Exact Calculation Procedures
for Multicomponent Distillation
Stage-by-stage calculations require good first guess of compositions at some point in the column. Method using matrix methods will be described: not restricted to cases where a good guess of composition is available. We will describe a simple matrix method using: \( \theta \)-convergence method.
MESH equations are the same (physical operation is unchanged)

We will rearrange the equations to enhance convergence especially when one good first guess is available

Solve equation by type instead of stage-by-stage

All mass balance equations for component $i$ are grouped and solve simultaneously (equations are written in matrix form)
Specify $F$, $z_i$, $T_F$, $N$, $N_F$, $P$, $T_{\text{reflux}}$, $L/D$ and $D$

Simulation problem with $D$ specified

Design problem:

Run a series of simulation problems with good guess for $N$ and $N_F$. 
Input Equilibrium and Enthalpy Data

Input specified conditions

Pick Initial $L_j, V_j$, and $T_j$ on every stage

Calculate $K$ values for all components on each stage

Solve the component mass balance and equilibrium equations in matrix form. Eqs. (6-1) to (6-13)

Direct substitution New $T_j$

Calculate Temperatures on each stage using $\theta$ convergence and bubblepoint calculations. Eqs. (6-17) to (6-25)

Convergence Check is $\theta = 1.00$?

No

Yes

Solve Energy balance on each stage Calculate $L_j$ and $V_j$. Eqs. (6-26) to (6-39)

Convergence Check Eqs. (6-40)

Not Satisfied

Satisfied

Finished

Figure 6-1. Flowchart for matrix calculation for multi-component distillation
(1) Guess vapor and liquid flow rates: $L_j$ and $V_j$ for each stage $j$
(can use CMO) / Guess $T_j$ for each stage $j$

(2) Calculate $K$ values

(3) Solve component mass balance equations

(4) Use $\theta$-convergence and bubble-point calculations to get $T$

   If $\theta \neq 1$ go to step (2) with new $T_j$

(5) Solve energy balance to get $L_j$ and $V_j$ for each stage $j$

   Convergence check not satisfied

   then go to step (3) with new $L_j$ and $V_j$
Component Mass Balance in Matrix Form

Mass balance for any component $i$ at stage $j$:

$$V_j y_j + L_j x_j - V_{j+1} y_{j+1} - L_{j-1} x_{j-1} = F_j z_j$$

Equilibrium relationships:

$$y_j = K_j x_j \quad \text{and} \quad y_{j+1} = K_{j+1} x_{j+1}$$
Liquid component flow rates:

\[ x_j = \frac{l_j}{L_j} \quad \text{and} \quad x_{j-1} = \frac{l_{j-1}}{L_{j-1}} \]

New form of the mass balance:

\[ (-1)l_{j-1} + \left( 1 + \frac{V_j K_j}{L_j} \right) l_j + \left( -\frac{V_{j+1} K_{j+1}}{L_{j+1}} \right) l_{j+1} = F_j Z_j \]
\[ A_j l_{j-1} + B_j l_j + C_j l_{j+1} = D_j \]
TABLE 6-1. Thomas algorithm for inverting tridiagonal matrices

Consider the solution of a matrix in the form of Eq. (6-13) where all $A_j$, $B_j$, $C_j$, and $D_j$ are known.

1. Calculate three intermediate variables for each row of the matrix starting with $j = 1$. For $1 \leq j \leq N$,
   
   $$(V1)_j = B_j - A_j(V3)_{j-1}$$
   
   $$(V2)_j = [D_j - A_j(V2)_{j-1}]/(V1)_j$$
   
   $$(V3)_j = C_j/(V1)_j$$

   since $A_1 \equiv 0$, $(V1)_1 = B_1$, and $(V2)_1 = D_1/(V1)_1$.

2. Initialize $(V3)_0 = 0$ and $(V2)_0 = 0$ so you can use the general formulas.

3. Calculate all unknowns $U_j$ [$l_j$ in Eq. (6-13), $V_j$ in Eq. (6-34), or $\Delta T_j$ in Eq. (12-58)]. Start with $j = N$ and calculate

   $$U_N = (V2)_N$$

   Then going from $j = N - 1$ to $j = 1$, calculate $U_{N-1}$, $U_{N-2}$, … $U_1$ from

   $$U_j = (V2)_j - (V3)_j U_{j+1}, \quad 1 \leq j \leq N-1$$
Initial guess for the flow rates:

Assume CMO

Rectifying section:

\[ L = \left( \frac{L_0}{D} \right) D \]

\[ V = L + D \]

Feed quality:

\[ q = \frac{H - h_{\text{feed}}}{H - h} \]

Stripping section:

\[ \bar{L} = L + qF \]

\[ \bar{V} = V + (1 - q)F \]
Bubble point calculations

\[ K_{ref}(T_{new}) = \frac{K_{ref}(T_{old})}{\sum_{i=1}^{c} (K_i x_i)_{calc}} \]

Estimate T

Calculate \( K_i(T, p, x_i) \)

Is \( \sum_{i=1}^{c} K_i x_i = 1.0 \) ?

Yes

\[ y_i = K_i x_i \]

FINISHED \( T = T_{BP} \)

No

Estimate new T
θ-convergence Method

This method defines a quantity θ that forces the equation below to be verified:

\[
D_{\text{specified}} = \sum_{i=1}^{C} \left( \frac{F Z_i}{1 + \theta \left( B x_{i,\text{bot}} / D x_{i,\text{dist}} \right)_{\text{calc}}} \right)
\]

with

\[
(B x_{i,\text{bot}})_{\text{calc}} = l_{N,i}
\]
\[
(D x_{i,\text{dist}})_{\text{calc}} = l_{1,i}/(L/D)
\]
\[ f(\theta) = \sum_{i=1}^{C} \left( \frac{FZ_i}{1 + \theta \left( B \frac{x_{i,\text{bot}}}{D} \frac{x_{i,\text{dist}}}{\text{calc}} \right)} \right) - D_{\text{specified}} = 0 \]

\[ \theta_{k+1} = \theta_k + \frac{f(\theta_k)}{f'(\theta_k)} \]
Once $\theta$ is found, one can compute the following:

$$
(D \ x_{i,\text{dist}})_{\text{cor}} = \frac{FZ_i}{1 + \theta \ (B \ x_{i,\text{bot}} / D \ x_{i,\text{dist}})_{\text{calc}}}
$$

$$
(B \ x_{i,\text{bot}})_{\text{cor}} = (D \ x_{i,\text{dist}})_{\text{cor}} \ \theta \ (B \ x_{i,\text{bot}} / D \ x_{i,\text{dist}})_{\text{calc}}
$$

$$
(l_{i,j})_{\text{cor}} = \frac{(D \ x_{i,\text{dist}})_{\text{cor}}}{(D \ x_{i,\text{dist}})_{\text{calc}}} \ (l_{i,j})_{\text{uncor}}
$$

$$
(l_{i,j})_{\text{cor}} = \frac{(B \ x_{i,\text{bot}})_{\text{cor}}}{(B \ x_{i,\text{bot}})_{\text{calc}}} \ (l_{i,j})_{\text{uncor}}
$$
Convergence Test:

\[ x_{i,j} = \frac{(l_{i,j})_{cor}}{\sum_{i=1}^{c} (l_{i,j})_{cor}} \]

\[ \theta = 1.0 \pm 10^{-5} \]

Calculate new \( T_j \)
Using the following equations, one gets a matrix equation:

\[ V_j H_j + L_j h_j = V_{j+1} H_{j+1} + L_{j-1} h_{j-1} + F_j h_{F_j} + Q_j \]

\[ L_j = V_{j+1} + D - \sum_{k=1}^{j} F_k \]

\[ L_{j-1} = V_j + D - \sum_{k=1}^{j-1} F_k \]
\[
\begin{bmatrix}
B_{E1} & C_{E1} & 0 & 0 & \cdot & 0 & 0 & 0 & 0 \\
0 & B_{E2} & C_{E2} & 0 & \cdot & 0 & 0 & 0 & 0 \\
0 & 0 & B_{E3} & C_{E3} & \cdot & 0 & 0 & 0 & 0 \\
\cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\
0 & 0 & 0 & 0 & 0 & 0 & B_{E_{N-1}} & C_{E_{N-1}} & \cdot \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & B_{E_N} & \cdot \\
\end{bmatrix}
\begin{bmatrix}
V_1 \\
V_2 \\
V_3 \\
V_{N-1} \\
V_N \\
\end{bmatrix}
=
\begin{bmatrix}
D_{E1} \\
D_{E2} \\
D_{E3} \\
D_{E_{N-1}} \\
D_{EN} \\
\end{bmatrix}
\]
New values for $L_j$ and $V_j$

\[
\left| \frac{L_{j,\text{calc}} - L_{j,\text{old}}}{L_{j,\text{calc}}} \right| < \varepsilon \quad \text{and} \quad \left| \frac{V_{j,\text{calc}} - V_{j,\text{old}}}{V_{j,\text{calc}}} \right| < \varepsilon
\]

\[\varepsilon = 10^{-5}\]

If not use new values in step (3) (i.e., mass balance matrix equations)