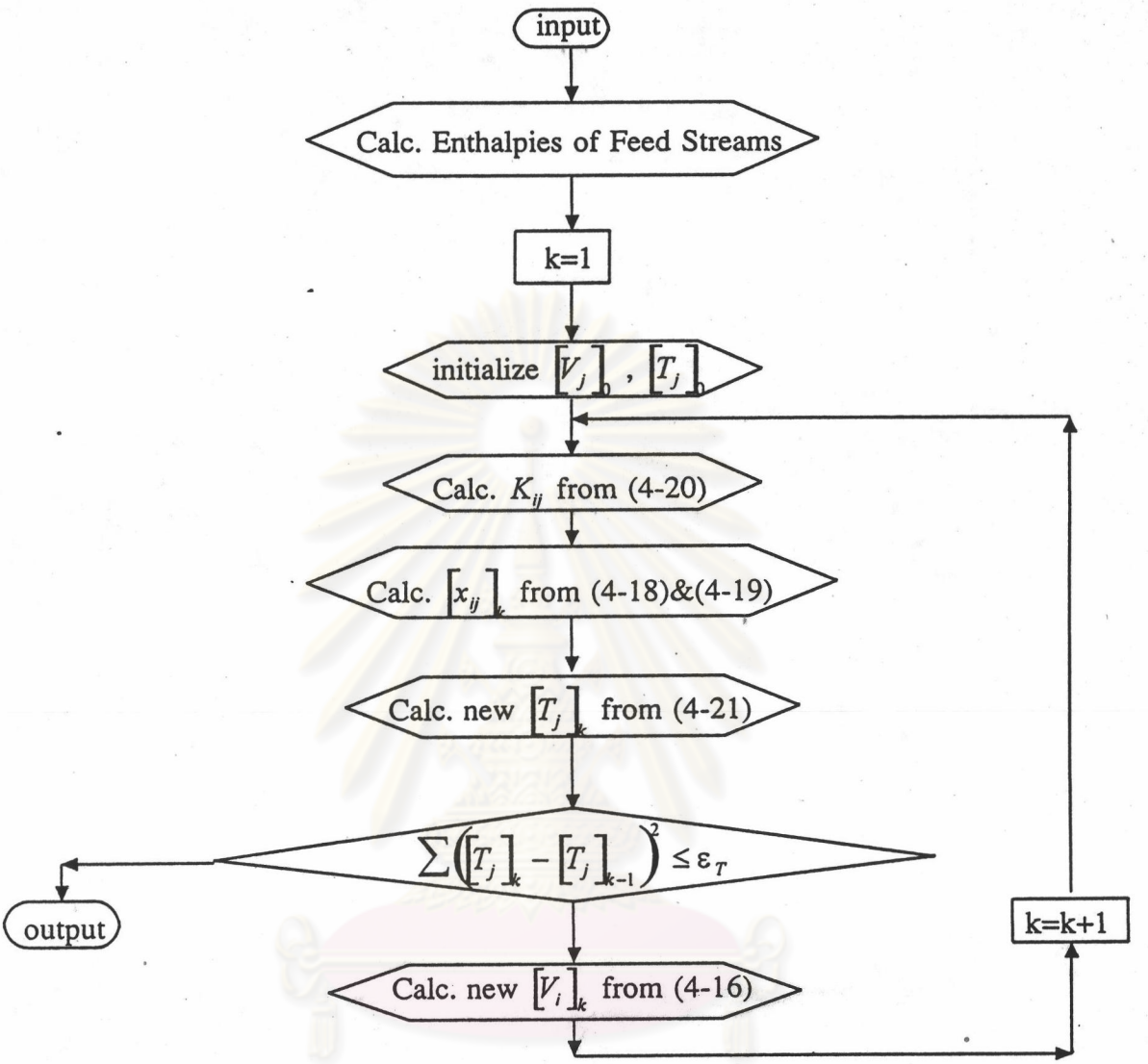

Figure 4.4 Tridiagonal Matrix Method Flowchart.