

2006 Engineering Design Seminar

Fractionation

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UOP LLC



A Honeywell Company

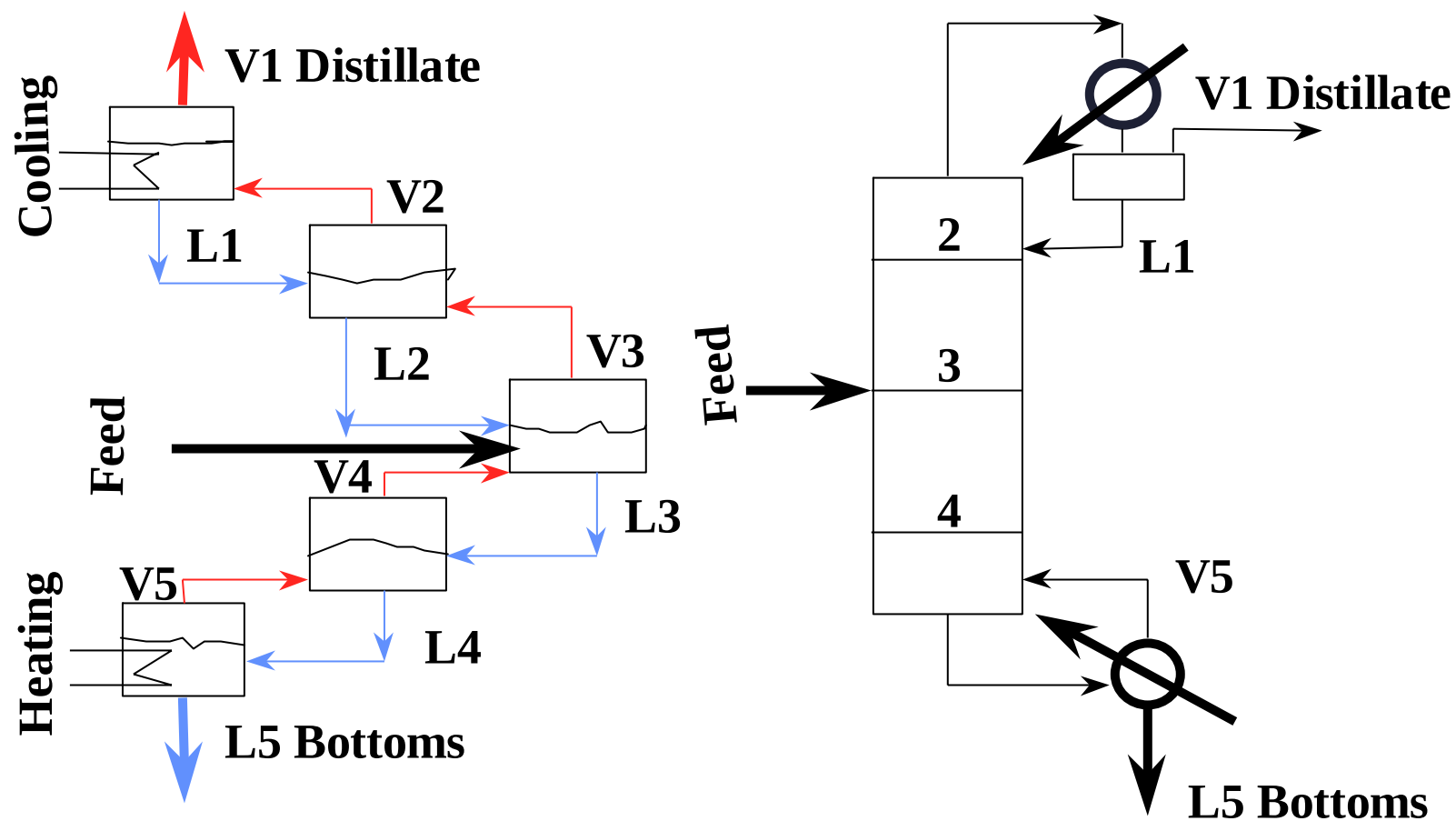
Fractionation

- **Fractionation Concepts**
 - Equilibrium and Relative Volatility
 - Heat and Material Balance
- **Shortcut/Approximate Methods**
 - Concept of Equimolar Overflow
 - McCabe - Thiele Graphical Method
 - Analytical Methods
- **Rigorous Methods**
- **Tray Efficiency**
- **Column Design and Optimization**
- **Design Cases**
- **Help in using programs**

Importance of Distillation

- **Key Separation Process**
 - **Used extensively in all refineries and chemical plants (probably the primary separation unit operation)**
 - **Capital and Energy Intensive**
 - **(Generally) non-proprietary**

Equilibrium Stages



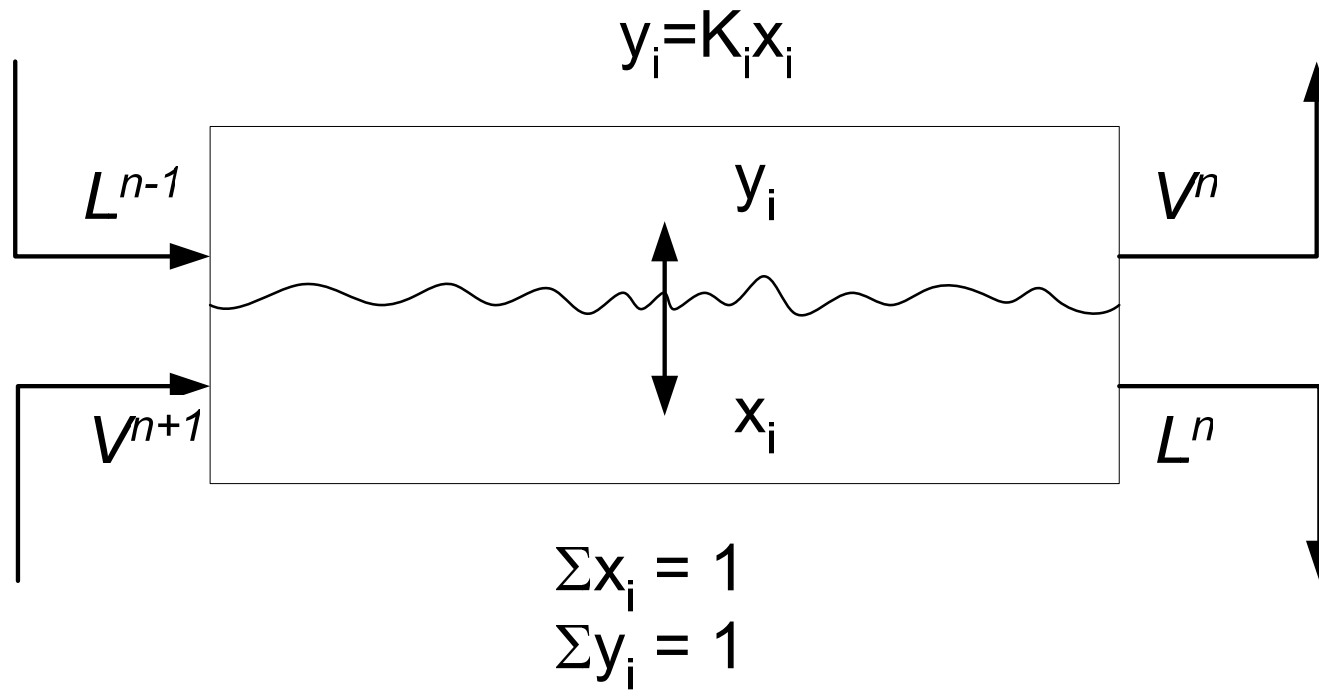
From "Distillation Design" H. Kister

Equilibrium

- Most distillation is modeled using “equilibrium stages” (which can be thought of a series of equilibrium flash calculations strung together).
- A component has a vapor liquid equilibrium K value that is defined as the mole ratio of its vapor concentration to its liquid concentration when these phases are in equilibrium.

$$K = \left(\frac{y}{x} \right)$$

Equilibrium Stage



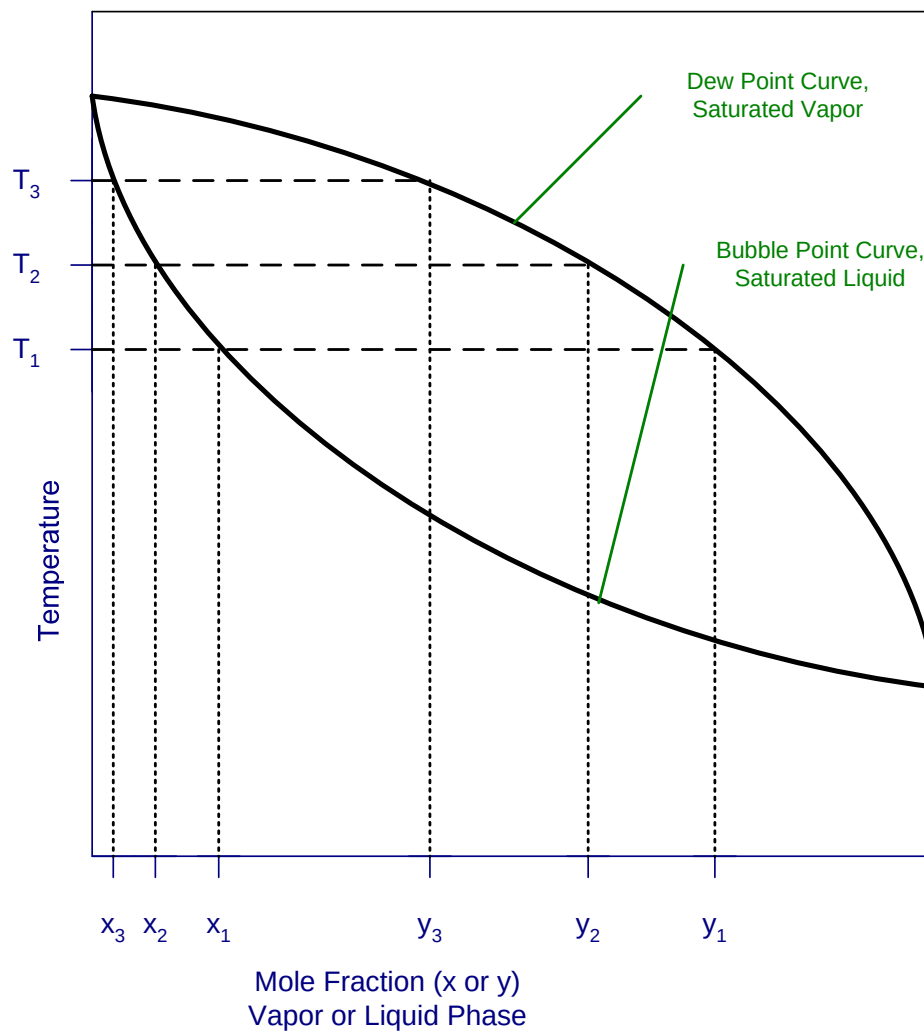
$$K = P_{vp}/\Pi$$

$$K = f(T, P, x, y)$$

Equilibrium K Value Definition

$$K = \frac{y}{x}$$

T-x Diagram



$$K = \frac{y}{x}$$

Equilibrium – Relative Volatility

- Alpha (relative volatility) is a measure of the intrinsic difficulty in using fractionation to separate two components
- It is the ratio of the vapor liquid equilibrium K values for two components

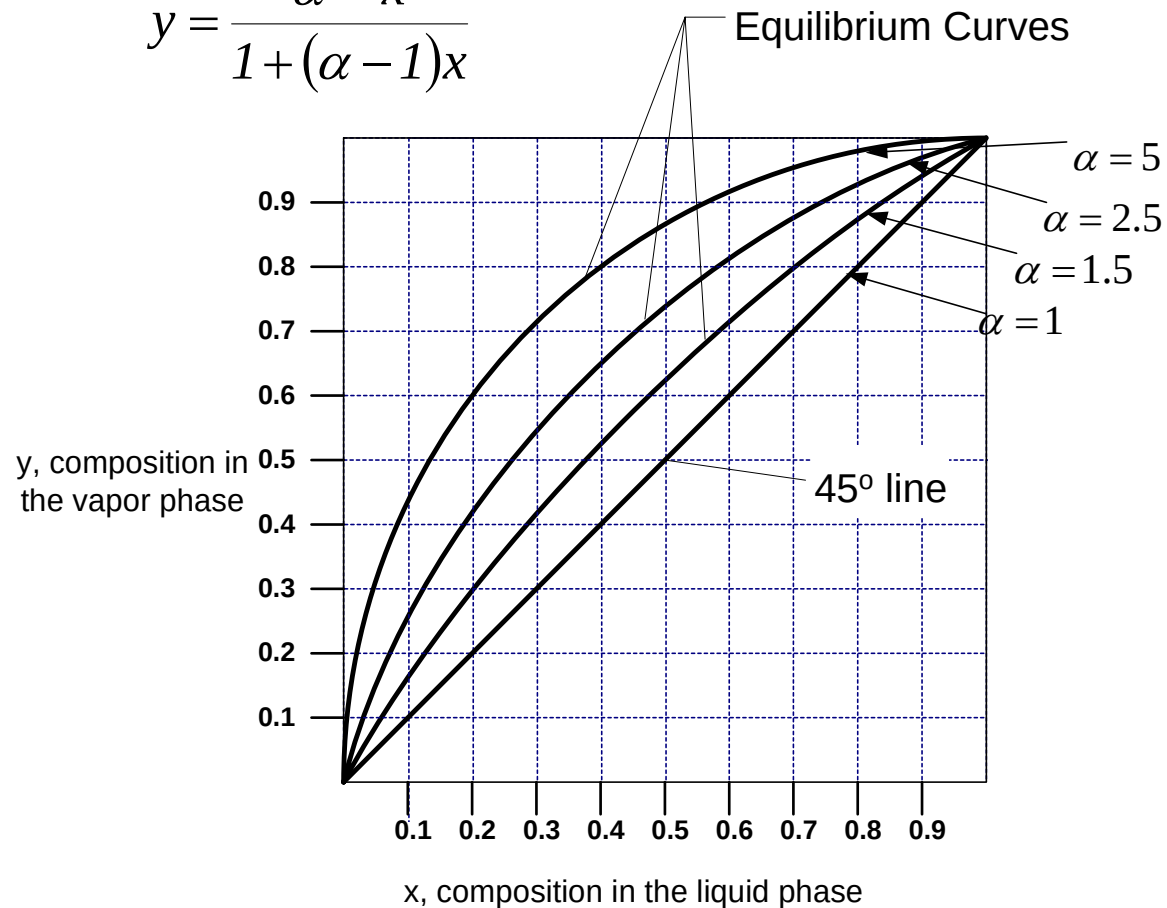
LK = Light Key Component

HK = Heavy Key Component

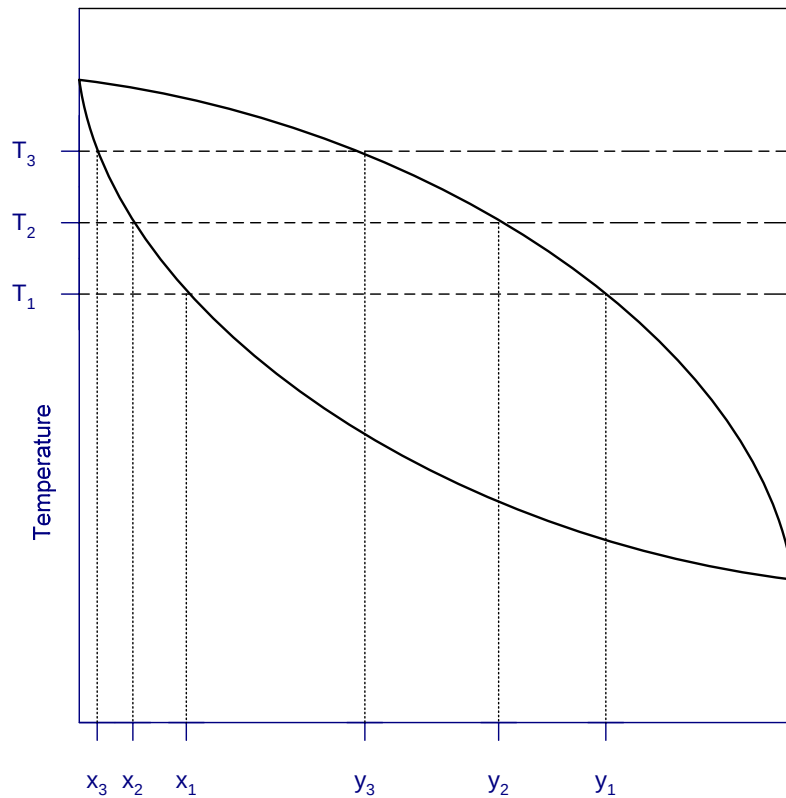
$$\alpha = \left(\frac{K_{LK}}{K_{HK}} \right)$$

Equilibrium Curve or x-y Diagram

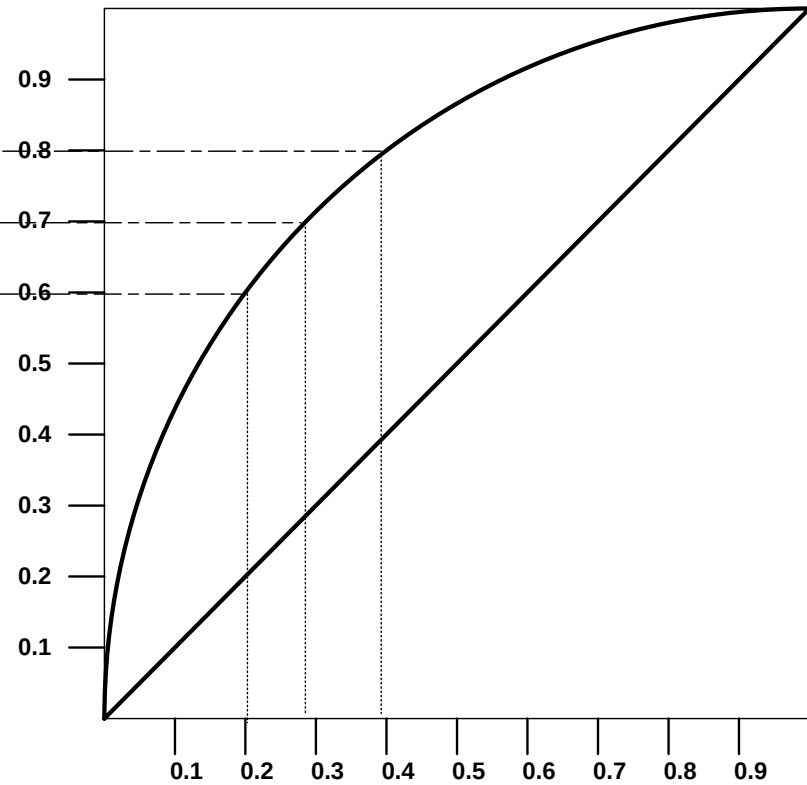
$$y = \frac{\alpha x}{1 + (\alpha - 1)x}$$



Equilibrium Curve from Equilibrium Data

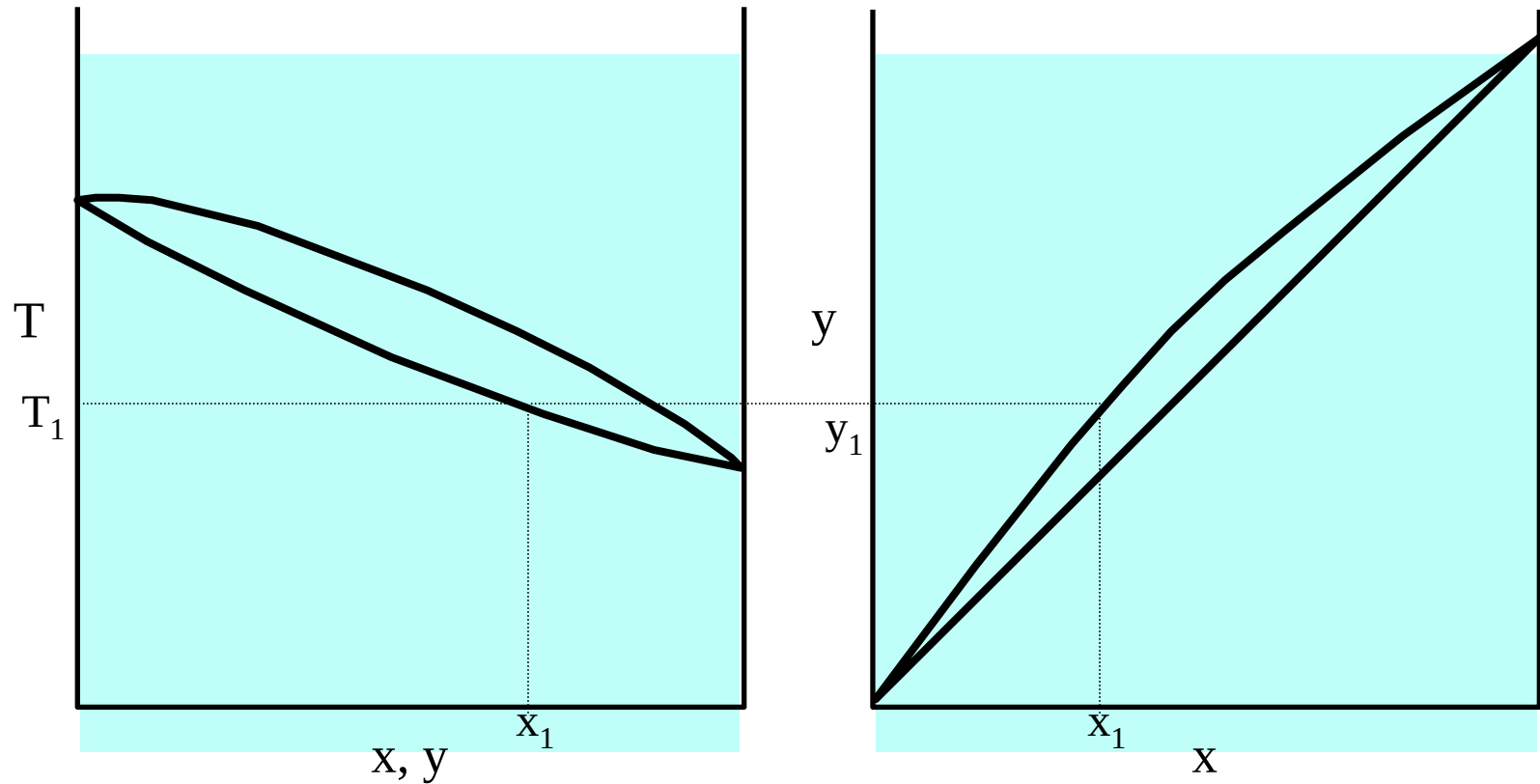


Mole Fraction (x or y)
Vapor or Liquid Phase



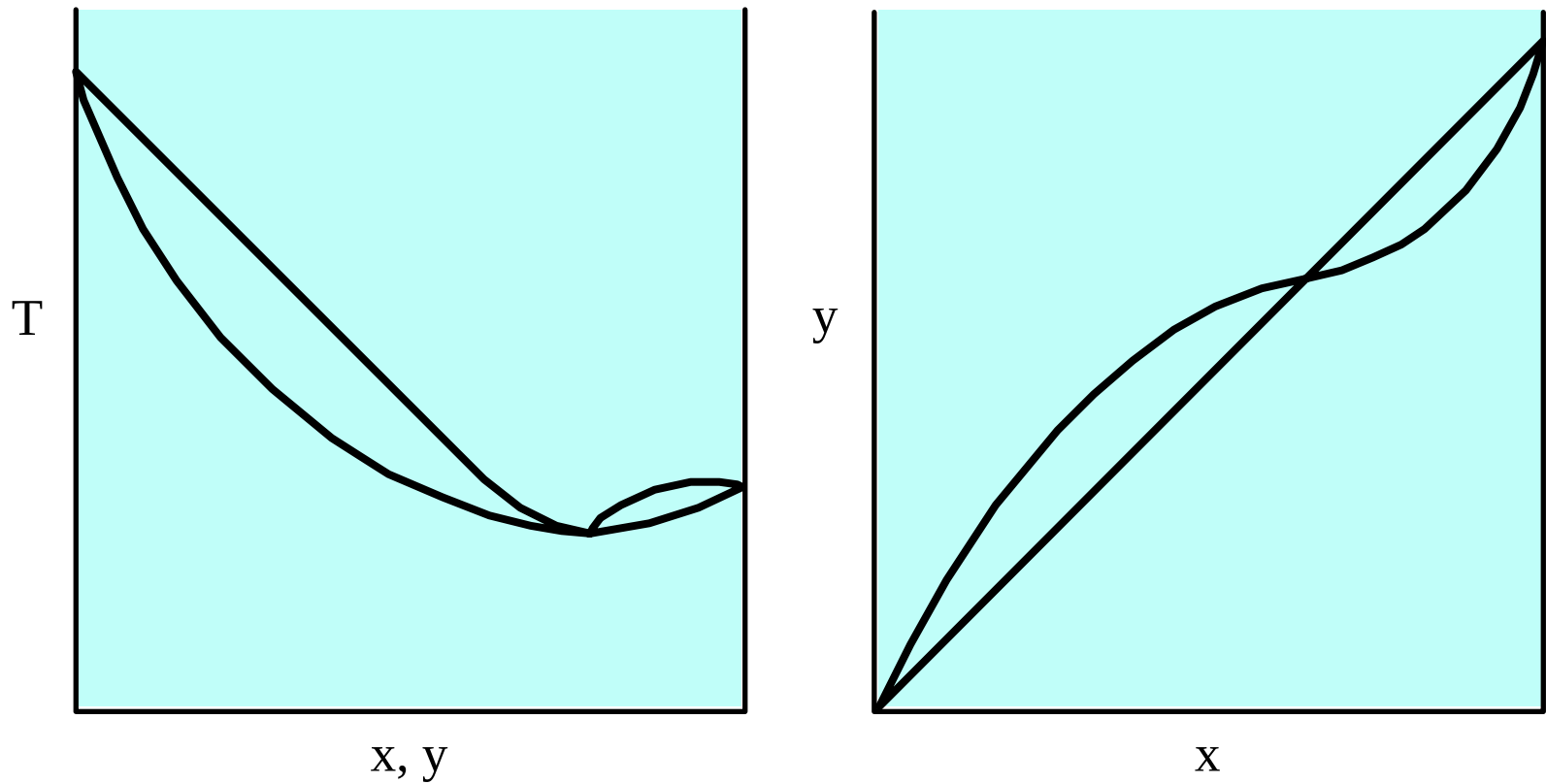
x, composition in the liquid phase

Equilibrium Pressure Constant



Ideal Vapor/Liquid Equilibria:
Systems that conform to Raoult's Law
(i.e. $p^* = P_v x$, $\therefore \alpha = \frac{P_v}{P_v^*} = 1$ = constant)

Equilibrium Pressure Constant



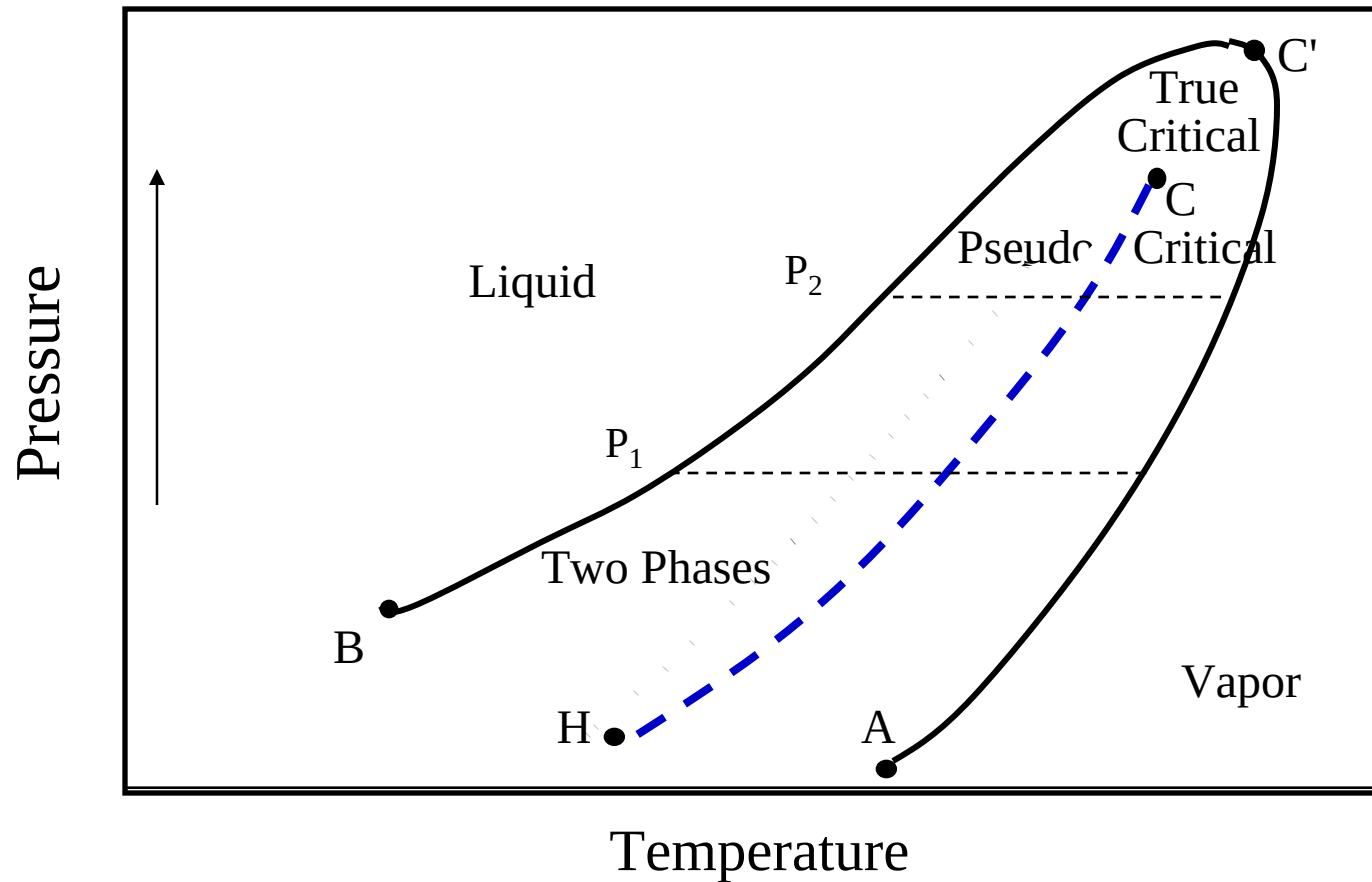
Large Deviation from Ideality:
e.g. Minimum boiling azeotrope

Alpha Variation

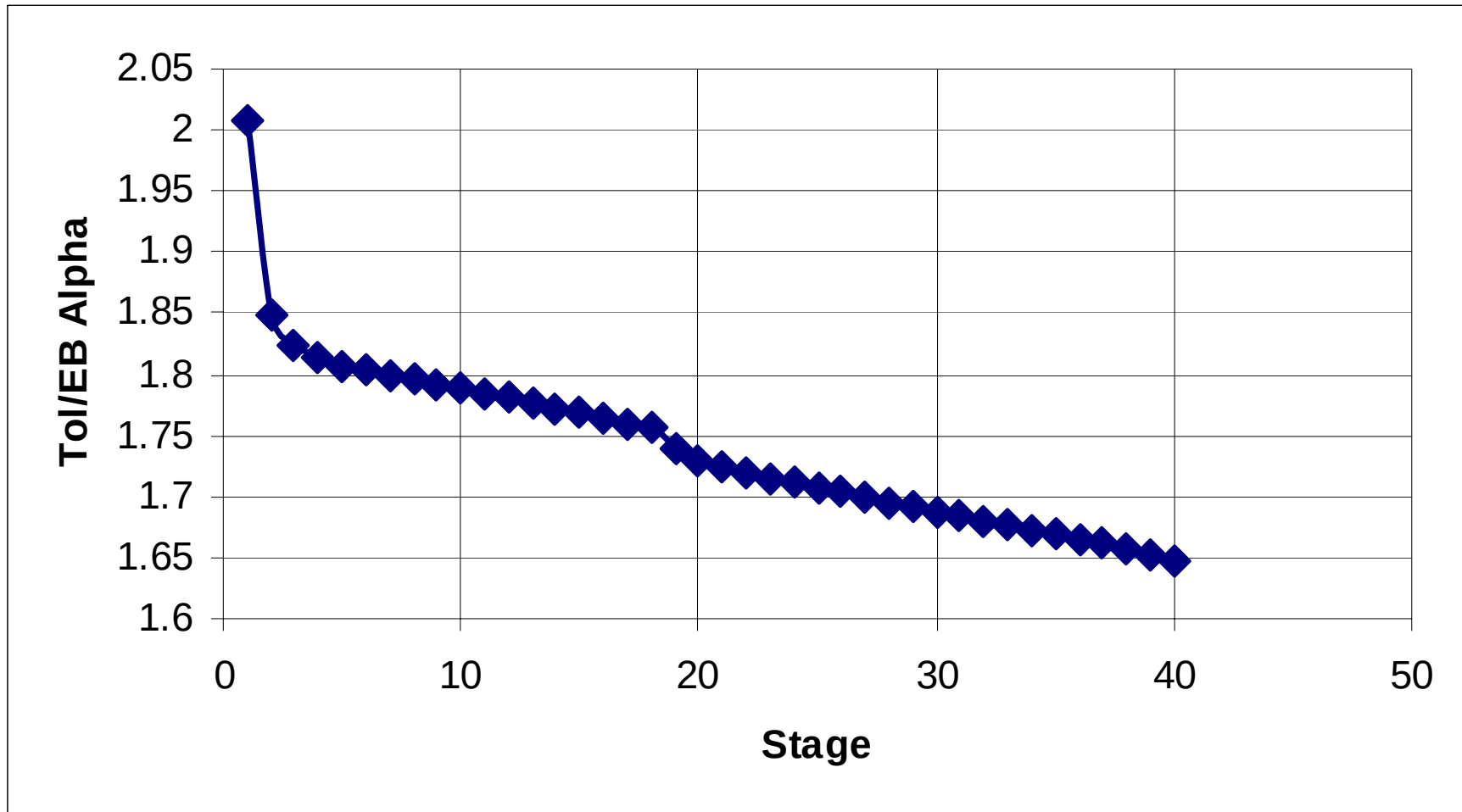
- A knowledge of the alpha value behavior is an important piece of information for designing distillation columns.
- Alpha varies by how K-values change.
 - Pressure
 - Composition
- $K = f(T, P, x, y)$

Pseudo-Critical Properties

Multi-Component Mixture



Alpha Variation



Water *K* Values

$$K = \frac{Y}{X}$$

$$Y = \frac{P^o(1 - X_{HW})}{\pi}$$

and

$$X = X_{wh}$$

$$K_w = \frac{(1 - X_{hw})P^o}{X_{wh}\pi}$$

Water Equilibrium Curve

$$Y = \frac{\alpha X}{1 + (\alpha - 1)X}$$

As X goes to 0

$$Y = \alpha X$$

and, therefore: $\ln(Y) = \ln(\alpha) + \ln(X)$

Approximate/Shortcut/Simplified Methods

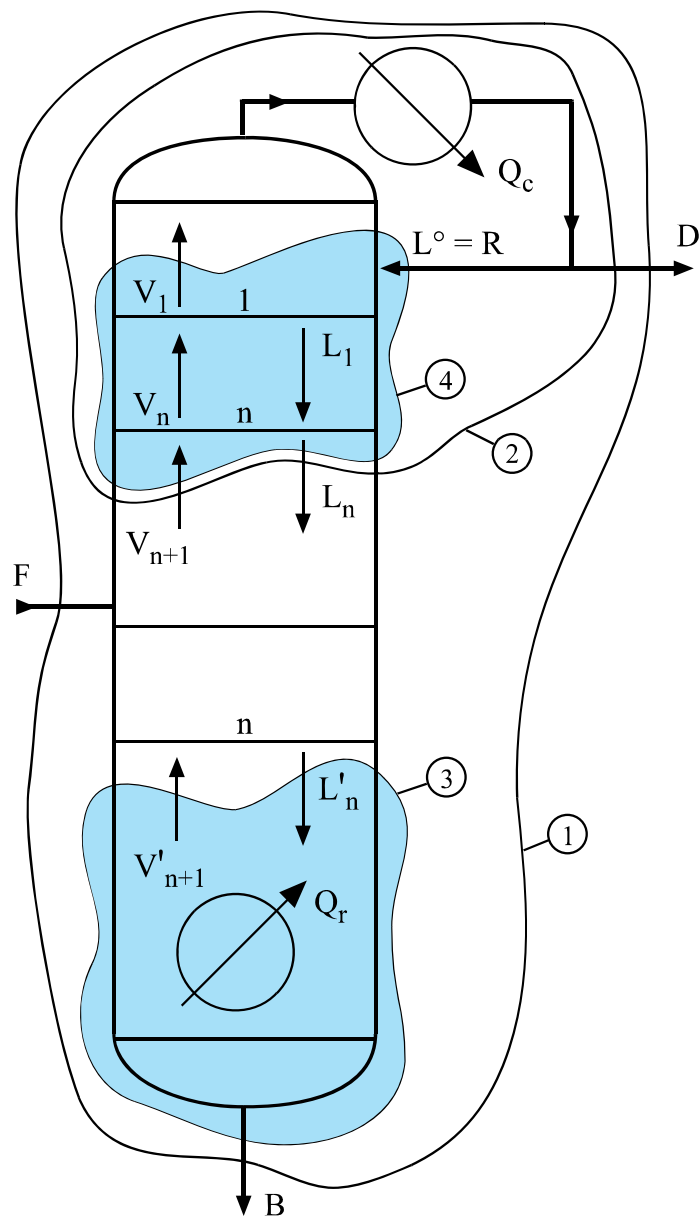
Approximate/Shortcut/Simplified Methods

■ **Fundamental Relations**

- **Heat balance**
- **Material balance**
- **Equilibrium**
- **McCabe-Thiele Method**

■ **Approximate Methods**

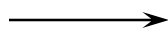
- **Fenske equation**
- **Underwood equation**
- **Gilliland graph**
- **Kremser for absorbers and strippers**
- **Naphtha fractionation**



Distillation Method Basics

ENVELOPE (1) - Overall Material and Heat Balance

Mass Balance

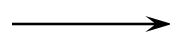


$$F = D + B$$

$$X_i^F F = X_i^D D + X_i^B B$$

(i = 1 to N components)

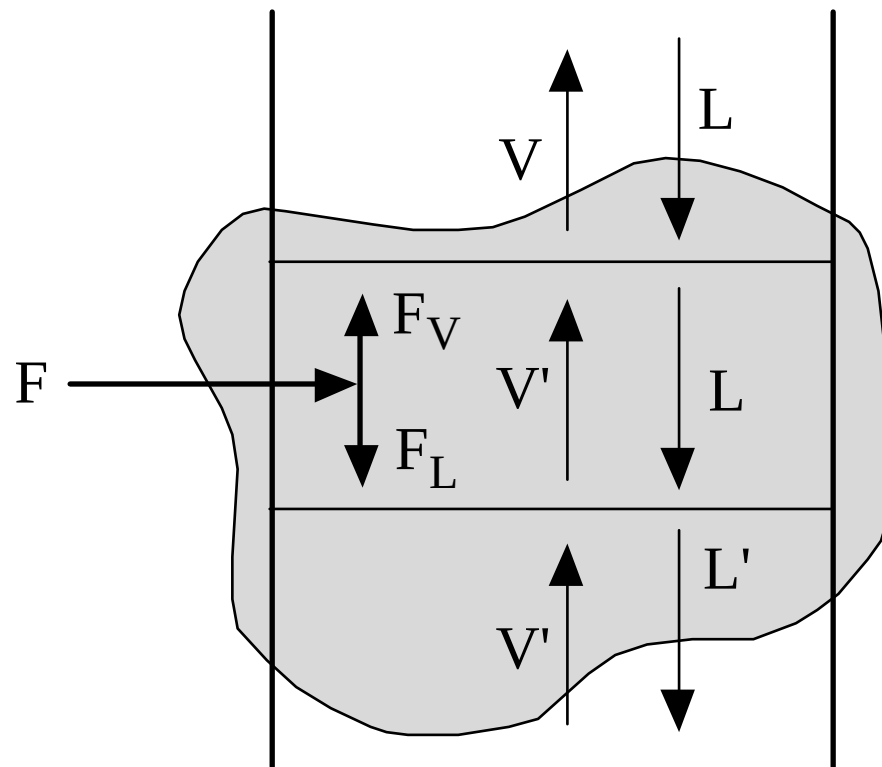
Heat Balance



$$h_F F + Q_R = h_D D + h_B B + Q_c$$

Distillation Method Basics

Envelope 4 – A single tray

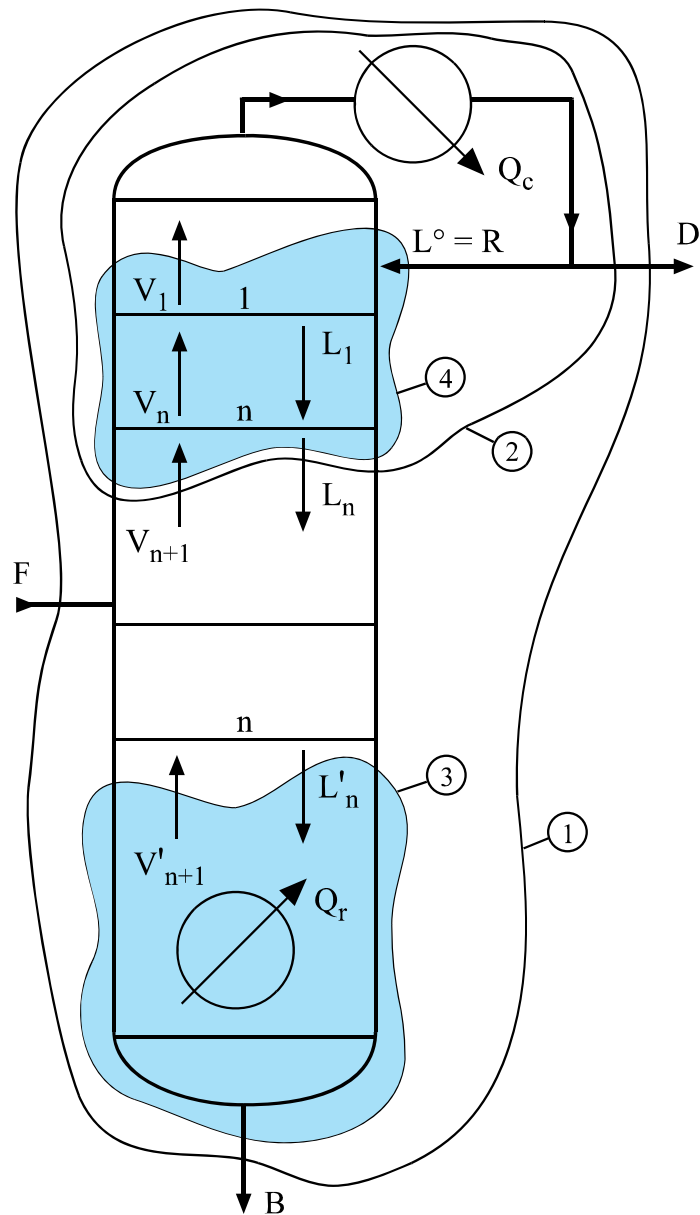


Distillation Method Basics

ENVELOPE (4) – A single tray

Mass Balance $\longrightarrow V^{n+1} + L^o = V^1 + L^n$

Heat Balance $\longrightarrow h_v^{n+1}V^{n+1} + h_L^o L^o = h_v^1V^1 + h_L^n L^n$



Distillation Shortcut Method Basics

ENVELOPE (1) - Overall Material and Heat Balance

Mass Balance $\longrightarrow$ $F = D + B$

$$X_i^F F = X_i^D D + X_i^B B$$

$(i = 1 \text{ to } N \text{ components})$

Heat Balance $\longrightarrow$ $h_F F + Q_R = h_D D + h_B B + Q_c$

Distillation Shortcut Method Basics

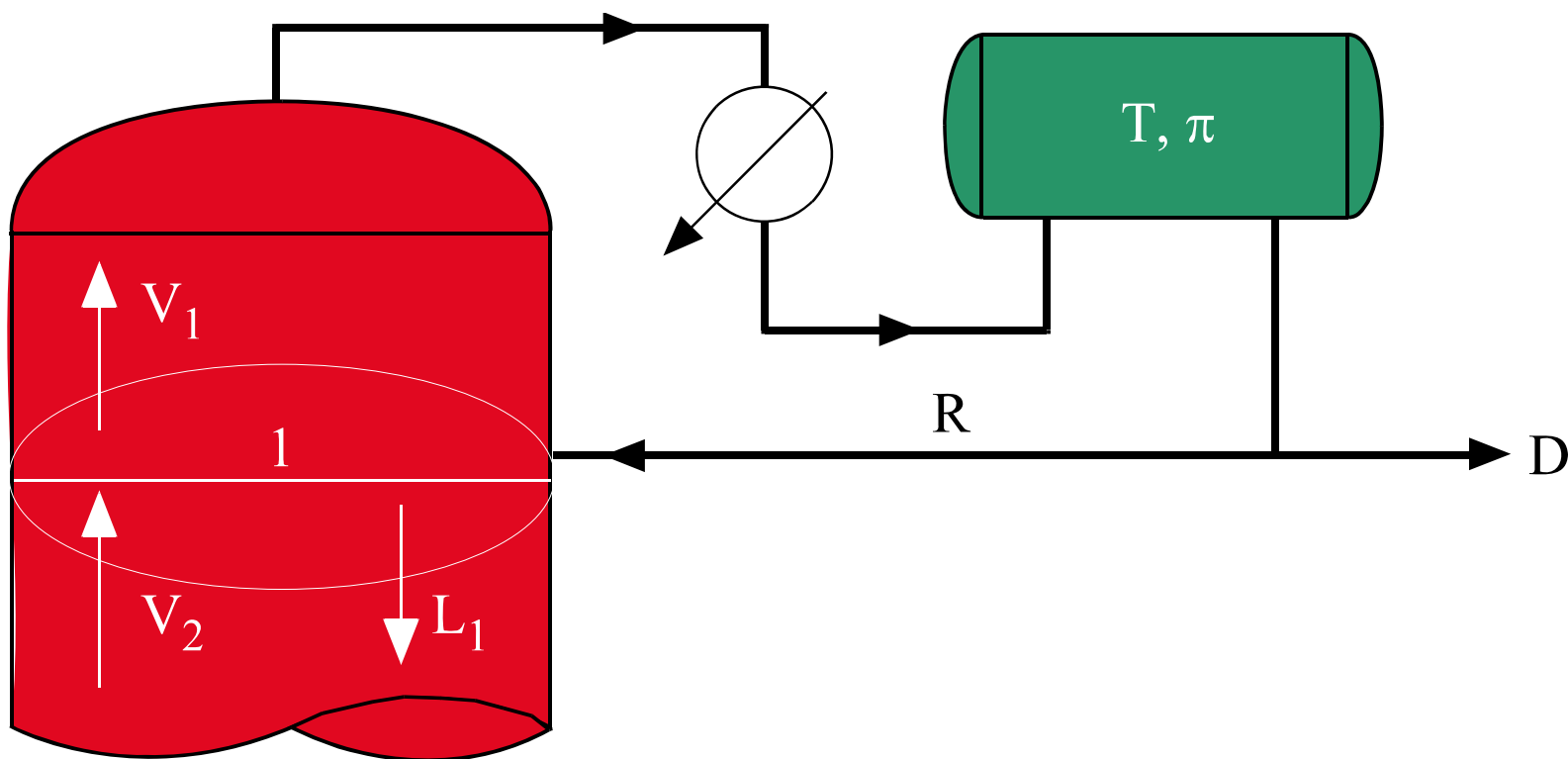
ENVELOPE (2) - Rectifying Section

Mass Balance $\longrightarrow V^{n+1} = L^n + D$

$$Y_i^{n+1}V^{n+1} = X_i^n L^n + X_i^D D$$

Heat Balance $\longrightarrow h_V^{n+1}V^{n+1} = h_L^n L^n + h_D D + Q_c$

Internal vs. External Reflux



Internal vs. External Reflux

$$h_{V2} V_2 + h_R R = h_{V1} V_1 + h_{L1} L_1$$

$$V_1 = R + D$$

$$V_2 = L_1 + D$$

Distillation Shortcut Method Basics

ENVELOPE (3) - Stripping Section

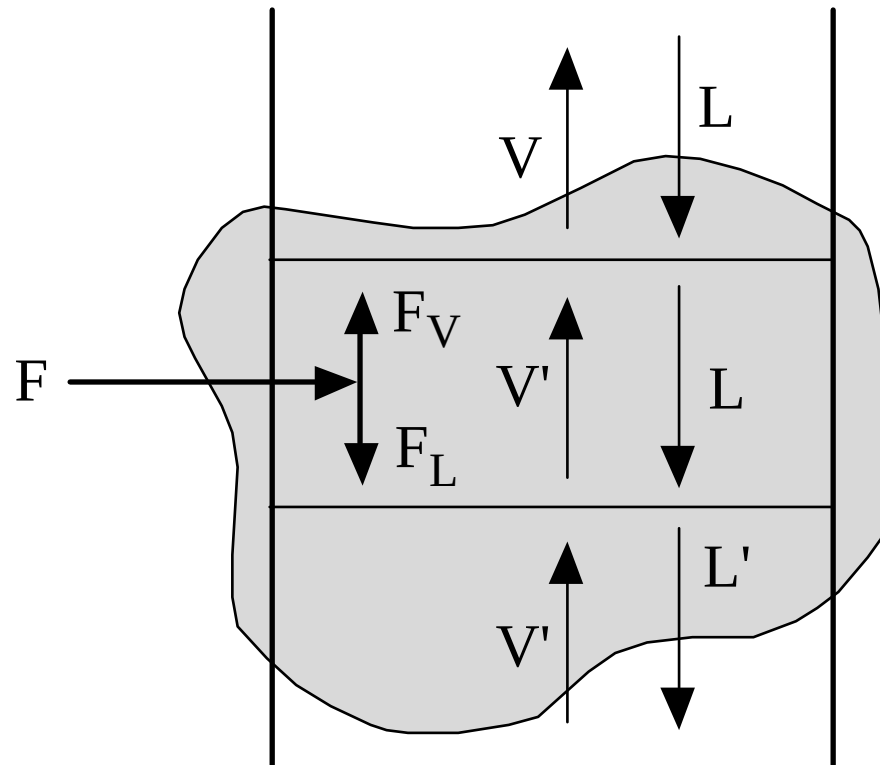
Mass Balance $\longrightarrow L^{n'} = V^{n+1'} + B$

$$x_i^n L^{n'} = y_i^{n+1} V^{n+1'} + X_i^B B$$

Heat Balance $\longrightarrow Q_R + h_L L^{n'} = h_v V^{n+1'} + h_b B$

Distillation Shortcut Method Basics

Envelope 4 – A single tray



Distillation Shortcut Method Basics

ENVELOPE (4) - A single tray

Mass Balance $\longrightarrow V^{n+1} + L^o = V^1 + L^n$

Heat Balance $\longrightarrow h_v^{n+1}V^{n+1} + h_L^o L^o = h_v^1V^1 + h_L^n L^n$

Distillation Shortcut Method Basics

ENVELOPE (4)

Rearranging the mass balance yields

$$V^{n+1} = V^1 + L^n - L^o$$

Inserting this into the heat balance

$$h_V^{n+1}V^1 + h_V^{n+1} L^n - h_V^{n+1}L^o + h_L^o L^o = h_V^1 V^1 + h_L^n L^n$$

Distillation Shortcut Method Basics

ASSUME

Sensible Heat Changes are Negligible

i) $h_L^0 = h_L^1 = h_L^n = h_L$

Molal Heats of Vaporization are Constant

ii) $\lambda^0 = \lambda^1 = \dots = \lambda^n$

Since $\lambda^n = h_V^n - h_L^n$

iii) $h_V^0 = h_V^1 = \dots = h_V^n = h_V$

Distillation Shortcut Method Basics

Heat Balance

$$h_V V^1 + h_V L^n - h_V L^o + h_L L^o = h_V V^1 + h_L L^n$$

$$(h_V - h_L) L^n = (h_V - h_L) L^o$$

Therefore $\longrightarrow L^n = L^o = \underline{\text{Constant}}$

Distillation Shortcut Method Basics

Constant Molal Overflow

$$L^n = \text{Constant}$$

- **Sensible Heat Changes are Negligible**
- **Molal Heats of Vaporization are Constant**

Equilibrium

- For constant molal overflow in a binary system, the equilibrium relationship of $K=y/x$ simplifies to:

$$\left(\frac{V}{K(R + D)} \right)$$

Distillation Shortcut Method Basics

Constant Molal Overflow

VALIDITY?

- **Boiling Point Range of Components is Narrow**
- **Molecular Characteristics of Components are Similar**
 - **For example: all paraffinic hydrocarbons or all aromatic hydrocarbons not mixture of paraffins and aromatics**

Distillation Shortcut Method Basics

McCabe-Thiele Method

ENVELOPE 2 - Rectifying Section

Mass Balance $\longrightarrow y_i^{n+1}V^{n+1} = x_i^n L^n + x_i^d D$

Equimolal Overflow

L = Constant

V = Constant

$$y_i^{n+1} = (L/V)x_i^n + (D/V)x_i^D$$

Binary Distillation Shortcut Methods

McCabe-Thiele Method

BINARY Separations

$$\mathbf{x}_i \longrightarrow \mathbf{x}_1, \mathbf{x}_2$$

$$\mathbf{x}_2 = 1 - \mathbf{x}_1$$

Used convention of dropping subscript i

$$\begin{array}{ll} \mathbf{x} = \mathbf{x}_1 & \text{Mole fraction of more volatile} \\ \mathbf{y} = \mathbf{y}_1 & \text{(lower boiling point) component} \end{array}$$

$$\mathbf{y}_{n+1} = (\mathbf{L}/\mathbf{V}) \mathbf{x}_n + (\mathbf{D}/\mathbf{V}) \mathbf{x}_D \quad \text{Trays above feed}$$

Binary Distillation Shortcut Methods

McCabe-Thiele Method

ENVELOPE 3 - Stripping Section

Mass Balance $\longrightarrow x_i^n L^n = y_i^{n+1} V^{n+1'} + x_i^B B$

Equimolal Overflow

$$L' = \text{Constant} \neq L$$

$$V' = \text{Constant} \neq V$$

$$y_{n+1} = (L'/V') x_n + (B/V') x_B$$

Trays below feed

Binary Distillation Shortcut Methods

McCabe-Thiele Method

Feed Stage

Mass Balance $F + V' + L = V + L'$

Heat Balance $h_F F + h'_V V' + h_L L = h_V V + h'_L L'$

$$V = L + D$$

$$V' = L' - B$$

Binary Distillation Shortcut Methods

McCabe-Thiele Method

ASSUME $h'_V = h_V$ **and** $h'_L = h_L$

Then $h_F F + h_V (L' - B) + h_L L = h_V (L + D) + h_L L'$

Rearranging $(h_V - h_L)L' = (h_V - h_L)L + h_V(D + B) - h_F F$

Since $D + B = F$

Then $L' = L + \left(\frac{h_V - h_F}{h_V - h_L} \right) F$

Binary Distillation Shortcut Methods

McCabe-Thiele Method

Define: $q = \frac{h_F^V - h_F}{h_F^V - h_F^L}$

Then: $L' = L + q F$

Also: $y^{n+1} = \left[\frac{q}{(q-1)} \right] x^n - \left[\frac{1}{(q-1)} \right] x_F$ **At Feed Tray**

Q Values

Condition	Value of q
BP Liquid	1.0
DP Vapor	0
Sub Cooled Liquid	>1.0
Superheated Vapor	<0
Partly Vapor	Mol Frac. Liquid

Binary Distillation Shortcut Methods

McCabe-Thiele Method

EQUILIBRIUM

$$y = K_1 x$$

$$(1 - y) = K_2 (1 - x)$$

$$x = \frac{1 - K_2}{(K_1 - K_2)}$$

$$y = K_1 x$$

$$x_2 = (1 - x_1)$$

$$y_2 = (1 - y_1)$$

Binary Distillation Shortcut Methods

McCabe-Thiele Method

EQUILIBRIUM

$$y = K_1 x$$

$$(1 - y) = K_2 (1 - x)$$

$$\frac{y}{(1 - y)} = \frac{K_1}{K_2} \frac{x}{(1 - x)}$$

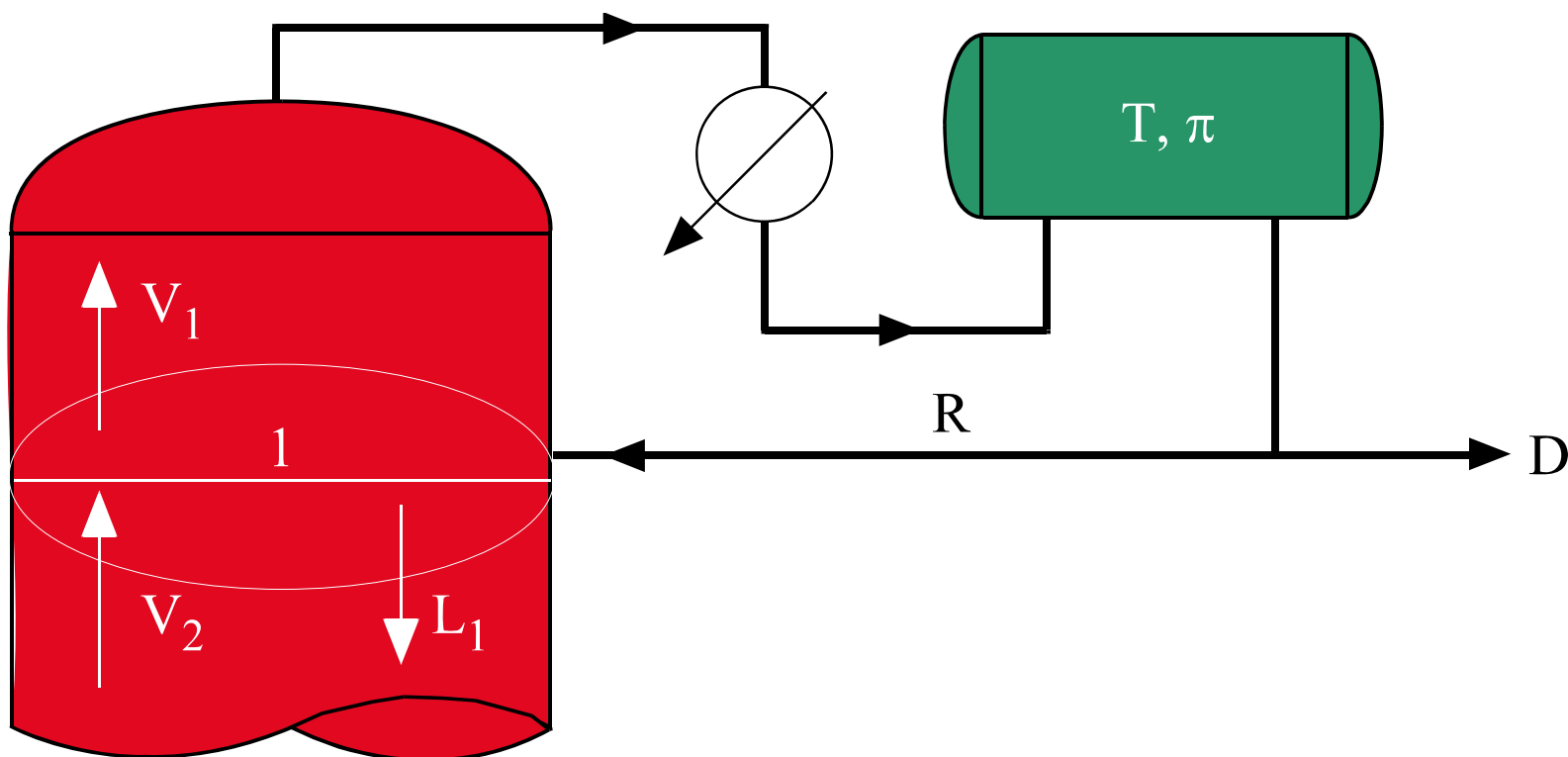
Define

$$\alpha = \frac{K_1}{K_2}$$

$$y = \frac{\alpha x}{1 + (\alpha - 1)x}$$

$$x = \frac{y}{K_1}$$

Internal vs. External Reflux



Internal vs. External Reflux

$$h_{V2} V_2 + h_R R = h_{V1} V_1 + h_{L1} L_1$$

$$V_1 = R + D$$

$$V_2 = L_1 + D$$

Internal vs. External Reflux

ASSUME: $h_{V1} = h_{V2}$

$$L = \frac{(h_V - h_R)}{(h_V - h_L)} R$$

h_V = saturated vapor enthalpy @ π
 h_L = saturated liquid enthalpy @ π
 h_R = liquid enthalpy @ T

Receiver Temp = 100°F

Receiver Press = 250 psia

Assume: Receiver liquid is 100% propane

$h_V = 168$ Btu/lb; $h_L = 47$ Btu/lb; $h_R = 27$ Btu/lb

$L = 1.16 R$

Summary of Equations

Equilibrium curve

$$x^n = \frac{(1 - K_2)}{(K_1 - K_2)},$$

$$y^n = K_1 x^n$$

or

$$y^n = \frac{\alpha x^n}{1 + (\alpha - 1)x^n}$$

$$\alpha = K_1 / K_2$$

Rectifying Section

$$y^{n+1} = (L/V)x^n + (D/V)x_D, \quad V = L + D$$

Note: When $x^n = x_D$

$$y^{n+1} = \left(\frac{L}{L + D} + \frac{D}{L + D} \right) x_D = x_D$$

can plot equation as a straight line with slope equal to $L/(L + D)$ that passes through the point (x_D, x_D)

Feed Q Line

$$y^{n+1} = \frac{q}{(q-1)} x^n - \frac{1}{(q-1)} x_F \qquad q = \frac{h_F^V - h_F}{h_F^V - h_F^L}$$

Note: When $x^n = x_F$

$$y^{n+1} = \left[\frac{q}{q-1} - \frac{1}{q-1} \right] x_F = x_F$$

can plot equation as a straight line with slope equal to $q/(q-1)$ that passes through the point (x_F, x_F)

Summary of Equations

Rectifying Section - upper operating line

$$y^{n+1} = (L/V)x^n + (D/V)x_D \qquad V = L + D$$

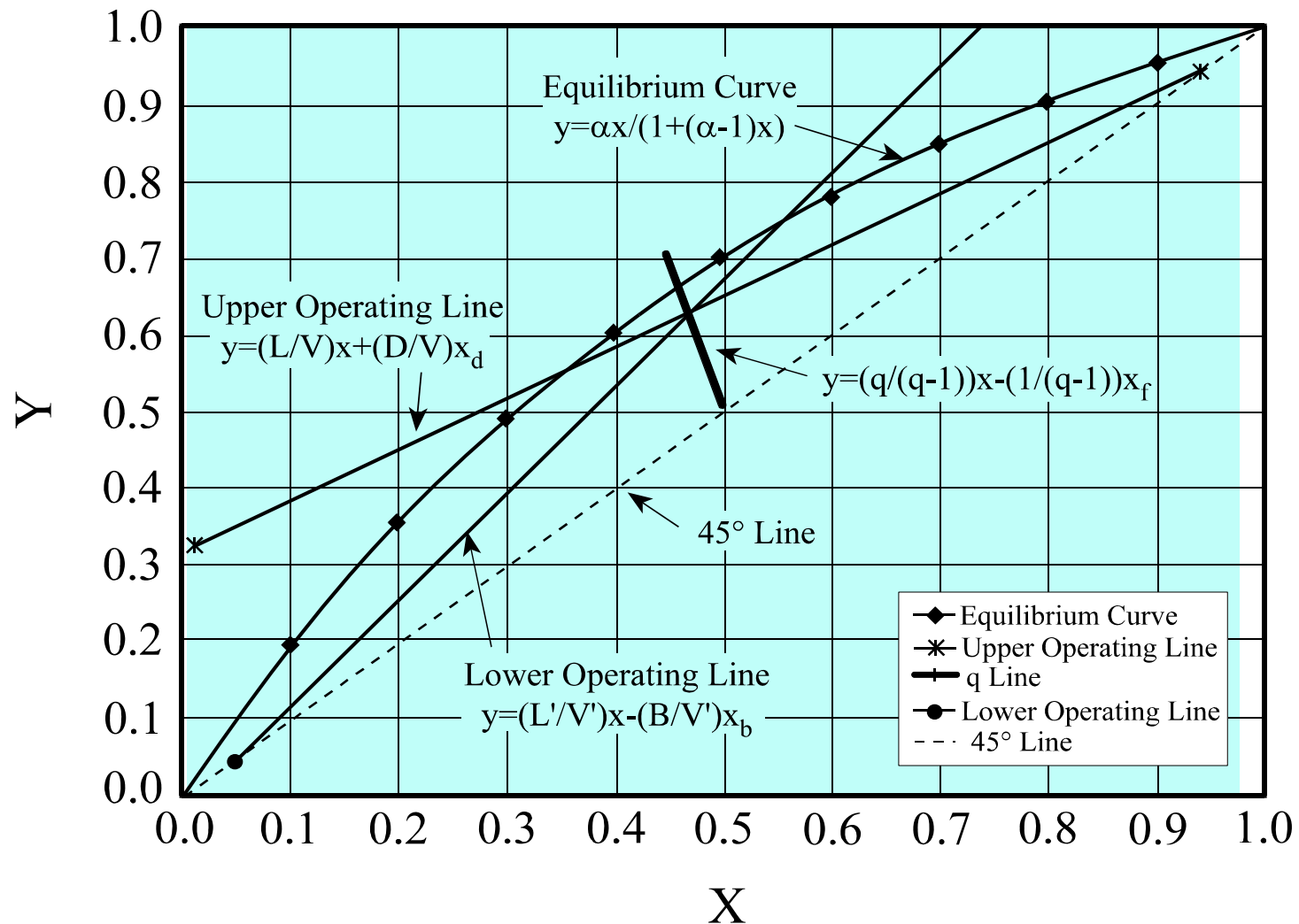
Stripping Section - lower operating line

$$y^{n+1} = (L'/V')x^n - (B/V')x_B \qquad V = L - B$$

Feed Tray - q-line

$$y^{n+1} = q/(q-1)x^n - 1/(q-1)x_F \qquad q = \frac{h_F^V - h_F}{\lambda_F}$$

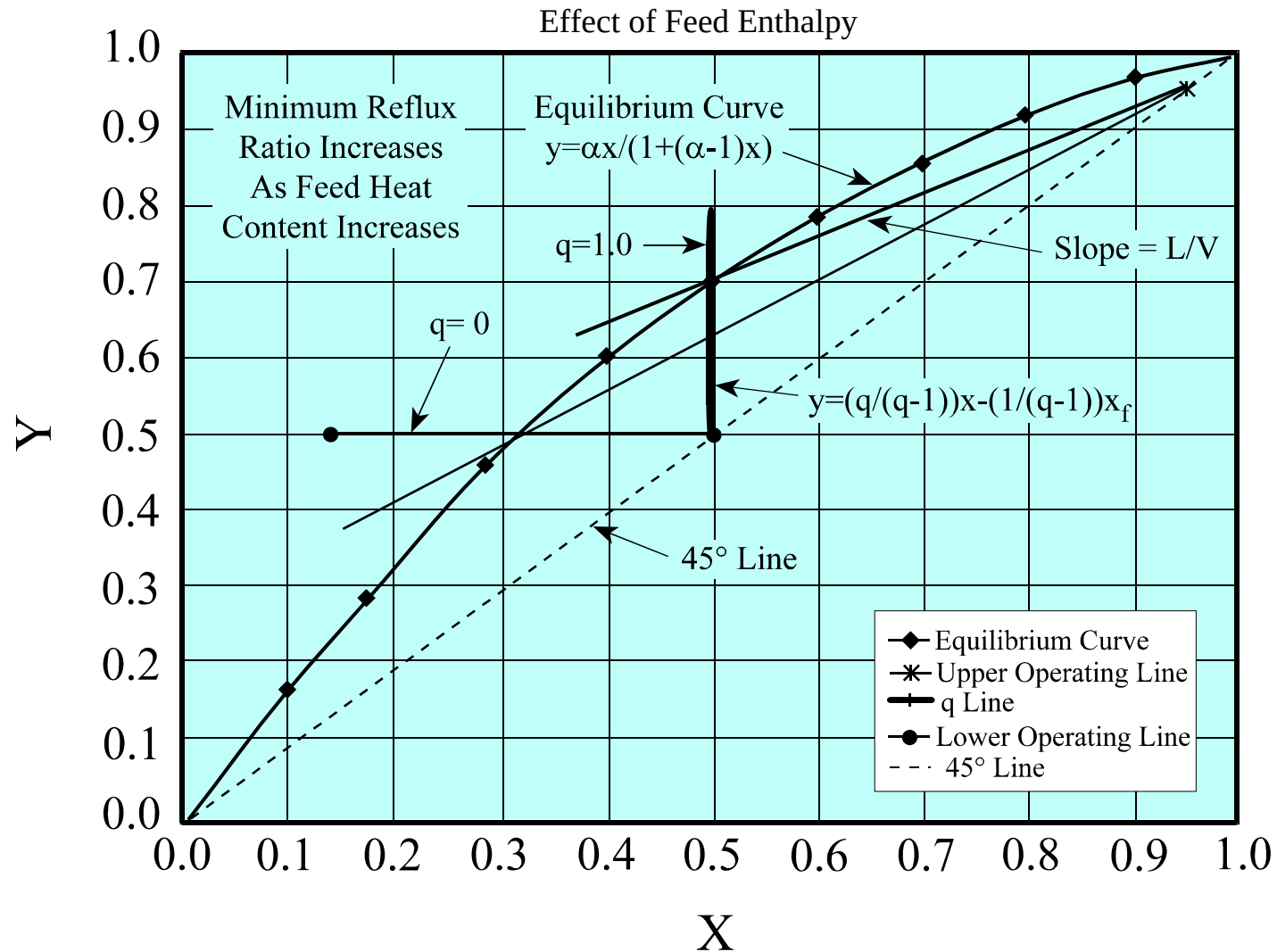
McCabe-Thiele



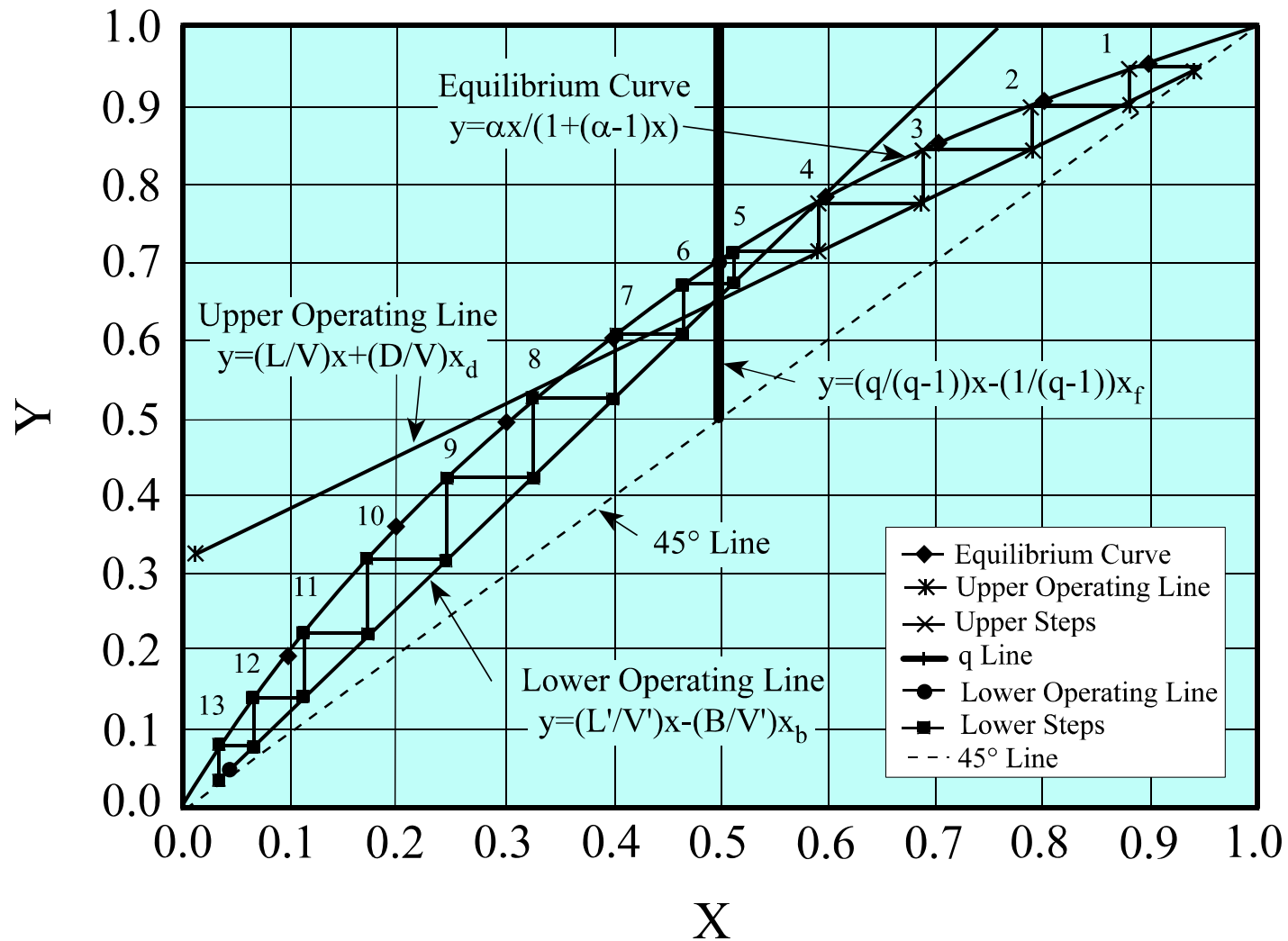
McCabe-Thiele

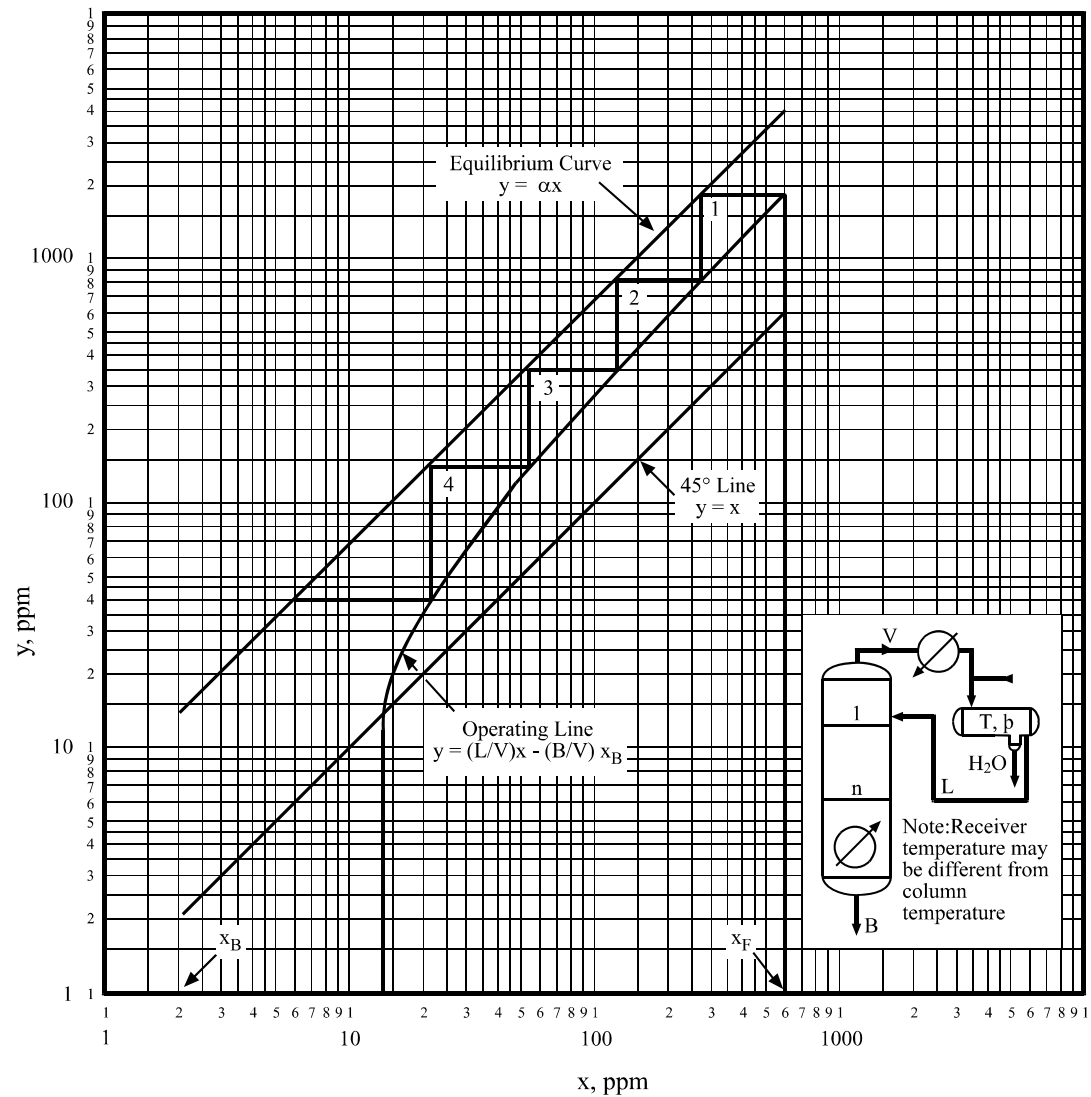
- **What insights do we draw from the McCabe Thiele diagrams?**
 - **Effect of alpha on design (alpha closer to 1 means many more stages for the same separation)**
 - **Effect of feed location and feed vaporization (correct feed location for a subcooled liquid would be the wrong location for a superheated vapor)**
 - **Effect of purity specification on number of stages (more pure products means many more stages)**

McCabe-Thiele



McCabe-Thiele





EDS-R01-0229

n (graphical) = 4.5 Stages

Analytical Approximation

$$n = \frac{\ln(X_F/X_B)}{\ln(\alpha V/L)} = \frac{\ln(610/12.2)}{\ln(6.5/3)}$$

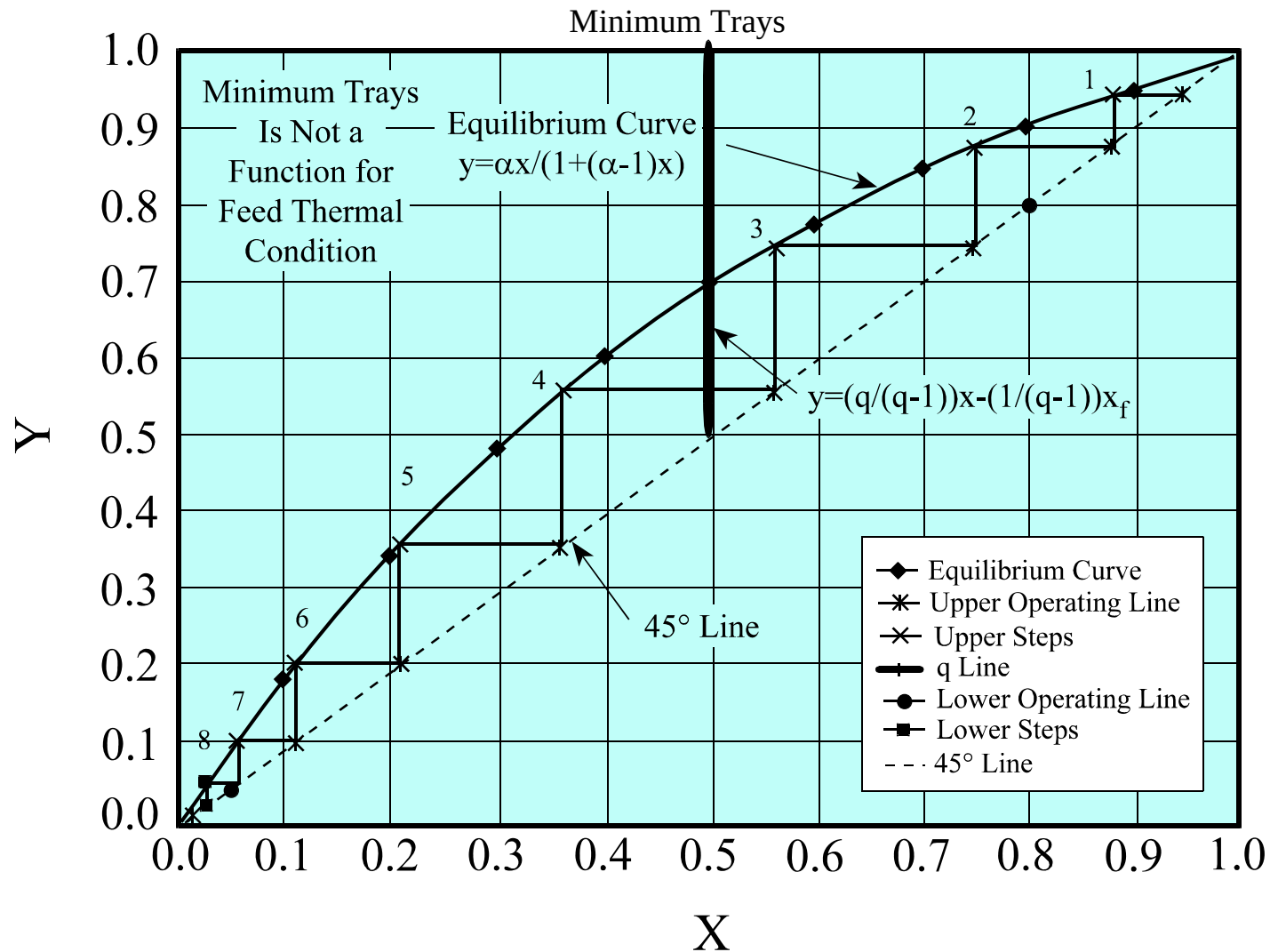
$n = 5.1$

McCabe-Thiele

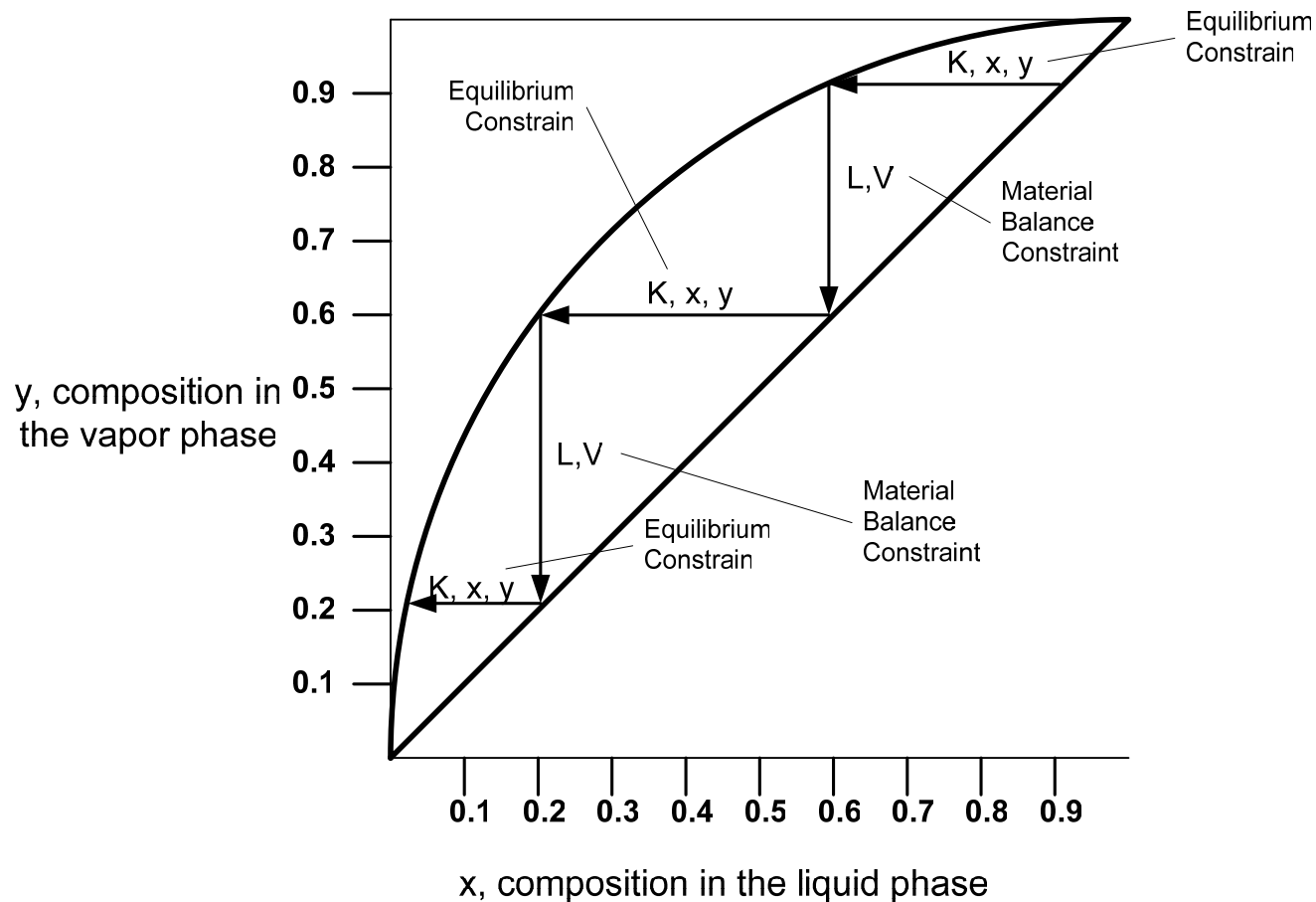
Limiting Conditions or Bounds of a Separation

- **Total reflux – minimum trays**
 - maximum separation but no feed or products
- **Minimum reflux – infinite trays, minimum duty**
 - pinch points
 - adjusting feed location and condition
 - operating reflux and duty

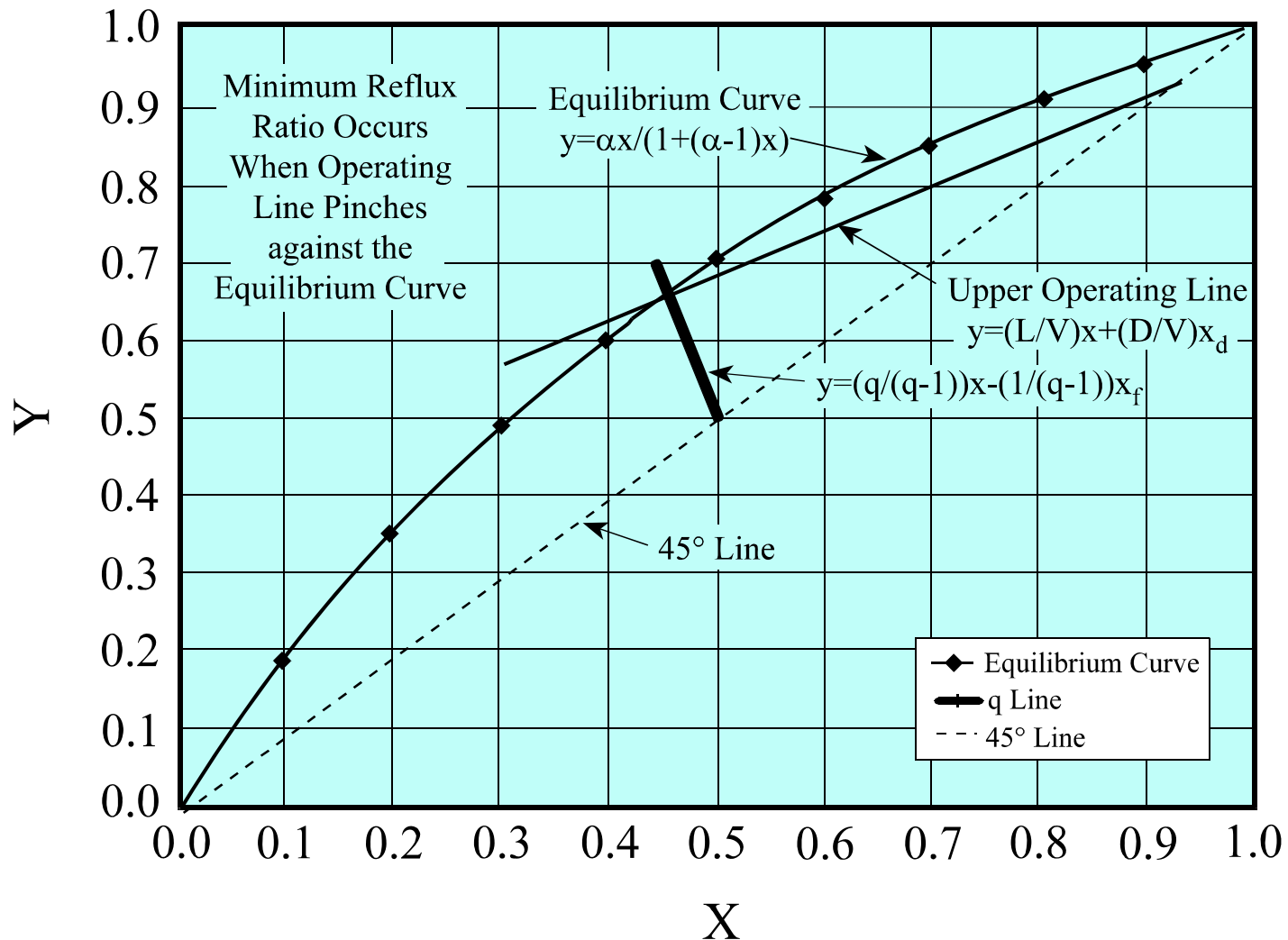
McCabe-Thiele



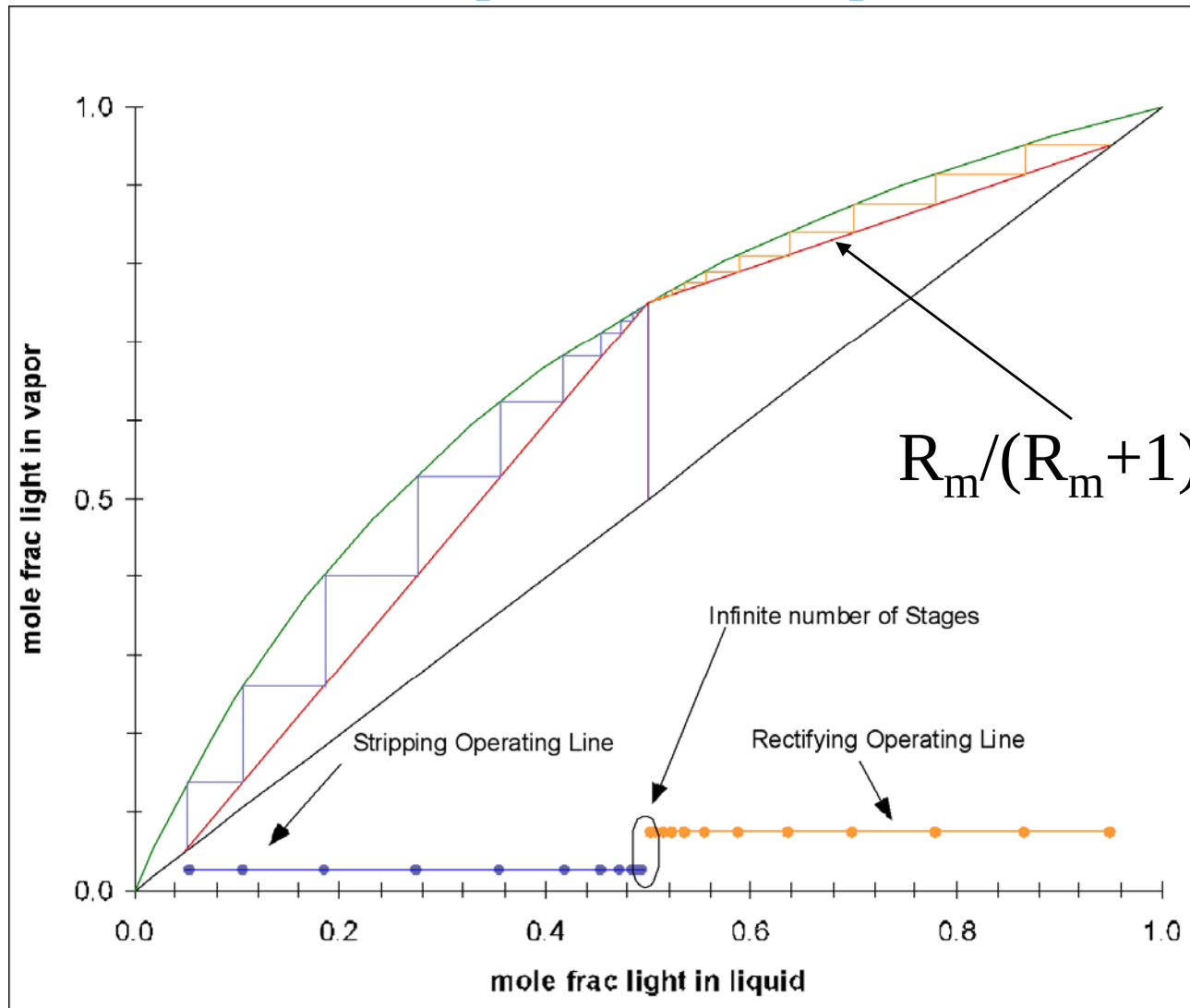
Minimum Stages – McCabe-Thiele Physical Reality



McCabe-Thiele



Minimum Reflux – Infinite Stages

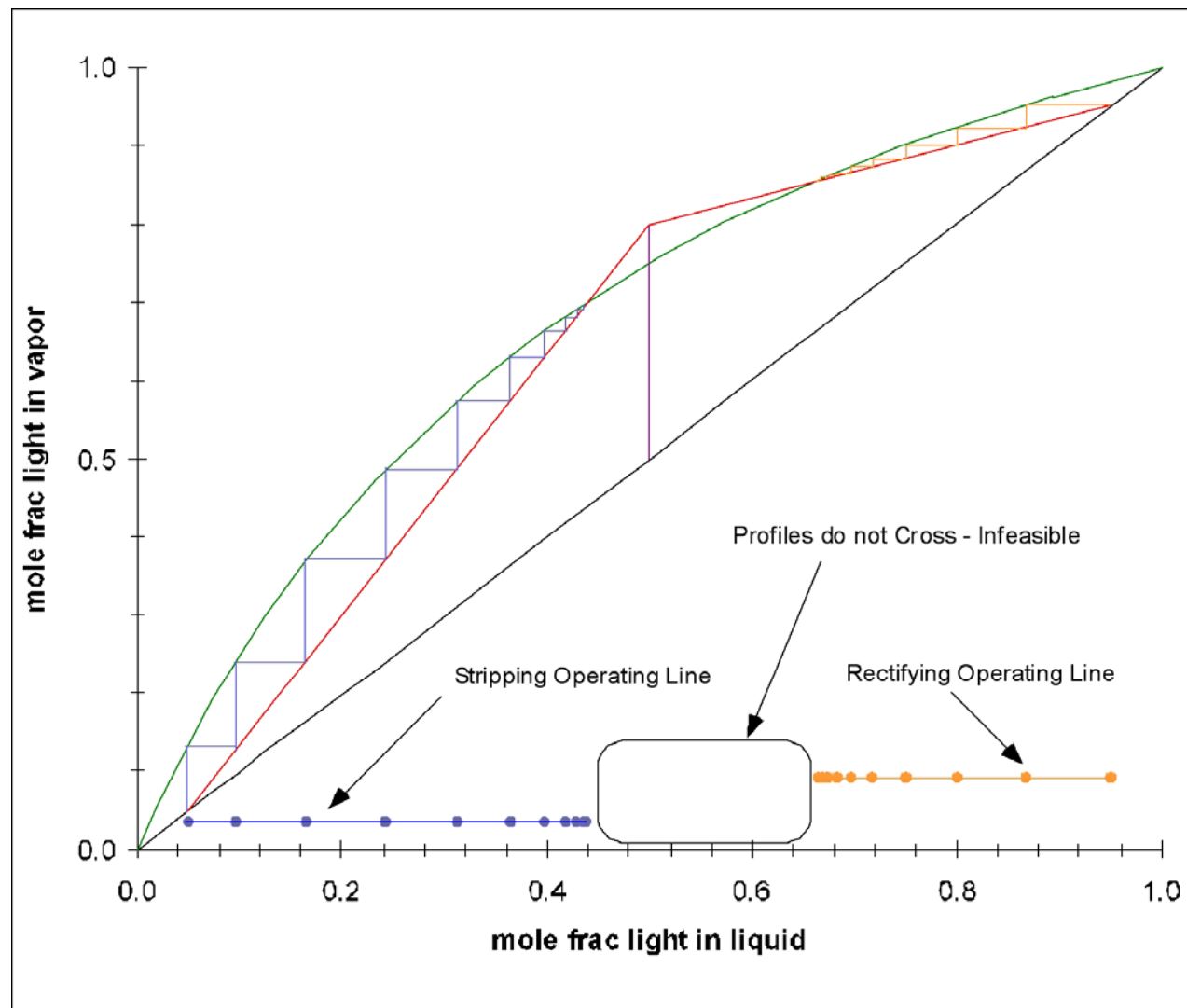


■ Rooks, R.E., Chemical Processing, May 2006

McCabe-Thiele Minimum Reflux

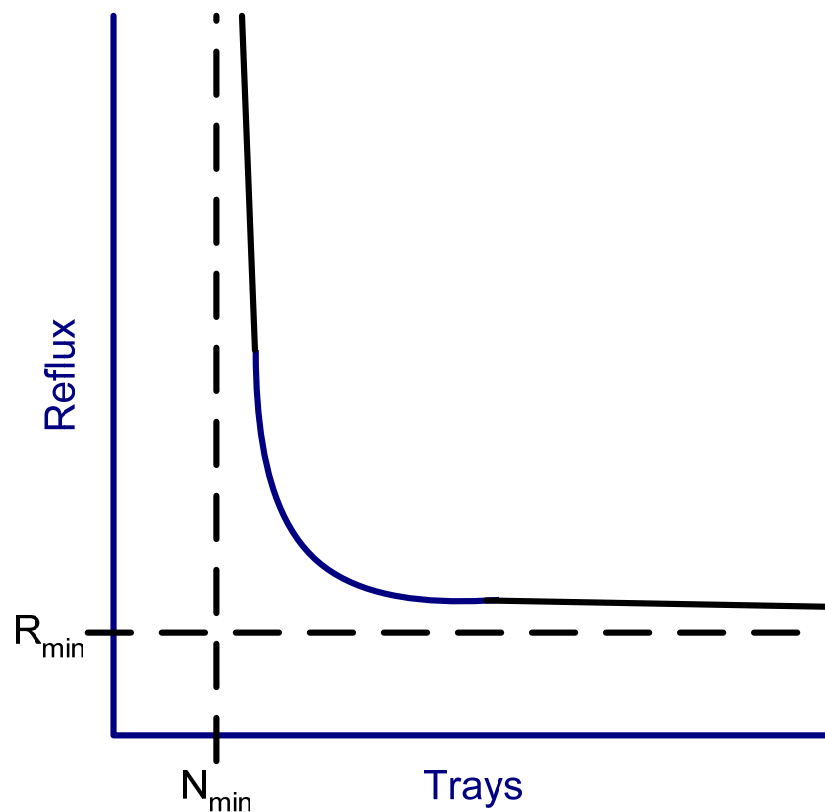
- At minimum, the slope of the upper operating line is:
 - slope = L/V
 - slope = $(x_D - y_F^*) / (x_D - x_F)$
 - where y_F and x_F are the compositions where the q-line meets the equilibrium line
 - $(R/D)_{\min} = L/V / (1 - L/V)$

Infeasible Separation

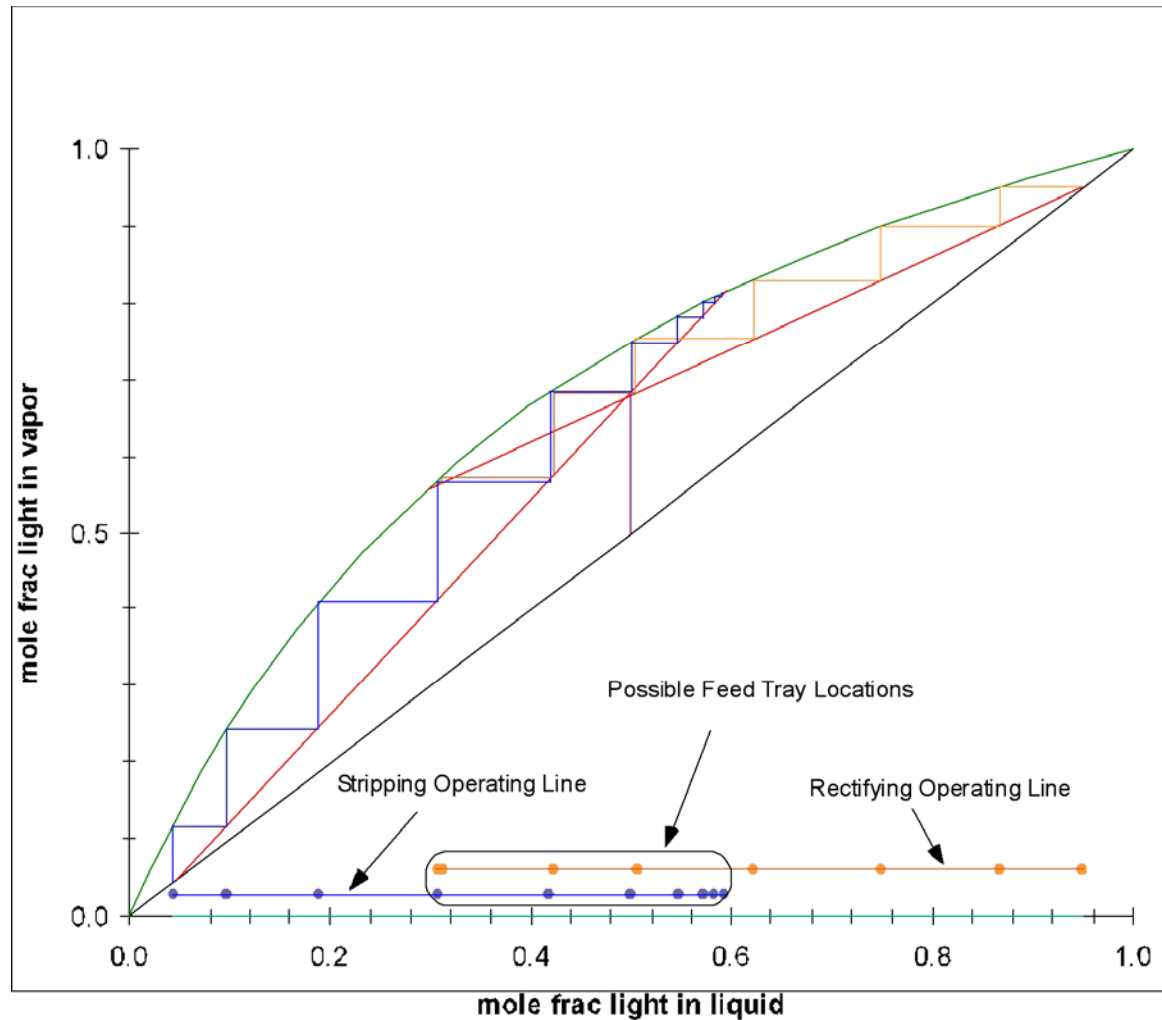


■ **Rooks, R.E., Chemical Processing, May 2006**

More Reflux or More Trays

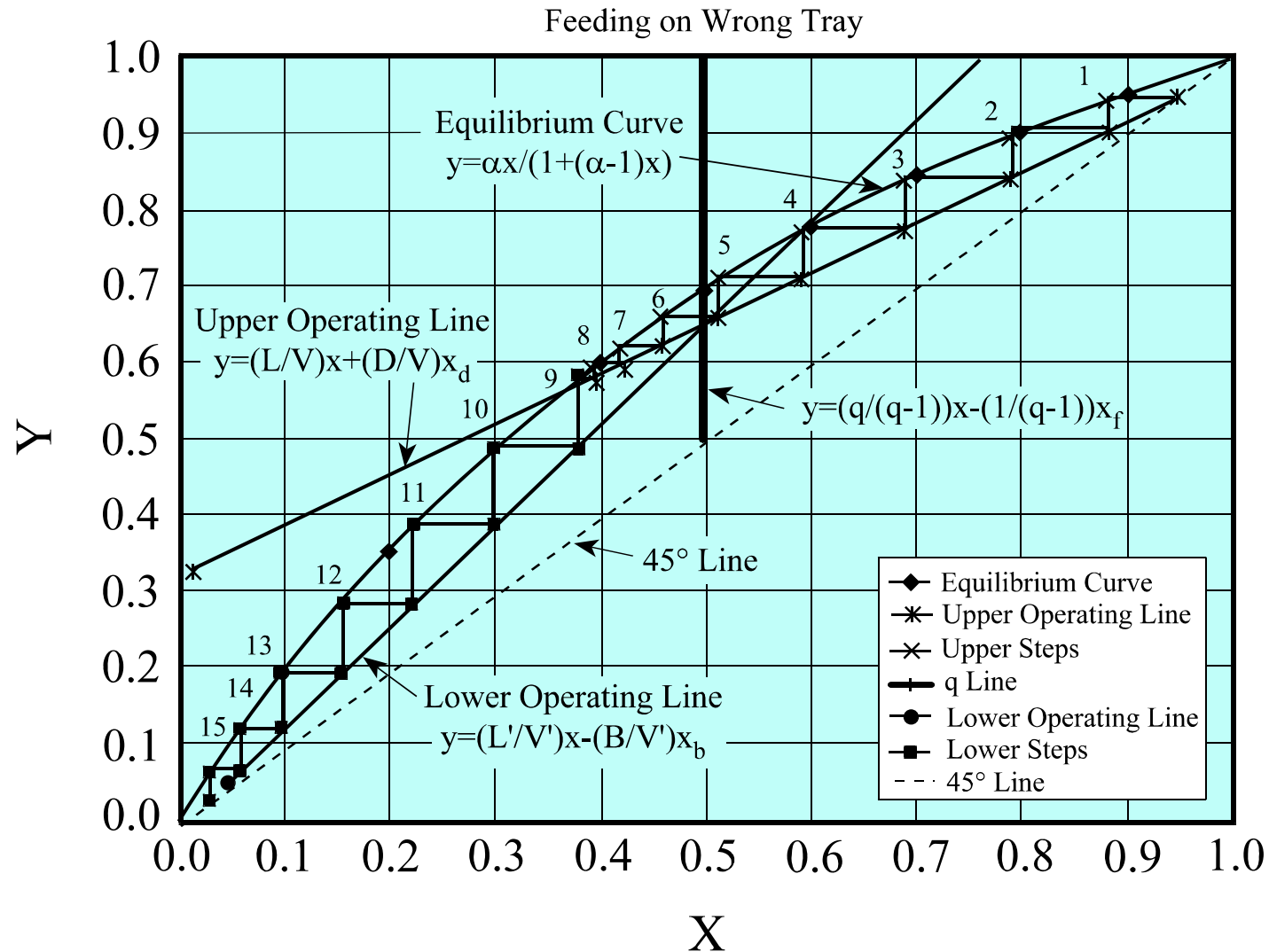


Feed Tray Location

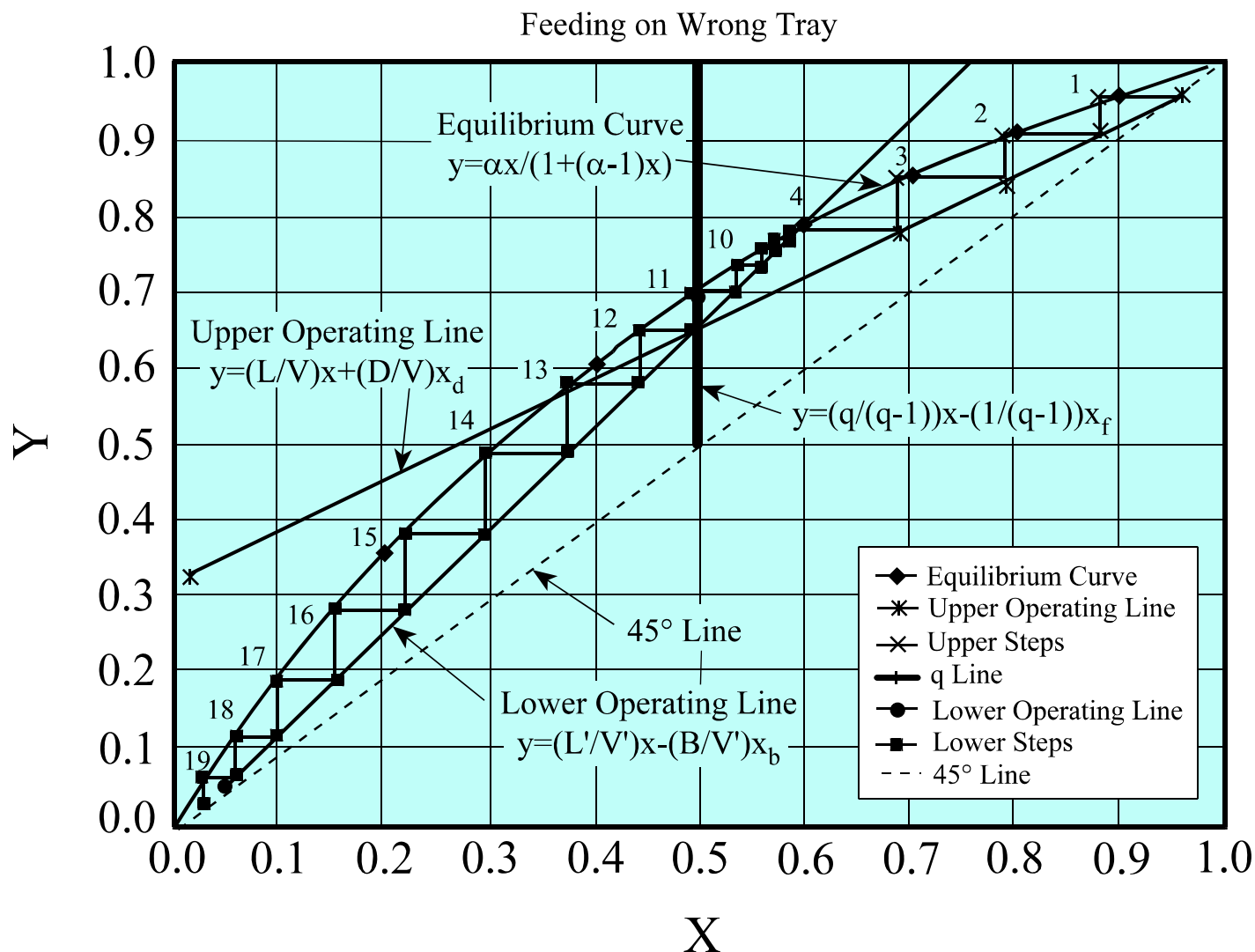


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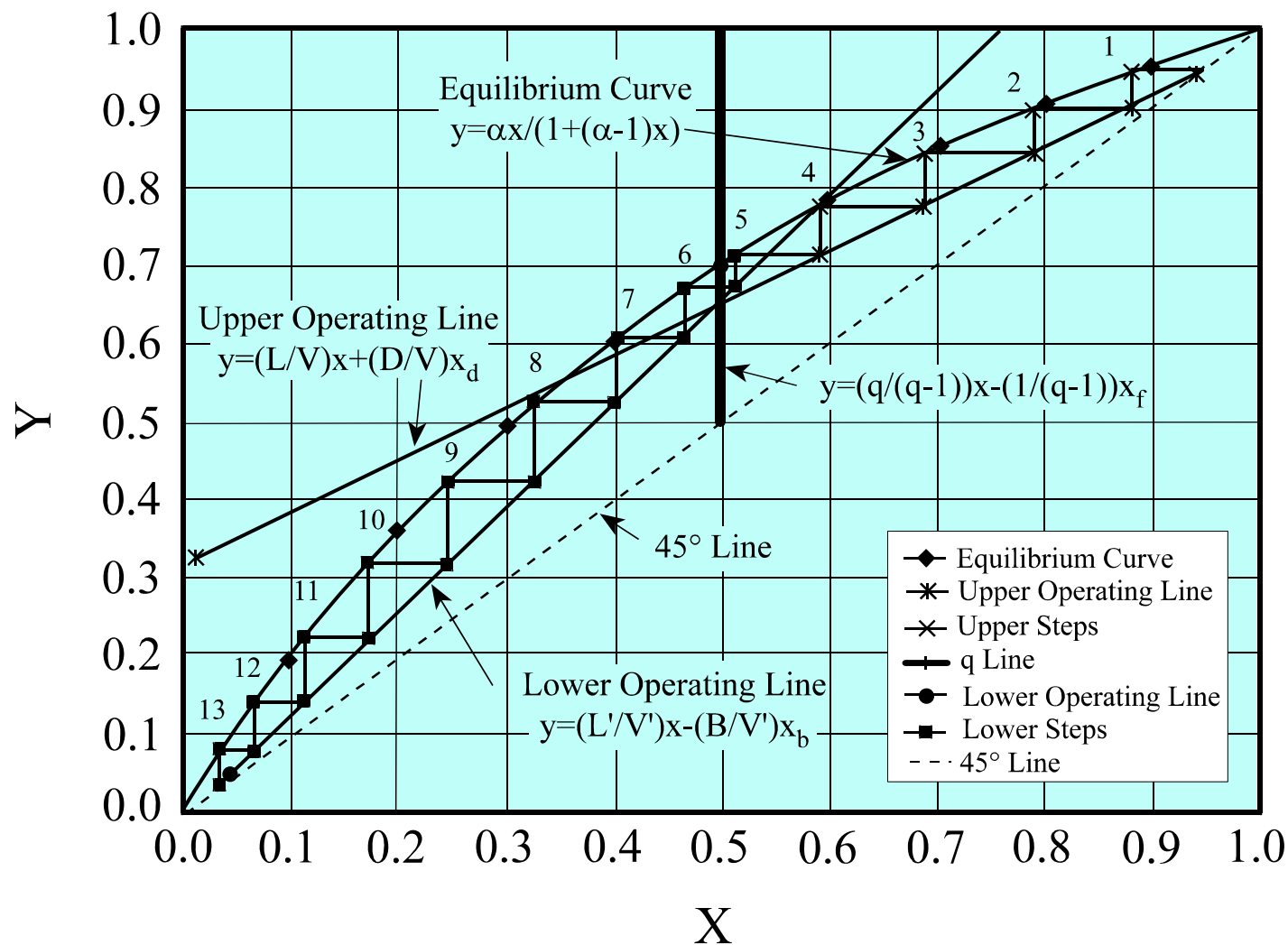
McCabe Thiele – Feed Tray Location



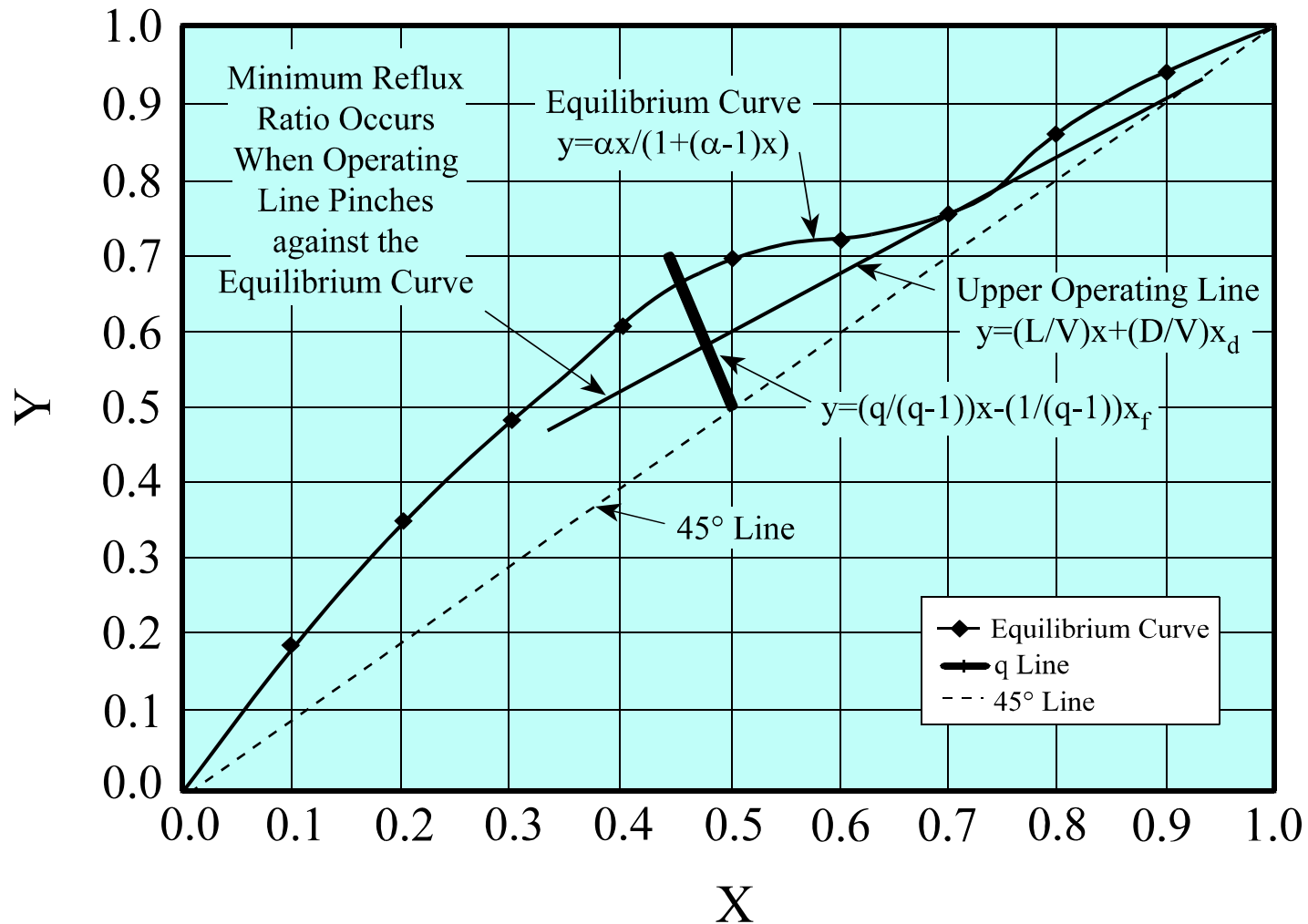
McCabe-Thiele – Feed Tray Location



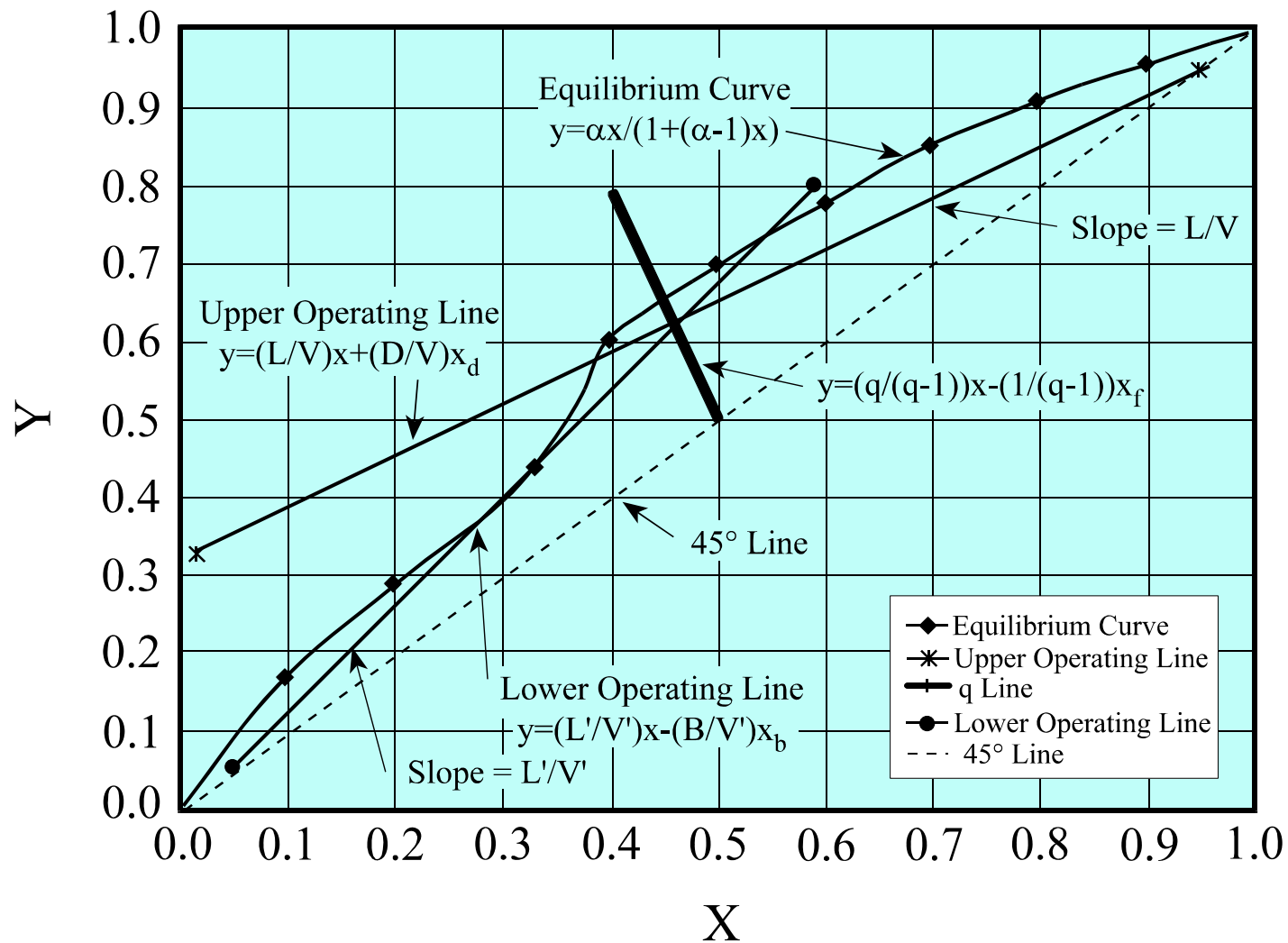
McCabe-Thiele – Feed Tray Location



McCabe-Thiele



McCabe-Thiele



McCabe-Thiele

- **What insights do we draw from the McCabe Thiele diagrams?**
 - **Effect of alpha on design (alpha closer to 1 means many more stages for the same separation)**
 - **Effect of feed location and feed vaporization (correct feed location for a subcooled liquid would be the wrong location for a superheated vapor)**
 - **Effect of purity specification on number of stages (more pure products means many more stages)**

Problem

- **Binary System: Propane-Normal Butane**
 - System pressure = 200 psia
 - Feed = 50 mol/h C₃ + 50 mol/h nC₄ at bubble point
 - Desired purities top and Bottom
$$x_D = 0.95 \qquad x_B = 0.05$$
 - Reflux rate (internal)
$$R = L = 100 \text{ mol/h}$$

Problem

Question: How Many Trays?

$$x_F = 50/100 = 0.50$$

$$x_F F = x_D D + x_B B$$

$$B = F - D$$

$$(0.5)(100) = (0.95)D + 0.05(100 - D) \rightarrow D = 50 \text{ mol/h}$$

Propane – Normal Butane

$\pi = 200$ psia

<u>°F</u>	<u>K₁</u>	<u>K₂</u>	<u>α</u>	<u>x₁</u>	<u>y₁</u>
110	1.058	0.4098	2.58	0.911	0.963
120	1.151	0.4622	2.49	0.781	0.899
130	1.249	0.5180	2.41	0.659	0.824
140	1.350	0.5769	2.34	0.547	0.739
150	1.456	0.6389	2.28	0.442	0.643
160	1.566	0.7036	2.23	0.344	0.538
170	1.681	0.7710	2.18	0.252	0.423
180	1.801	0.8408	2.14	0.166	0.299
190	1.925	0.9130	2.11	0.086	0.165
200	2.051	0.9875	2.08	0.102	0.024

Rectifying Section

For This Problem

$$L = 100 \text{ Mol/h}$$

$$D = 50 \text{ Mol/h}$$

$$\text{Slope} = \frac{L}{V} = \frac{L}{L + D}$$

$$\text{Slope} = \frac{100}{100 + 50} = 0.67$$

Feed Q Line

For This Problem

$$h_F = h_F^L \quad \text{(bubble point liquid feed)}$$

Therefore,

$$q = 1$$

$$q \text{ Line Slope} = \frac{1}{1-1} = \infty$$

Binary System: Propane/Isobutane

■ Specified

- Feed = 200 mol/h C₃ + 200 mol/h iC₄ at bubble point
- Distillate = 196 mol/h
- Reflux = 400 mol/h at 100°F
- Column pressure = 250 psia
- Number of trays = 24, feed on 13

■ Problem

- Find x_D and x_B
- $L = 1.16 F = 464 \text{ mol/h}$ $L/F = \frac{464}{400} = 1.16$

Binary System: Propane/Isobutane

**Rigorous Heat and Weight
Balanced Tray-to-Tray
Method**

$$x_D = 0.927$$

$$x_B = 0.090$$

**Equimolal Overflow
Simplified Tray-to-Tray
Method**

$$0.917$$

$$0.098$$

Binary System: Propane/Benzene

■ Specified

- Feed = 50 mol/h C₃ + 50 mol/h Bz at bubble point
- Distillate = 50 mol/h
- $x_D = \underline{0.99}$
- Column pressure = 215 psia
- Number of trays = 10, Feed on 6

■ Problem

- Find reflux rate (temp = 100°F)

Binary System: Propane/Benzene

**Equimolal Overflow
Simplified Tray-to-Tray
Method**

$R = 5 \text{ Mol/hr}$

**Rigorous Heat and Weight
Balance Tray-to-Tray
Method**

$R = 14 \text{ Mol/h !!}$

If 5 Mol/h, $x_D = \underline{0.967}$

Tray to tray energy and total material balance makes a difference

Analytic Methods

- **For multicomponent mixtures or to ease the use of graph paper, we use the shortcut/approximate methods**
- **Smokers**
- **Fenske**
- **Underwood**
- **Gilliland**

Smoker's Equation

- **Simplified form**

$$N = \frac{\ln(S)}{\ln \left[\alpha \sqrt{1 - \frac{R + q}{(R + 1)(Rx_F + q)}} \right]}$$

- **where S is a separation parameter**

$$S = (x_{LK} / x_{HK})_D (x_{HK} / x_{LK})_B$$

$$R = L / D$$

Minimum Trays

Fenske Equation

$$n_m = \frac{\text{Log}(r_D/r_B)}{\text{Log } \alpha}$$

$$r_D = \frac{X_D}{1 - X_D}$$

$$r_B = \frac{X_B}{1 - X_B}$$

Minimum Reflux

Underwood Method

$$1) \quad \frac{1 - x_F}{1 - \phi} + \frac{\alpha x_F}{\alpha - \phi} = 1 - q, 1 < \phi < \alpha$$

$$2) \quad (L/D)_{\min} = \frac{(1 - x_D)}{(1 - \phi)} + \frac{\alpha x_D}{(\alpha - \phi)} - 1$$

Solve equation 1 for the proper root of the quadratic for ϕ .

Solve equation 2 for $(L/D)_{\min}$ using the ϕ from equation 1.

Minimum Reflux

Note: If terms are multiplied out, equation 1 becomes

$$(1 - q)\phi^2 + (q + \alpha q + \alpha x_F - \alpha - x_F)\phi - q\alpha = 0$$

$$A\phi^2 + B\phi + C = 0$$

$$\phi = \frac{-B \pm \sqrt{B^2 - 4AC}}{2A}$$

Minimum Reflux

Underwood Method

If feed is bubble point liquid:

$$q = 1$$

The Underwood equations reduce to

$$(L/D)_m = \frac{1}{\alpha - 1} \left[\frac{x_D}{x_F} - \frac{\alpha(1 - x_D)}{(1 - x_F)} \right]$$

Minimum Reflux

Note: For perfect separation ($x_D = 1$)

$$(L/D)_m = \left(\frac{1}{\alpha - 1} \right) \left(\frac{1}{x_F} \right)$$

$$x_F = D/F$$

Since $x_F F = x_D D + x_B B$

Then $x_F = D/F$

When $x_D = 1$

Therefore $(L/F)_m = \frac{1}{\alpha - 1}$

For perfect separation with bubble point feed.

Feed Tray Location

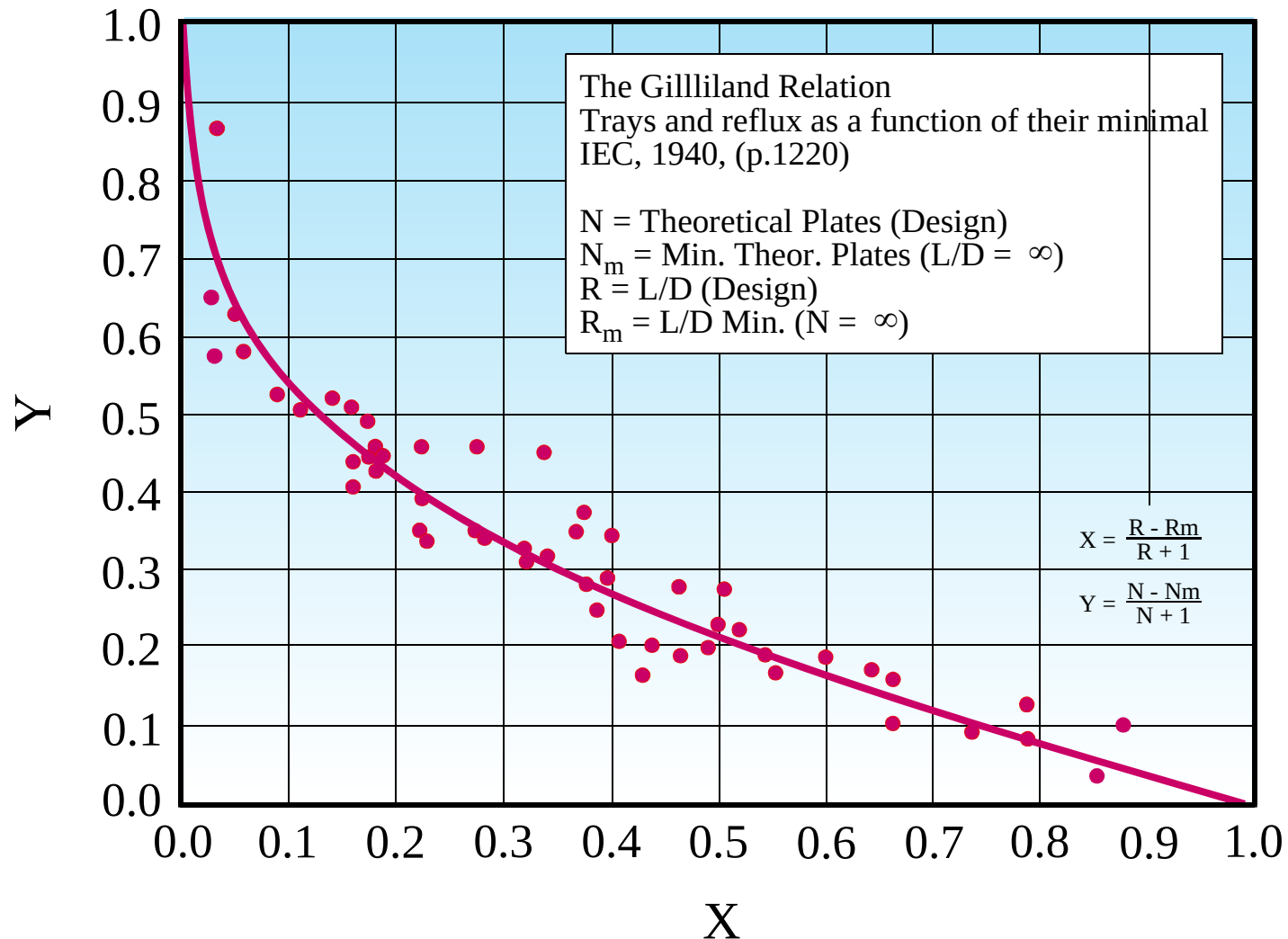
For Bubble Point Feed

$$n_m^R = \frac{\text{LOG}(r_D/r_F)}{\text{LOG } \alpha} \quad \left\{ \begin{array}{l} \text{Fenske Equation} \\ \text{rectifying section} \end{array} \right.$$

Then

$$\frac{n_m^R}{n_m} = \frac{\text{LOG}(r_D/r_F)}{\text{LOG}(r_D/r_B)} \quad \left\{ \begin{array}{l} \text{Assume ratio holds} \\ \text{for any reflux ratio} \end{array} \right.$$

Analytical Techniques



Analytical Techniques

$$X = \frac{R - R_m}{R + 1}$$

$$R = \frac{R_m + X}{1 - X}$$

$$Y = \frac{N - N_m}{N + 1}$$

$$N = \frac{N_m + Y}{1 - Y}$$

X + Y are parameters, not compositions

Determine:

R_m from Underwood Equation

N_m from Fenske Equation

Example #1

$$\begin{array}{llll} X_F = 0.5 & r_F = 1.0 & & \\ X_D = 0.927 & r_D = 12.7 & D/F = 0.49 & \\ X_B = 0.090 & r_B = 0.0989 & & \\ \alpha = 1.76 & q = 1.0 & & \end{array}$$

Given $n = 24$, calculate needed reflux

UNDERWOOD

$$(L/D)_m = \frac{1}{\alpha - 1} \left[\frac{X_D}{X_F} - \frac{\alpha(1 - X_D)}{(1 - X_F)} \right]$$

Example #1

FENSKE

$$n_m = \frac{\text{LOG}(r_D/r_B)}{\text{LOG}\alpha} = 8.59$$

$$\frac{n_m^R}{n_m} = \frac{\text{LOG}(r_D/r_F)}{\text{LOG}(r_D/r_B)} = 0.523$$

$$n \text{ (real in rectifying section)} = 0.523 \times 24 = 12.6$$

Example #1

GILLILAND

$$Y = \frac{N - N_m}{N + 1} = 0.616 \quad \rightarrow \quad X = 0.055$$

$$L/D = \frac{(L/D)_m + X}{1 - X} = 2.28 \quad \rightarrow \quad R/F = 1.12$$

Example #1

$$N = 24$$

$$L/D = 2.28$$

$$n_m = 8.59$$

$$L/D_m = 2.10$$

Multicomponent: Debutanizer C4- from Naphtha

	Approximate Method	Rigorous Method
R/D	14.1	10.1
Condenser Duty	15.8 Gcal/hr	11.5 Gcal/hr
Stages Above Feed	6	10
Actual Above Feed	11	17
Stages Below Feed	21	21
Actual Below Feed	33	33
Reboiler Duty	21.6 Gcal/hr	17.3 Gcal/hr
Tray to tray energy, material balances and equilibrium still make a difference the further we move from assumptions		

Shortcut/Approximate Methods

- **McCabe-Thiele – Binary Distillation**
- **Fenske – Minimum tray**
- **Underwood – Minimum reflux**
- **Kremser – Absorbers and Strippers**

Underwood Method

(Minimum Reflux)

Underwood's Method Assumptions: Constant Molal Overflow and Constant α

$$\text{a) } \sum_1^n \frac{\alpha_i X_{i,F}}{\alpha_i - \phi} = 1 - q$$

X - Mol fraction in total stream

Φ - Underwood parameter

Q - Feed thermal conditions

$$\text{b) } \sum_1^n \frac{\alpha_i X_{i,D}}{\alpha_i - \phi} = (L/D)_{\text{MIN}} + 1$$

I - A component

N - Total number of components

All possible roots of equation (a) lie between the α 's of the feed components

Substitution of these roots into (b) yields $(L/D)_{\text{MIN}}$

Example #1

$$\begin{array}{llll} X_F = 0.5 & r_F = 1.0 & & \\ X_D = 0.927 & r_D = 12.7 & D/F = 0.49 & \\ X_B = 0.090 & r_B = 0.0989 & & \\ \alpha = 1.76 & q = 1.0 & & \end{array}$$

Given $n = 24$, calculate needed reflux

UNDERWOOD

$$(L/D)_m = \frac{1}{\alpha - 1} \left[\frac{X_D}{X_F} - \frac{\alpha(1 - X_D)}{(1 - X_F)} \right]$$

Example #1

FENSKE

$$n_m = \frac{\text{LOG}(r_D/r_B)}{\text{LOG}\alpha} = 8.59$$

$$\frac{n_m^R}{n_m} = \frac{\text{LOG}(r_D/r_F)}{\text{LOG}(r_D/r_B)} = 0.523$$

$$n \text{ (real in rectifying section)} = 0.523 \times 24 = 12.6$$

Example #1

GILLILAND

$$Y = \frac{N - N_m}{N + 1} = 0.616 \quad \rightarrow \quad X = 0.055$$

$$L/D = \frac{(L/D)_m + X}{1 - X} = 2.28 \quad \rightarrow \quad R/F = 1.12$$

Example #1

$$N = 24$$

$$L/D = 2.28$$

$$n_m = 8.59$$

$$L/D_m = 2.10$$

Minimum Reflux Sample Problem

Comp	α	← Mols/Hr →		
		Feed	Ovhd	Bottoms
A	6	40	40	-
B - LK	2	20	20	-
C - HK	1	20	-	20
D	0.5	20	-	20
		100	60	40

Bubble Point Feed

Minimum Reflux Underwood

1st Equation

$$\sum_1^n \frac{\alpha_i X_{i,F}}{\alpha_i - \phi} = 1 - q$$

$$\frac{(6)(0.4)}{(6 - \phi)} + \frac{(2)(0.2)}{(2 - \phi)} + \frac{(1)(0.2)}{(1 - \phi)} + \frac{(0.5)(0.2)}{(0.5 - \phi)} = 1 - 1$$

$$\frac{2.4}{(6 - \phi)} + \frac{(0.4)}{(2 - \phi)} + \frac{0.2}{(1 - \phi)} + \frac{0.1}{(0.5 - \phi)} = 0$$

$1 \leq \phi \leq 2$ (ϕ between 1 and light/heavy key alpha)

$\phi = 1.2267$ By Trail and Error

Minimum Reflux Underwood

2nd Equation

$$\sum_1^n \frac{\alpha_i X_{i,D}}{\alpha_1 - \phi} = \left(\frac{L}{D} \right)_{MIN} + 1$$

$$\frac{6 \left(\frac{40}{60} \right)}{6 - 1.2267} + \frac{2 \left(\frac{20}{60} \right)}{2 - 1.2267} = \frac{L}{D} + 1$$

$$\frac{L}{D} = 0.700 \rightarrow L = (0.7)(60) = 42.0 \text{ Mols/Hr}$$

Fenkse Equation (Minimum Trays)

$$n = \frac{\log\left(\frac{r_D}{r_B}\right)_K}{\log(\alpha_K)}$$

n = minimum trays

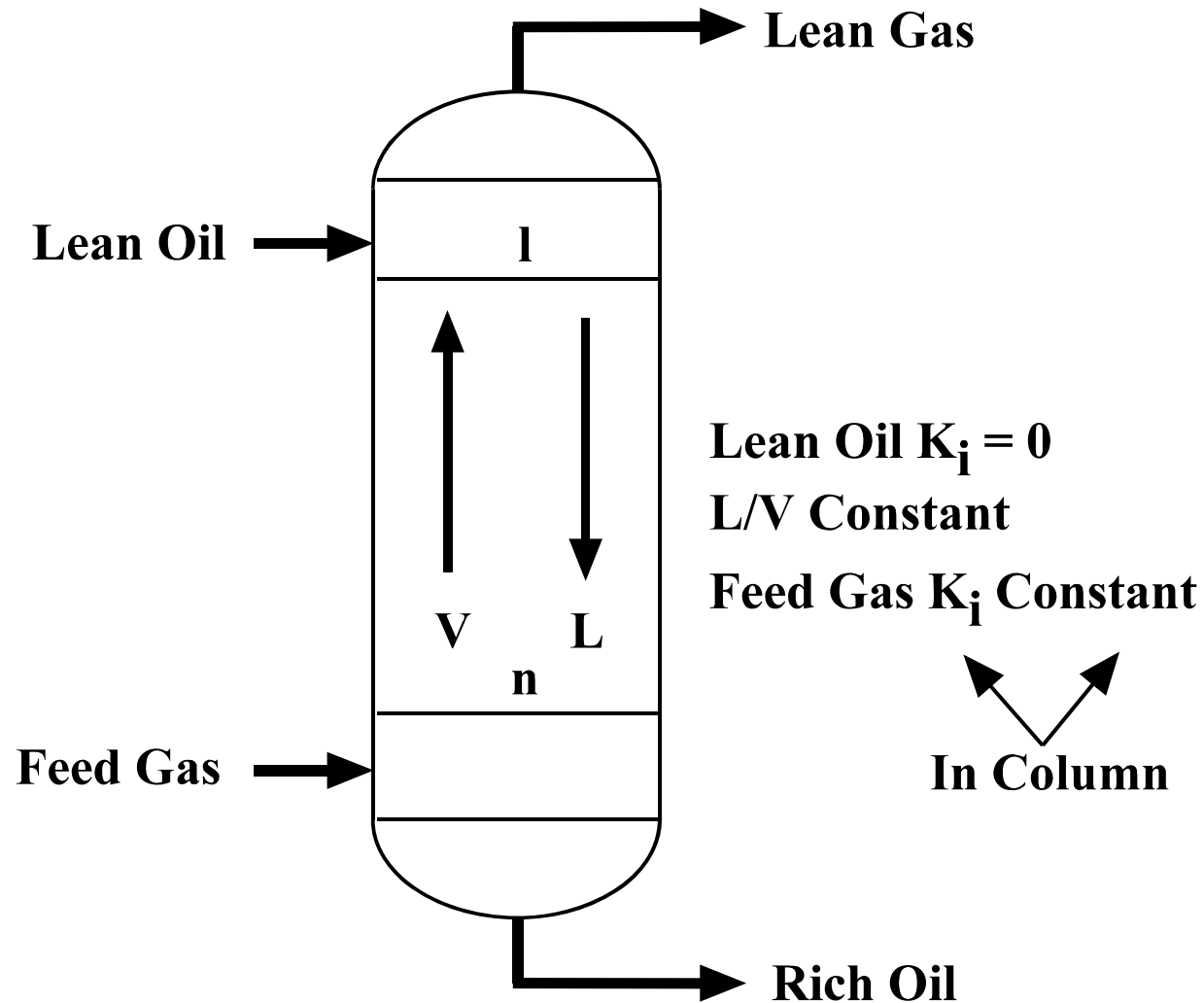
r_D = ratio of light and heavy key material in distillate

r_B = ratio of light and heavy key material in bottoms

Fenkse Equation (Sample Problem)

$$n = \frac{\log\left(\frac{r_D}{r_B}\right)_K}{\log(\alpha_K)} = \frac{\log\left(\frac{553.4 / 1.9}{5.6 / 127.1}\right)}{\log(1.74)} = 15.9$$

Kremser Simple Absorber



Kremser Simple Absorber

- Define $A = L/KV$

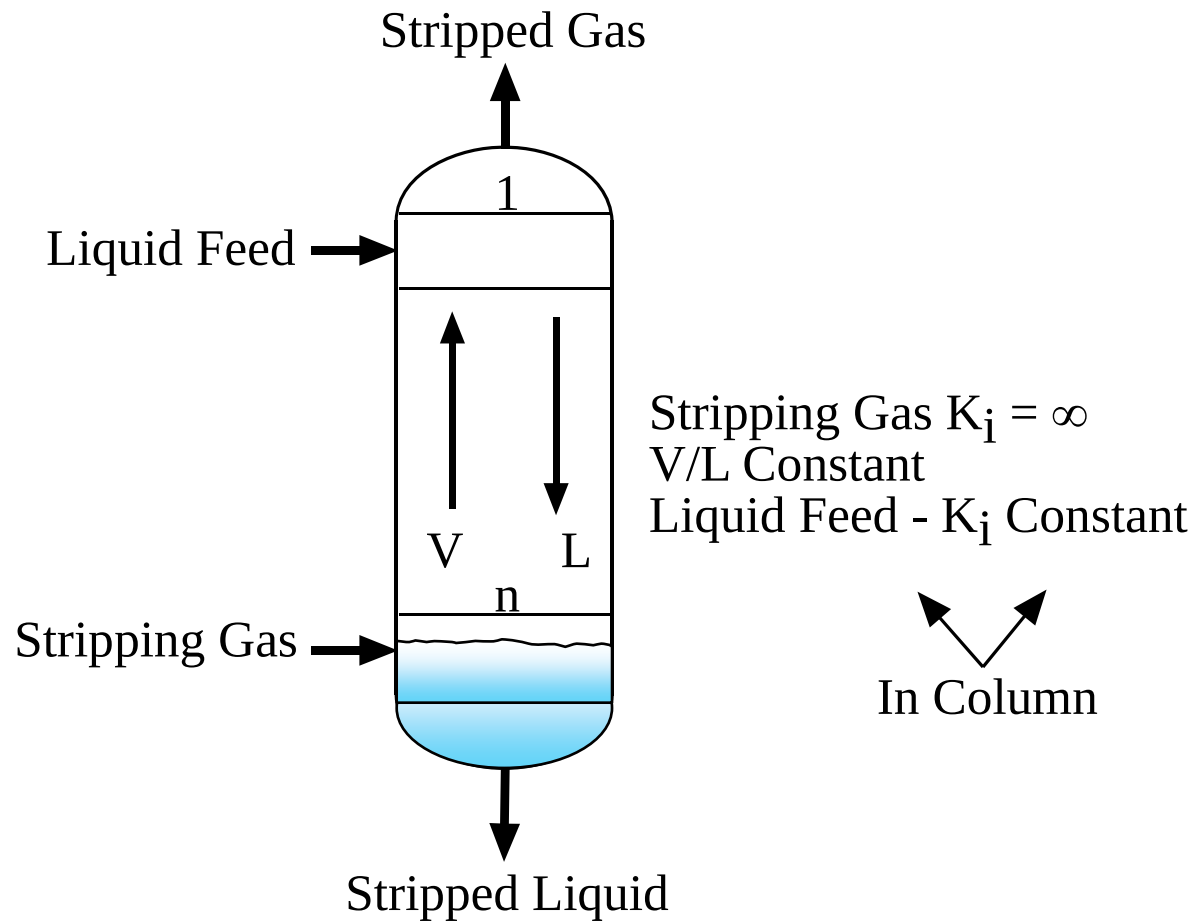
↖
— Absorption Factor

- Fraction of Gas Component Absorbed = $f(A)$

$$f(A) = \left(A^{n+1} - A / A^{n+1} - 1 \right)$$

Note: Liquid phase non-ideality corrections are usually significant for absorbers.

Kremser Simple Stripper



Kremser Simple Stripper

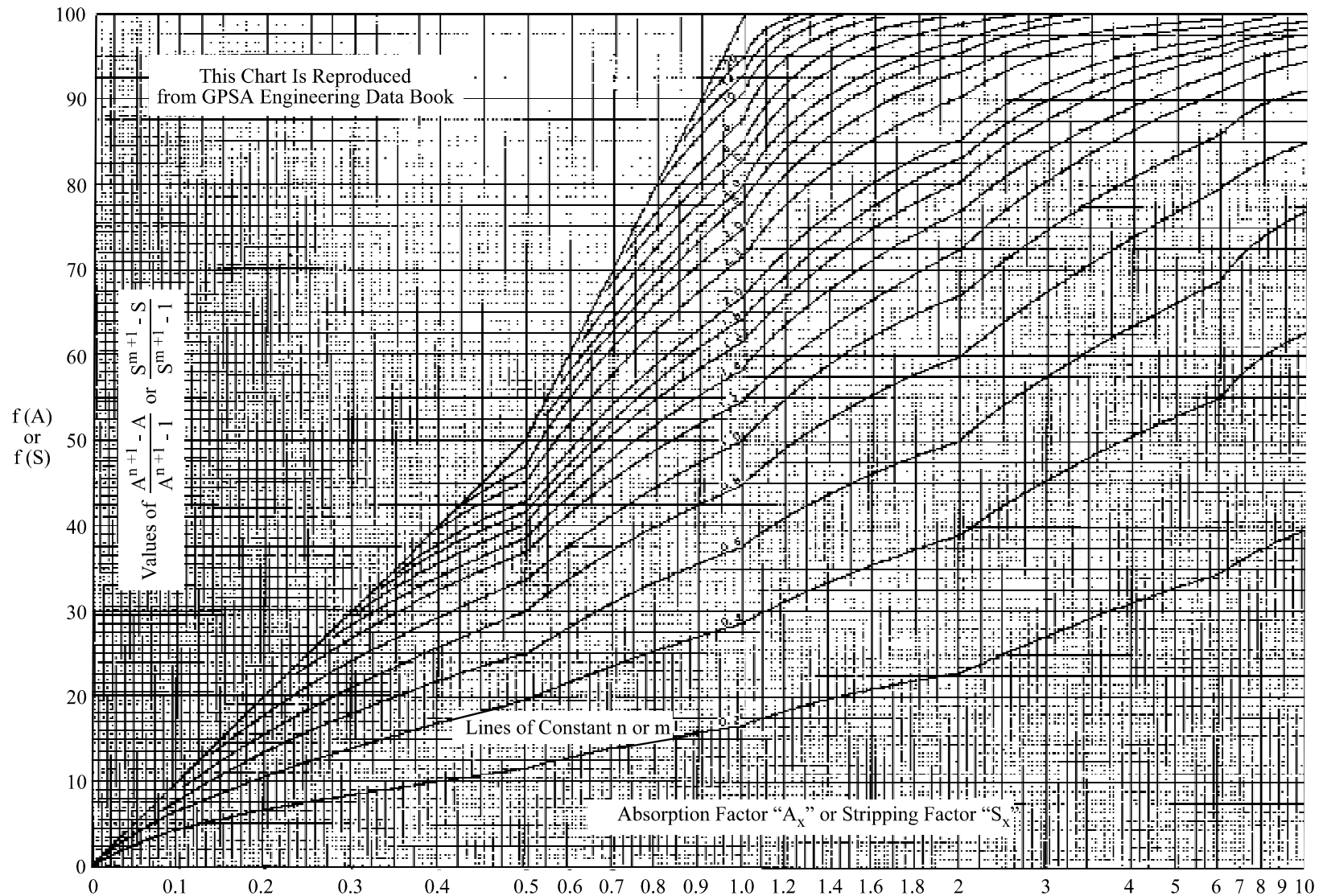
- Define $S = KV/L$

↖
— Stripping Factor

- Fraction of Liquid Component Stripped = $f(S)$

$$f(S) = \left(S^{n+1} - S / S^{n+1} - 1 \right)$$

Absorption and Stripping Factor Correlation



Kremser

Example – Simple Absorber

Gas at 100°F and 250 psia

6 Theoretical Trays

125°F Average (Use Intercoolers)

For 90% Propane Recovery -

Complete Absorber Material Balance

Kremser

Example – Simple Absorber

Comp.	Gas to Abs. (R+V ₀)	K 250psig 125°F	A <u>L</u> KV	100f(A) % Abs'd	Abs'd Mtl R	Off Gas V ₀
H ₂	172	68.2	0.017	1.7	3	169
N ₂	151	12.5	0.093	9.3	14	137
C ₁	339	9.26	0.126	12.6	43	296
C ₂	361	2.437	0.479	47.9	173	188
C ₃	95	1.029	1.135	90.0	86	9
iC ₄	52	0.558	2.093	100	52	
nC ₄	61	0.434	2.691	100	61	
iC ₅	42	0.222	5.261	100	42	
nC ₅	18	0.178	6.562	100	18	
nC ₆	<u>16</u>	0.0728	16.0	100	<u>16</u>	<u> </u>
	1307				508	799

Average L / V = (L / KV)(K) = 1.135 x 1.029 = 1.168

Kremser

Example – Simple Absorber

- Define Average $L/V = (L_0 + R/2)/(V_0 + R/2)$
 - The absorption oil rate, L_0 , is calculated:

$$L_0 = \frac{(L/V)(2V_0 + R) - R}{2}$$

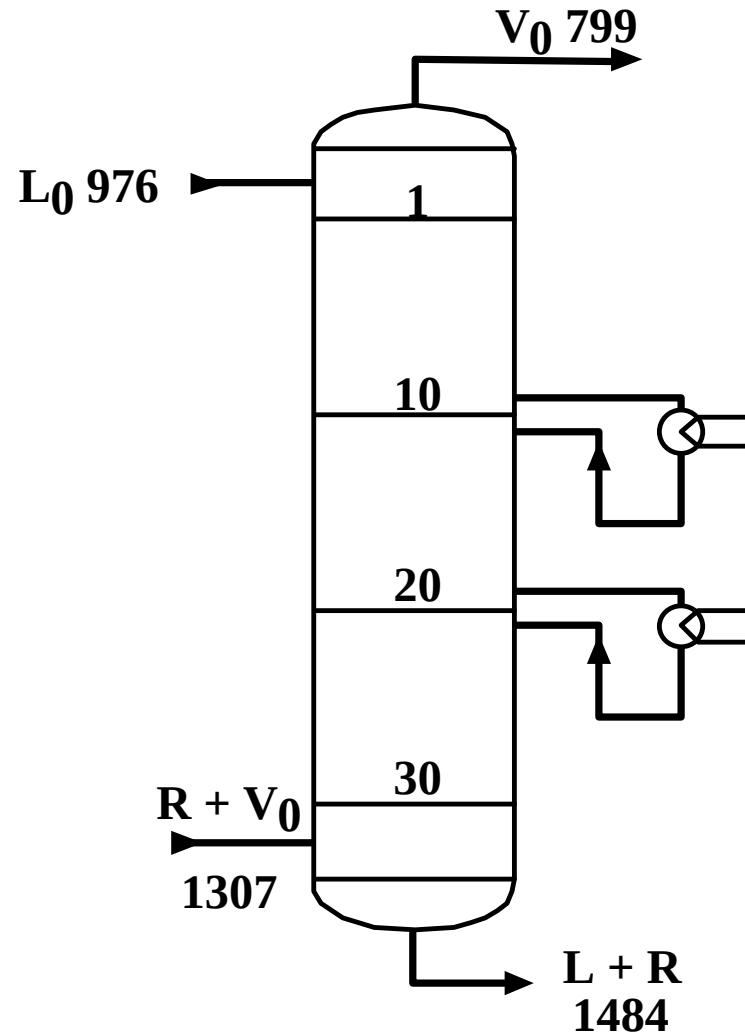
$$L_0 = \frac{(1.168)((2)(799) + 508) - 508}{2}$$

$$L_0 = 976 \text{ moles per hour}$$

- Estimating a tray efficiency of 20%, use 30 trays

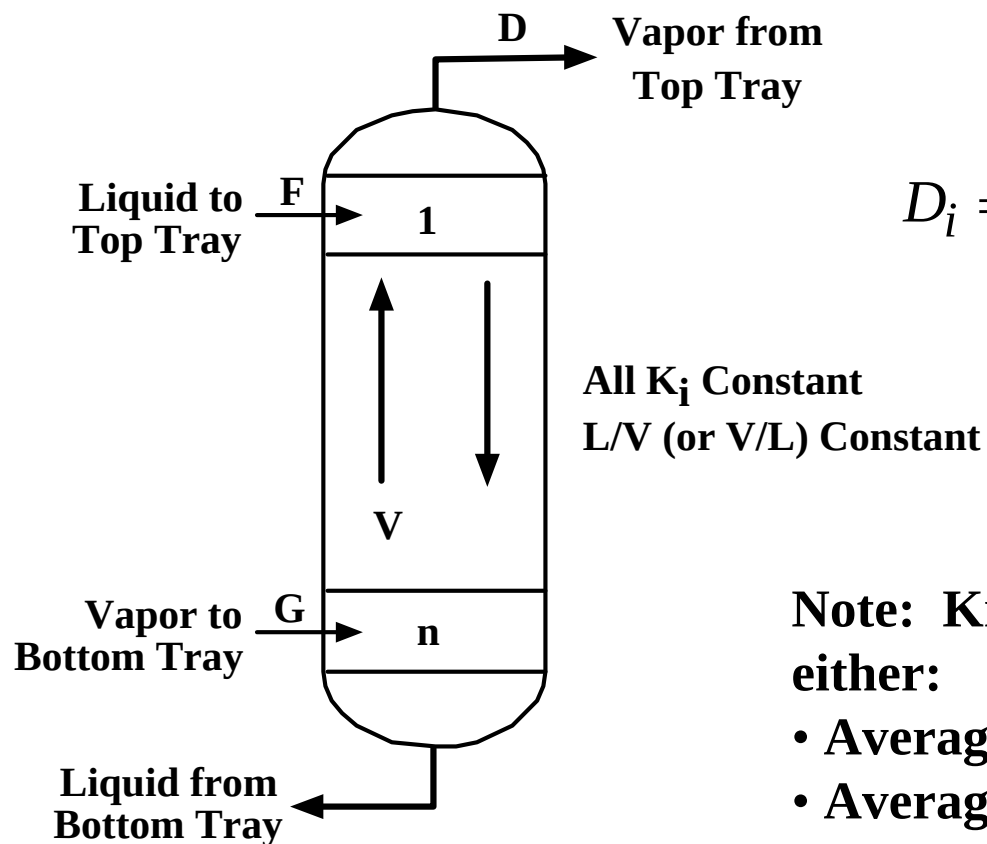
Kremser

Example – Simple Absorber



Kremser

General Case Absorber or Stripper



$$D_i = F_i [f(S_i)] + G_i [1 - f(A_i)]$$

Note: Kremser L/V may be based on either:

- Average L divided by average V
- Average of top V/L and bottom V/L

Aspen Problem No. 1

Shortcut Distillation

- **Open ReformateSplitter0.bkp**
- **Add a DSTWU column**
- **Connect feed (stream 1) and add distillate vapor, distillate liquid and bottoms streams**
- **Open column**
 - **40 Stages**
 - **15.7 psi Condenser pressure**
 - **30.7 psi Reboiler pressure**

Aspen Problem No. 1

Shortcut Distillation

- **Light key Toluene**
 - **0.99 Recovered in distillate**
- **Heavy key EB**
 - **0.015 Recovered in distillate**
- **Calculation options**
 - **Generate table of reflux/stages**
 - **20 to 60 stages**
- **Start calculations**

Aspen Problem No. 1

Results

Minimum reflux ratio:	1.231	
Actual reflux ratio:	1.368	
Minimum number of stages:	15.3	
Number of actual stages:	40	
Feed stage:	19.0	
Number of actual stages above feed:	18.0	
Reboiler heating required:	46.78	MMBtu/hr
Condenser cooling required:	40.98	MMBtu/hr
Distillate temperature:	188	F
Bottom temperature:	337	F
Distillate to feed fraction:	0.578	

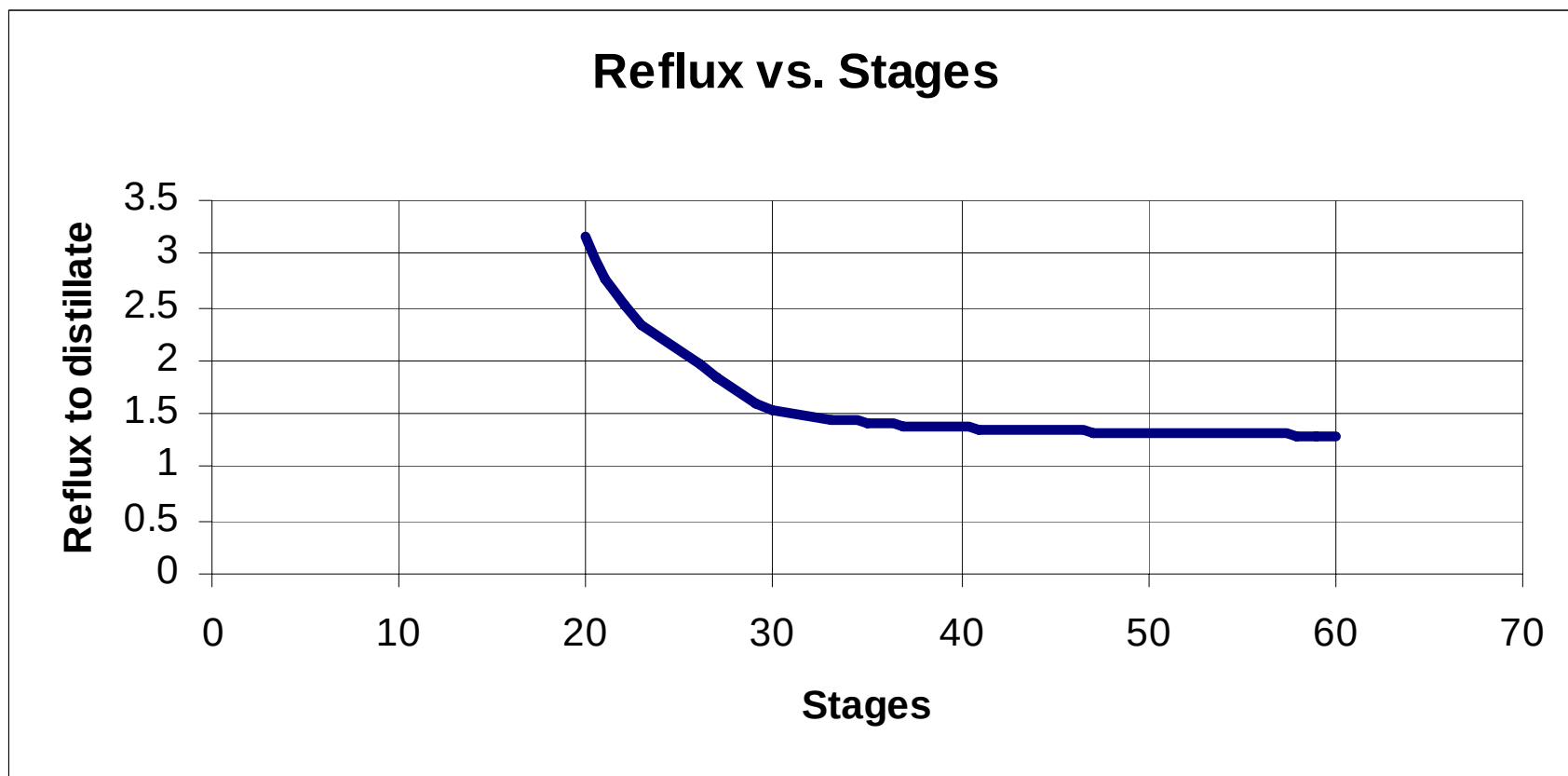
Aspen Problem No. 1

Results

Reflux/Feed	0.711
Reflux/Min Reflux	1.111
Stages/Min Stages	2.611

Aspen Problem No. 1

Results



Estimating Component Distribution

Why Valuable?

- **To Estimate Column Material Balance**
- **To Start a Tray-to-Tray Calculation**

Estimating Component Distribution

Approximate Method

- Components lighter than light key $\longrightarrow$ all to overhead
- Components heavier than heavy key $\longrightarrow$ all to bottoms
- Only valid if not key components and α 's are considerably different than α of keys
- No distributed components

Estimating Component Distribution

Fenske Equation Method

$$n = \frac{\log\left(\frac{r_D}{r_B}\right)_K}{\log(\alpha_K)}$$

Component Distribution

1	2	3	4	5	6	7	8
<u>Component</u>	<u>Alpha</u>	<u>Log(Alpha)</u>	<u>Log (r_D/r_B)</u>	<u>r_D/r_B</u>	<u>F_i</u>	<u>D_i</u>	<u>B_i</u>
A	1.65	0.217	5.7002	501361	196.1	195.8	0.3
B -LK	1.49	0.173	4.5391	34604	122.6	119.6	3.0
C	1.445	0.160	4.1901	15490	95.8	90.7	5.1
D	1.188	0.075	1.9609	91	68.4	6.5	61.9
E	1.14	0.057	1.4914	31	86.8	3.0	83.8
F -HK	1	0.000	0.0000	1	86.9	0.1	86.8

$$r_D/r_B = (119.6/0.1)/(3.0/86.8) = 34604$$

$$n = \text{Log} (r_D/r_B)/\text{Log} (\alpha) = 4.539/.173 = 26.21$$

$$\text{Log}(r_D/r_B) = n * \text{Log} (\alpha)$$

$$D_i = (r_{Di}/r_{Bi}) F_i D_H / (B_H + (r_{Di}/r_{Bi}) D_H)$$

$$B_i = F_i - D_i$$

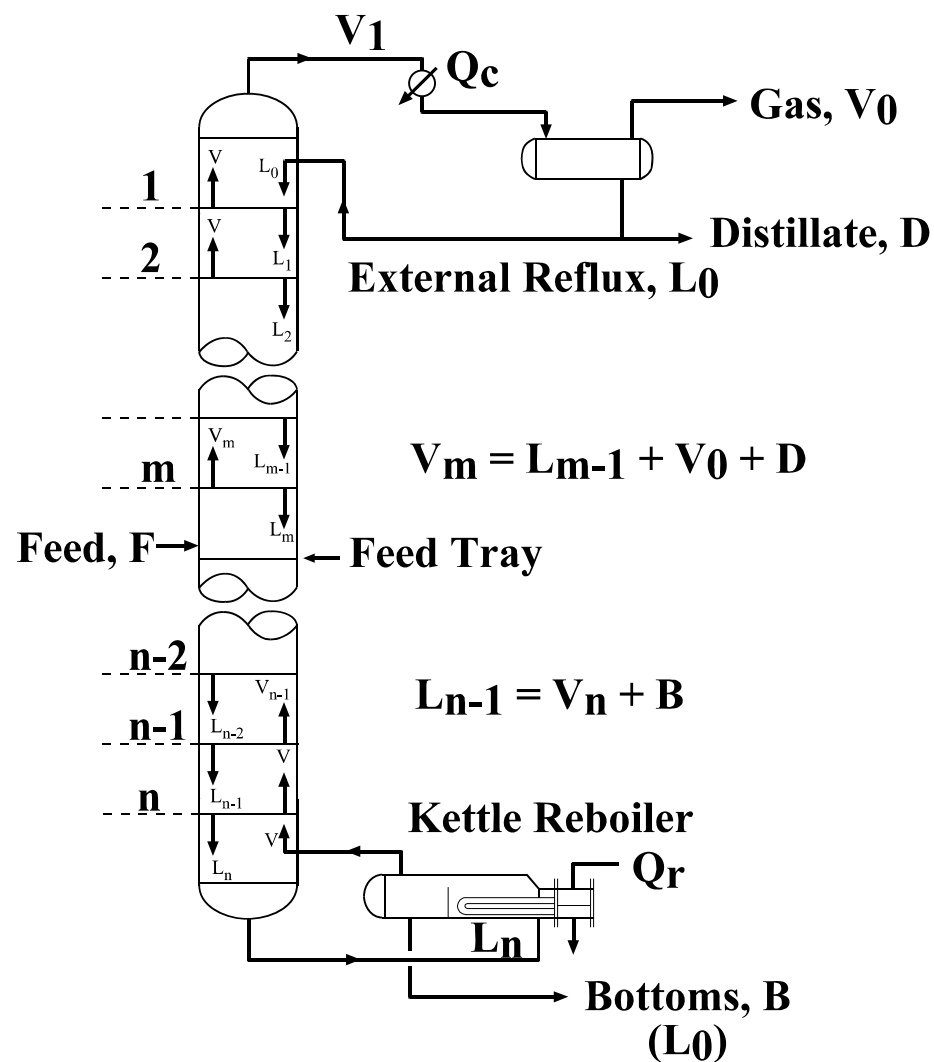
Distillation

Rigorous Computer Methods

Multicomponent Distillation

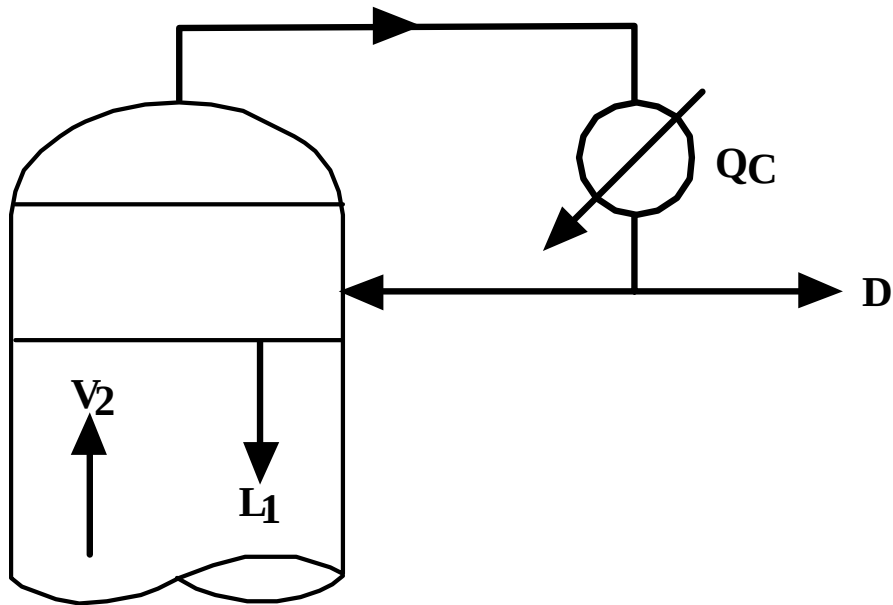
- **Tray to Tray Calculation Fundamental Relations**
 - Heat balance
 - Material balance
 - Equilibrium
- **Methods Descriptions**
 - Simultaneous equations
 - Top down/bottom up
 - Trays are always specified, not calculated
- **Example Problems**

Distillation Column Nomenclature



Procedure with Heat Balance

Liquid Composition Known:



Estimate a liquid rate.

Find vapor rate by material balance.

$$V_2 = L_1 + D + V_0 \text{ (if any)}$$

Calculate dew point on vapor and find vapor enthalpy.

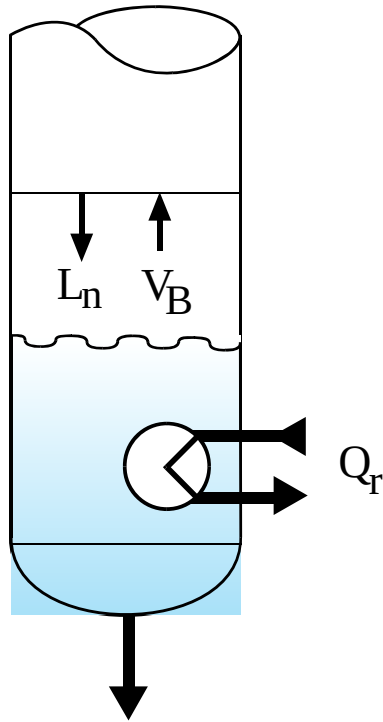
Check heat balance.

$$L_1 H_{L_1} + D H_D + Q_C = V_2 H_{V_2}$$

Repeat above steps until a satisfactory heat balance is obtained. Note vapor dew point calculation gives liquid composition to next tray down.

Procedure with Heat Balance

Vapor Composition Known:



MCF-R00-23

Estimate a vapor rate. Find liquid rate by material balance.

$$L_n = V_B + B$$

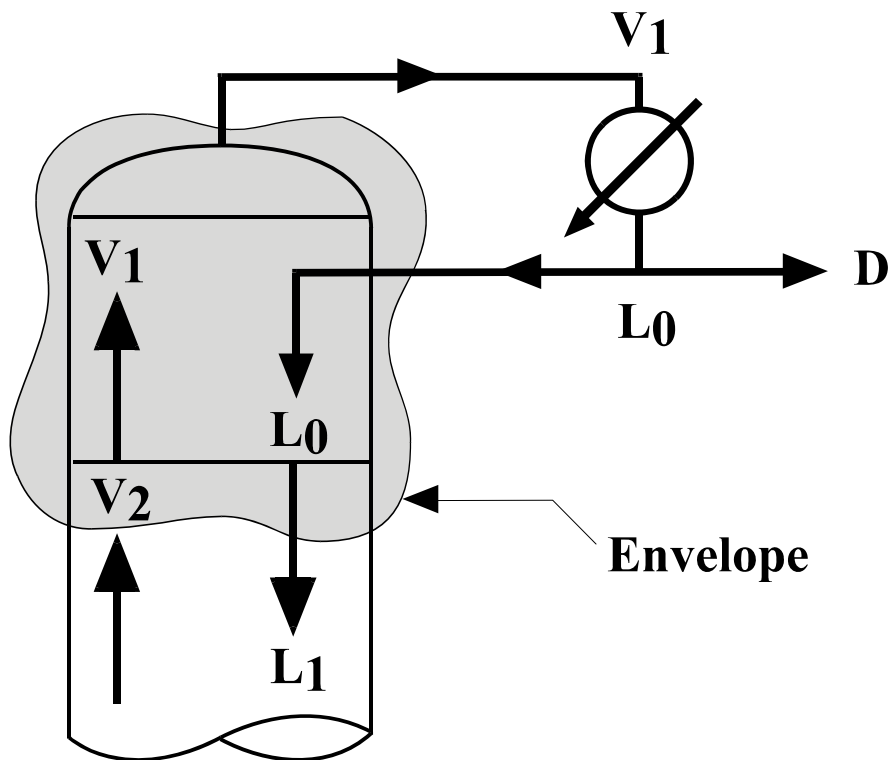
Calculate bubble point on liquid and find liquid enthalpy.

Check heat balance.

$$V_B H_{V_B} + B H_B = L_n H_{L_n} + Q_R$$

Repeat above steps until a satisfactory heat balance is obtained. Note liquid bubble point calculation gives liquid composition to next tray up.

External/Internal Reflux Relationships



Internal reflux material and heat balance:

$$L_0 + V_2 = V_1 + L_1$$

$$L_0 H_{L_0} + V_2 H_{V_2} = V_1 H_{V_1} + L_1 H_{L_1}$$

External/Internal Reflux Relationships

- **Additional Material Balances**

$$V_1 = L_0 + D$$

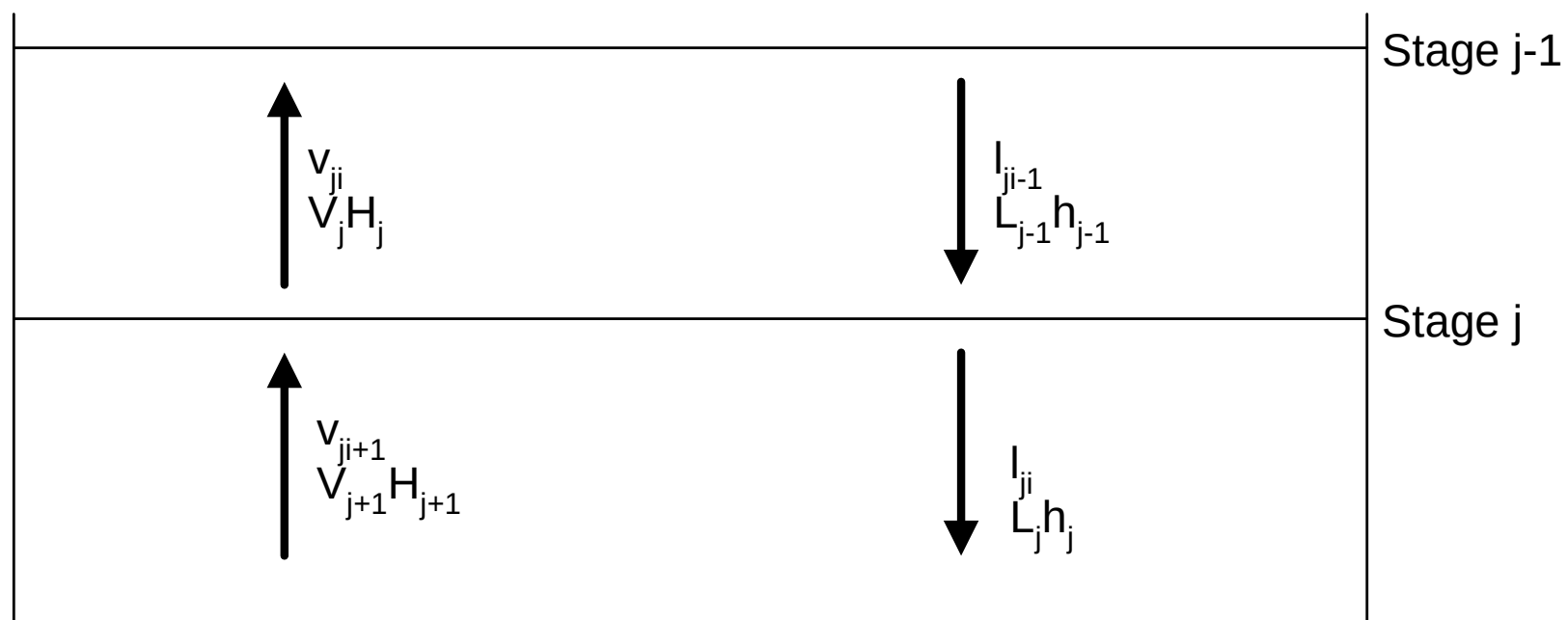
$$V_2 = L_1 + D$$

- **If $H_{V_2} = H_{V_1}$, it may be shown that**

$$L_1 = L_0 \frac{(H_{V_1} - H_{L_0})}{(H_{V_1} - H_{L_1})}$$

Note: The denominator can be considered a latent heat.

Basic Tray Model



Basic Equations (MESH)

- Material balances, component and total.

$$v_{ij+1} + l_{ij-1} - v_{ij} - l_{ij} = 0 \quad (1 \text{ per component, per stage})$$

$$V_{j+1} + L_{j-1} - V_j - L_j = 0 \quad (1 \text{ per stage})$$

- Equilibrium equations.

$$y_{ij} = K_{ij} x_{ij} \quad (1 \text{ per component, per stage})$$

- Summation or composition constraints.

$$\sum_{i=1}^C y_{ij+1} \quad \text{and} \quad \sum_{i=1}^C x_{ij-1} \quad (1 \text{ each per stage})$$

- Heat or energy balances.

$$V_{j+1}H_{j+1} + L_{j-1}h_{j-1} - V_jH_j - L_jh_j = 0 \quad (1 \text{ per stage})$$

Basic Variables

Design variables

- Stage temperatures, T_j 's.
- Total vapor and liquid rates, V_j 's and L_j 's.
- Stage compositions, y_{ji} 's and x_{ji} 's.

Basic thermodynamic parameters

- $K_{ji} = K_{ji}(T_j, P_j, x_{ji}, y_{ji})$
- $H_j = H_j(T_j, P_j, y_{ji})$
- $h_j = h_j(T_j, P_j, x_{ji})$

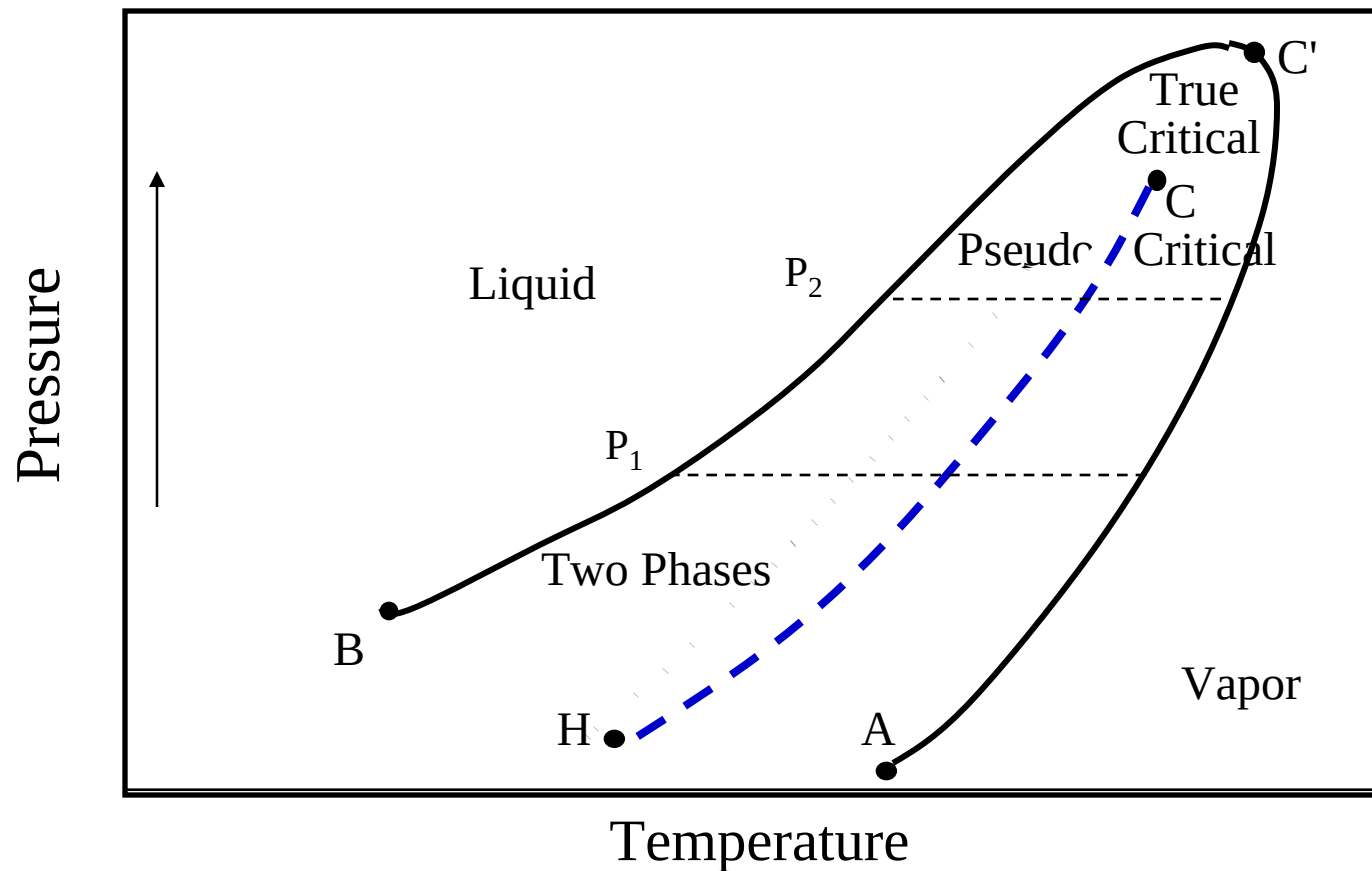
Basic Equations

- There are $(2NC + 2N + P)$ equations and variables to solve in a column, where
 - N = Number of stages
 - C = Number of components
 - P = Number of products

- This makes for a very big matrix of equations
 - $[f_{1,1}, f_{1,2}, \dots, \dots, f_{1,n}]$
 - $[f_{2,1}, f_{2,2}, \dots, \dots, f_{2,n}]$
 - $[\dots, \dots, \dots, \dots, \dots]$
 - $[f_{j,1}, f_{j,i}, \dots, \dots, f_{j,n}]$
 - $[\dots, \dots, \dots, \dots, \dots]$
 - $[f_{n,1}, f_{n,2}, \dots, \dots, f_{n,n}]$

The Phase Envelope

The Equation of State is supposed to predict the values we need to solve a column for a multi-component mixture.
Often it does not.



Inside-Out Method

K-values

- $\ln K_{bj} = A_j + B_j (1 / T_j - 1 / T^*)$
- $\alpha_{ji} = K_{ji(\text{actual})} / K_{bj\text{Ref}}$
- $\ln \gamma^*_{ij} = a_{ij} + b_{ij} x_{ij}$
- $K_{ji(\text{simple})} = K_{bj} \alpha_{ji} \gamma^*_{ij}$

Enthalpies

- $H_j = H^0_j + \Delta H_{Vj}$
- $h_j = h^0_j + \Delta H_{Lj}$
- $\Delta H_{Vj} = C_j - D_j (T_j - T^*)$
- $\Delta H_{Lj} = E_j - F_j (T_j - T^*)$

Inside Out Procedure

- Given, a feed, and operating pressure
- Set initial values for the stage temperatures and total flow rates
- Initialize the outside loop variables K_{bj} , α_{ji} , A_j , B_j , C_j , D_j , E_j , F_j from the actual K-value and enthalpy methods such as from an equation of state
- In the inside loop, use these simplified methods K-value and enthalpy to calculate tray compositions and update temperatures and flow rates from the MESH equations above
- In turn, update the outside variables from those update in the inside loop
- Continue until little changes (converged)

Aspen Problem No. 2

RadFrac Distillation

- **Open ReformatSplitter0.bkp**
- **Add a RadFrac column**
- **Connect feed (stream 1) and add distillate and bottoms streams**
- **Open column**
 - **40 Stages**
 - **Total condensing**
 - **1264 lb-mol/h distillate**
 - **1500 lb-mol/h reflux**
 - **Feed above tray 21**

Aspen Problem No. 2

RadFrac Distillation

- 15.7 psia condenser pressure
- 8 psi condenser pressure drop
- 0.15 stage pressure drop
- Start calculation
- Review the results in:
 - Results summary folder
 - Profile folder
 - Stream results folder

Aspen Problem No. 2

Results Summary – Split Fraction

BZ	1.0000	0.0000
NC7	1.0000	0.0000
MCH	0.9997	0.0003
TOL	0.9928	0.0072
NC8	0.8199	0.1801
ECH	0.2320	0.7680
EB	0.6308	0.3692
PX	0.5810	0.4190
MX	0.5313	0.4687
OX	0.4815	0.5185

Aspen Problem No. 2

Profile – Liquid Composition

Stage	NC4	NC5	NC6	MCP	BZ
1	0.030841	0.318960	0.182529	0.002289	0.105690
2	0.003165	0.079114	0.110759	0.001582	0.082278
3	0.001528	0.042748	0.073445	0.001105	0.060195
4	0.001440	0.038462	0.063160	0.000950	0.051832
5	0.001440	0.038038	0.060647	0.000905	0.049109
6	0.001444	0.038055	0.060009	0.000892	0.048209

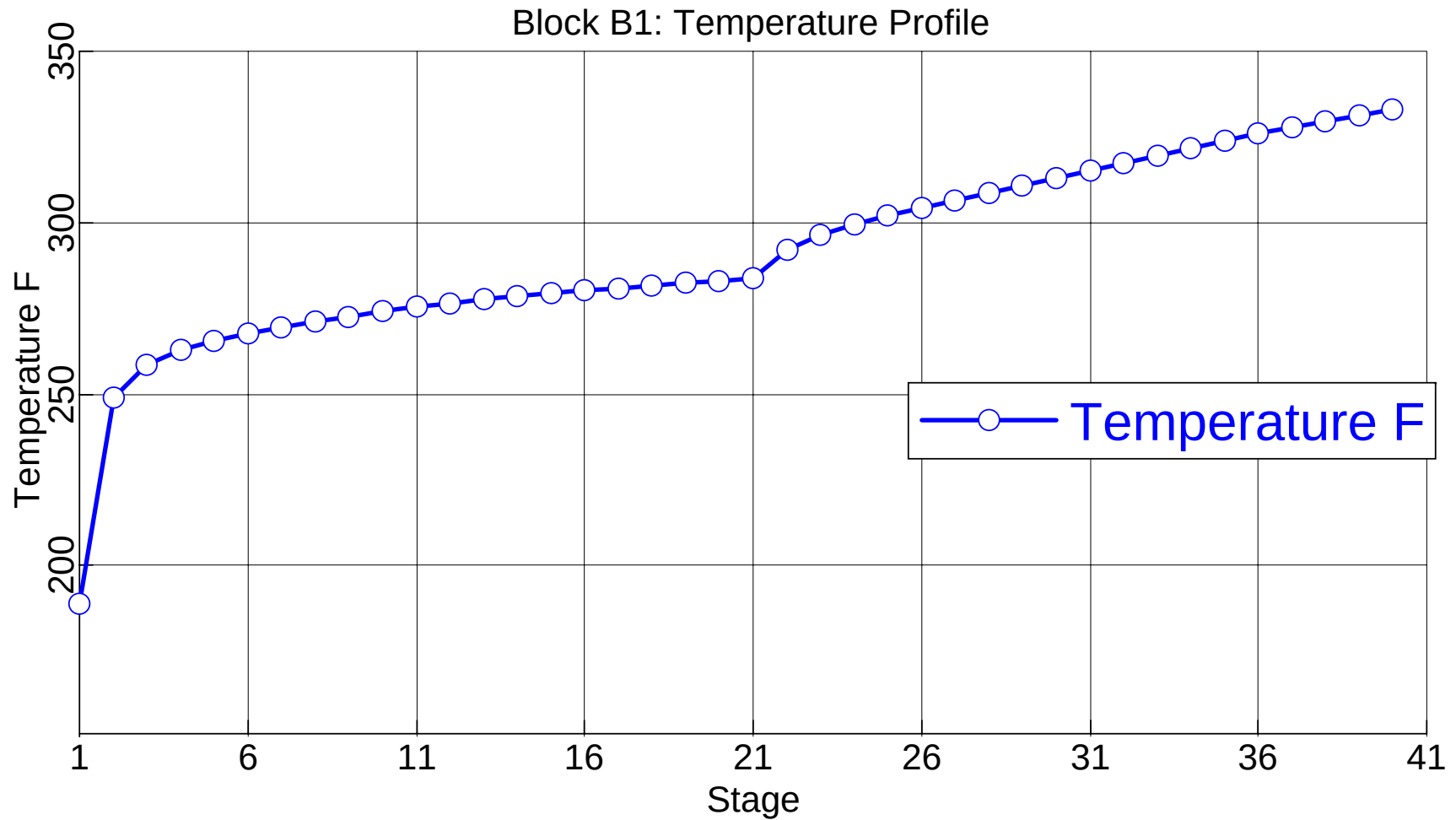
Aspen Problem No. 2

Profile – Equil. K Values

Stage	NC4	NC5	NC6	MCP	BZ	NC7
1	9.74643151	4.03195	1.64804	1.446388	1.284489	0.715115
2	11.1493236	5.23342	2.456419	2.131372	1.894904	1.208961
3	11.9326988	5.68353	2.72748	2.360773	2.100105	1.364629
4	12.2243702	5.85812	2.838803	2.455306	2.18711	1.429443
5	12.3978635	5.96635	2.908672	2.513371	2.239762	1.470676
6	12.5391268	6.05564	2.965656	2.558504	2.27848	1.504652
7	12.6681043	6.13707	3.01702	2.597033	2.309313	1.535464

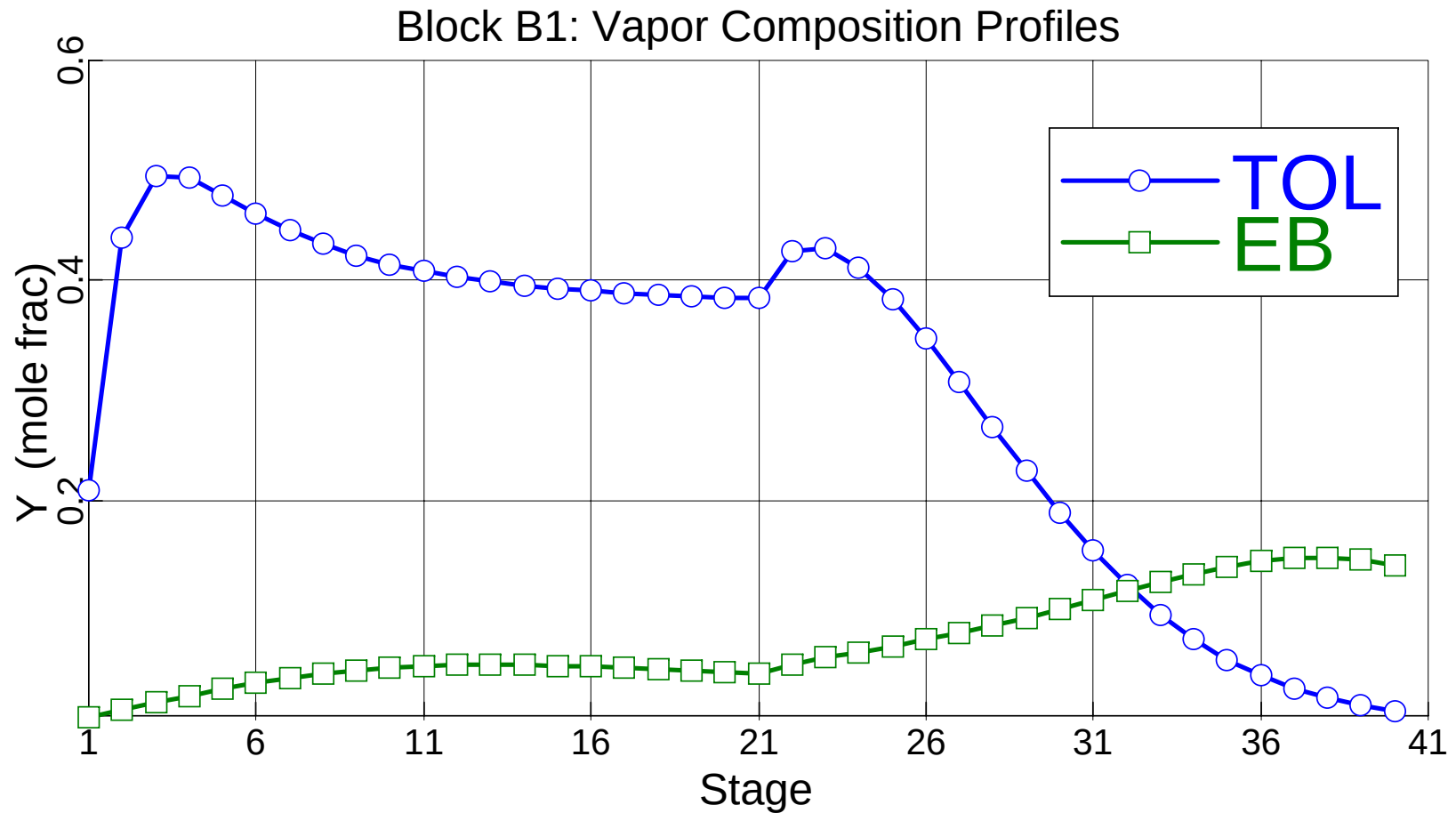
Aspen Problem No. 2

Profile – Plots



Aspen Problem No. 2

Profile – Plots



Aspen Problem No. 2

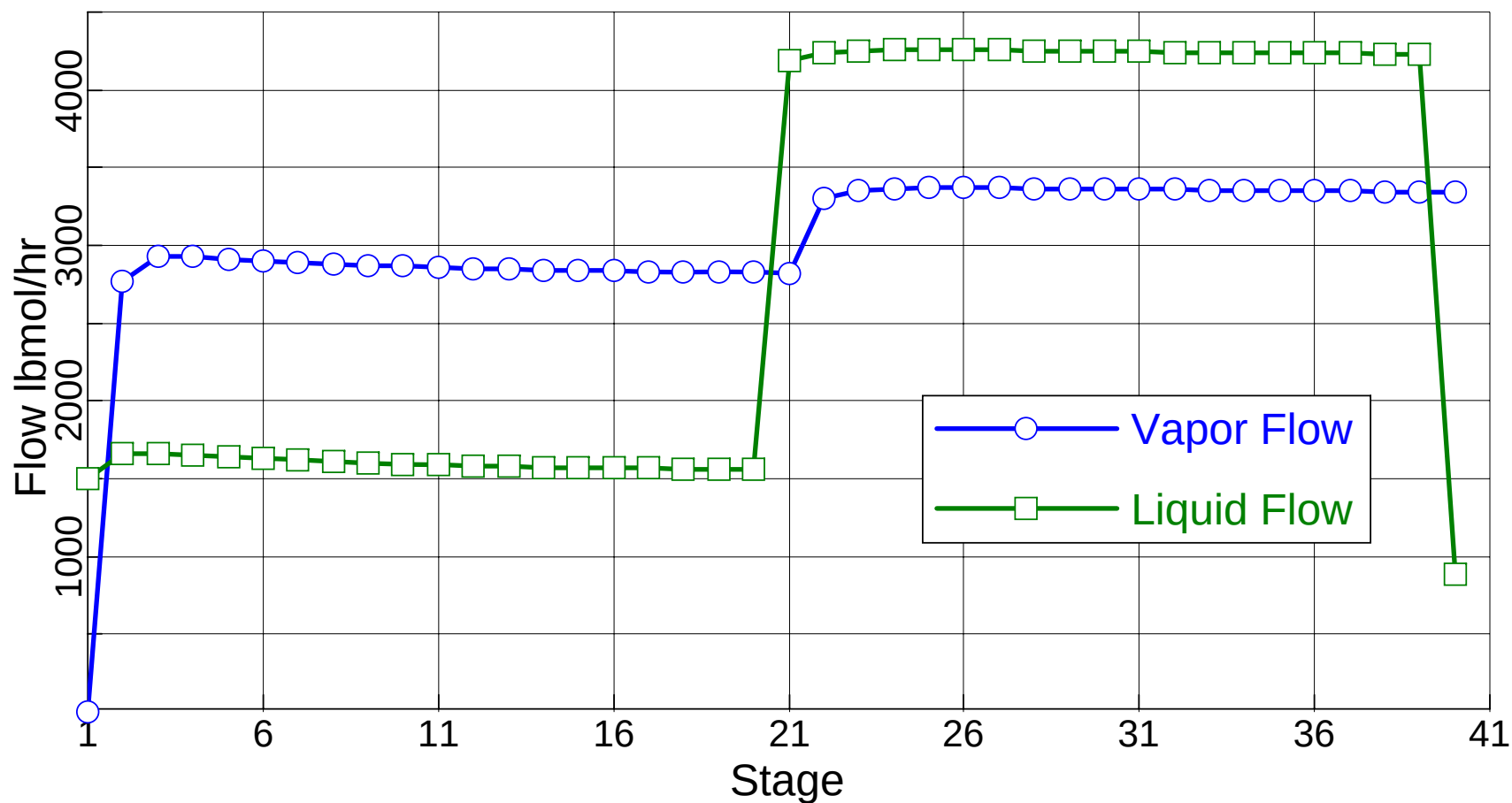
Profile – TPFQ

Stage	Temp	Pres	Heat duty	Liquid flow	Vapor flow
	F	psi	MMBtu/hr	lbmol/hr	lbmol/hr
1	189	15.7	-44.35	1500.00	0.00
2	249	23.7	0	1663.63	2764.00
3	259	23.9	0	1660.75	2927.63
4	263	24.0	0	1649.75	2924.75
5	265	24.2	0	1638.30	2913.75
6	268	24.3	0	1627.70	2902.30

Aspen Problem No. 2

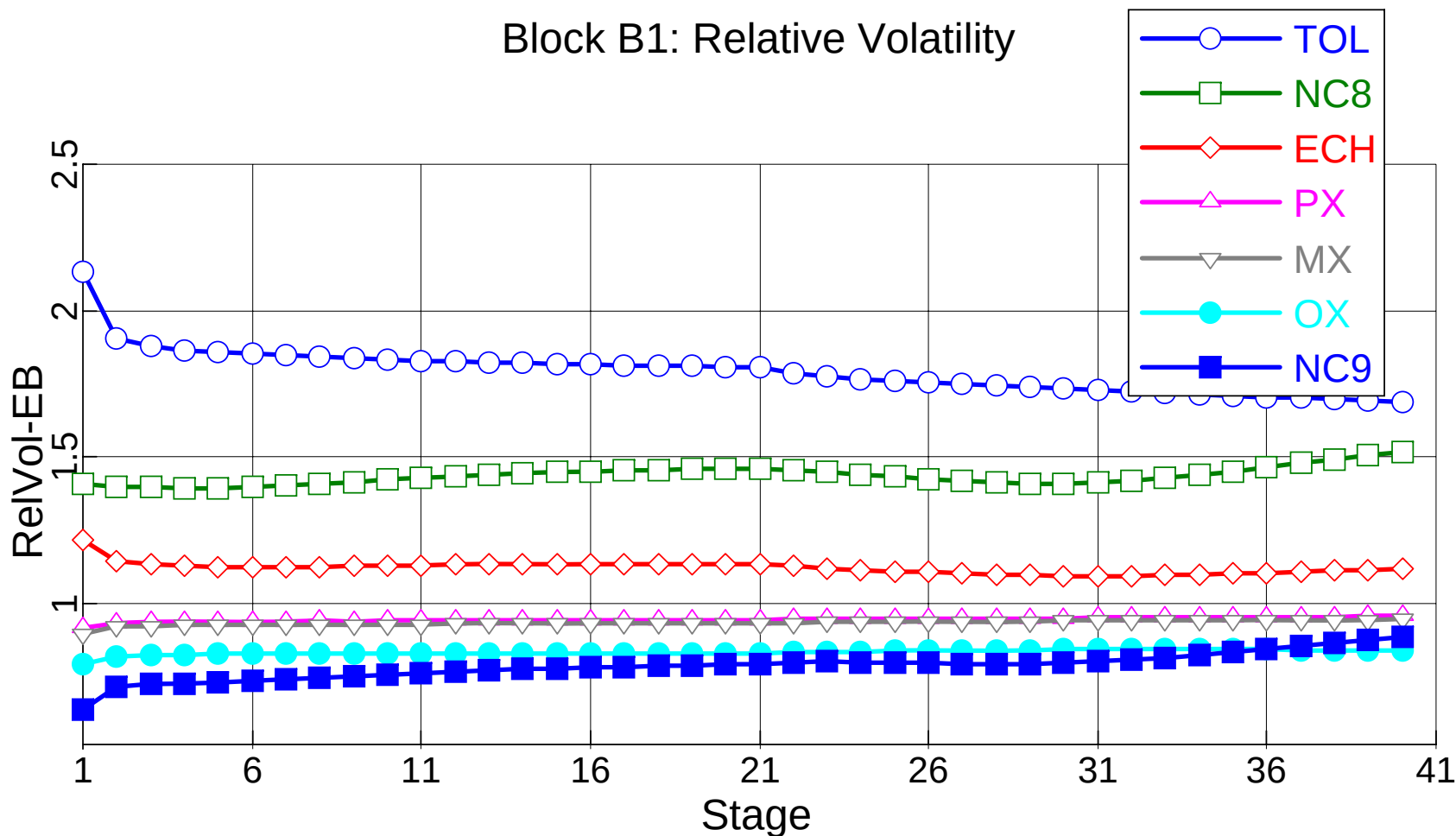
Profile – Plots

Block B1: Molar Flow Rate



Aspen Problem No. 2

Profile – Plots



Aspen Problem No. 2

Stream Results

	1	2	3
Vapor Frac	0.0000	0.0000	0.0000
Temperature F	200	189	333
Pressure psig	285.3	1	14.7
Pressure mmHg	15514	812	1520
*** ALL PHASES ***			
Mass Flw lb/hr	211467	116846	94621
Mole Flw lbmol/hr	2151	1264	887
Enthalpy MMBtu/hr	-48.281	-41.227	-1.527
Enthalpy Btu/lb	-228.315	-352.829	-16.143
MW	98.31	92.44	106.68

Aspen Problem No. 2

Stream Results

Components	Feed Mole Frac	Overhead Mole Frac	Bottoms Mole Frac
MCH	0.001395	0.00237	0.000001
TOL	0.259879	0.43907	0.00453
NC8	0.069735	0.0973	0.03045
ECH	0.004649	0.00184	0.008659
EB	0.059972	0.0092	0.132323
PX	0.061367	0.00464	0.1422
MX	0.142724	0.00904	0.333235
OX	0.13947	0.00141	0.336217

Aspen Problem No. 2

- **Add design specs**
 - 1.0 mol % Toluene recovered to bottoms
 - 1.5 mol % EB recovered to overhead
- **Add varies**
 - **Distillate rate**
 - 0 lb-mol/h lower bound
 - 2000 lb-mol/h upper bound
 - **Reflux rate**
 - 0 lb-mol/h lower bound
 - 4000 lb-mol/h upper bound
- **Start calculations**
- **Review results**

Multicomponent Distillation

Example Problem: A Deethanizer

- **Receiver Conditions**
 - **0°F**
 - **300 psig**

- **No Net Overhead Liquid**

Multicomponent Distillation

Example Problem: A Deethanizer

- **Key Components are C₂ and C₃**
 - **1.0 mol/hr C₂ in bottoms**
 - **Only enough C₃ in overhead to make reflux**
 - **Methane and lighter in overhead**
 - **Butane and heavier in bottoms**

Multicomponent Distillation

Example Problem: A Deethanizer

- **External Reflux Is 275.3 Mols/Hr**
- **Constant Molal Internal Reflux**
- **No Liquid Phase Non-Ideality**
- **H₂ Doesn't Affect Vapor Phase Fugicity**
- **Constant Pressure on All Trays**

Example Problem: A Deethanizer

Deethanizer Mole Balance					
	Total Feed Mol/H	Vapor Feed Mol/H	Liquid Feed Mol/H	Net Ovhd. (As Gas) Mol/H	Bottoms Mol/H
H₂	14.2	13.1	1.1	14.2	-
C₁	12.4	7.4	5.0	12.4	-
C₂	31.1	7.0	24.1	30.1	1.0
C₃	117.5	13.1	104.4	4.1	113.4
iC₄	44.9	2.0	42.9	-	44.9
nC₄	69.5	1.9	67.6	-	69.5
iC₅	50.9	0.4	50.5	-	50.9
nC₅	32.4	0.2	32.2	-	32.4
iC₆	9.8	0.1	9.7	-	9.8
Total	382.7	45.2	337.5	60.8	321.9

Example Problem: A Deethanizer

Tray-to-Tray Calculation (continued)

- Calculate the amount of C_3 in the overhead vapor product

	V_{y1} Vapor Mol/H	K @ 315 psia 0°F	V_{y1}/K	Vapor Mol/H	Composition External Reflux V/K
H_2	14.2	74.5	0.2	14.2	0.2
C_1	12.4	4.0	3.1	12.4	3.1
C_2	30.1	0.79	38.1	30.1	38.1
C_3	<u>Z</u>	<u>0.21</u>	<u>Z / 0.21</u>	<u>4.1</u>	<u>19.4</u>
	56.7 + Z		41.4 + Z/0.21	60.8	60.8

$$56.7 + Z = 41.4 + Z/0.21$$

$$Z = 4.1$$

Example Problem: A Deethanizer

Example Problem - Tray-to-Tray Calculation

(continued)

- Calculation of top tray temperature and composition of internal reflux leaving first tray. Try 60°F.

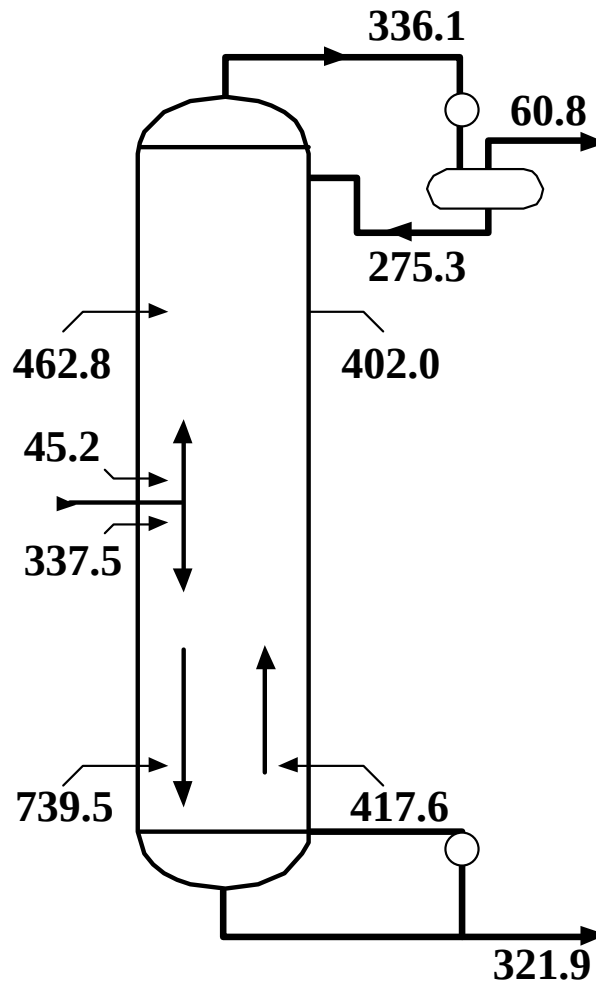
	Net Ovhd Gas V_0	Reflux L_0	$V_1 =$ $V_0 + L_0$	K 315 psia, 60°F	V_1/K
H ₂	14.2	0.9	15.1	63.9	0.2
C ₁	12.4	14.0	26.4	5.50	4.8
C ₂	30.1	172.6	202.7	1.317	153.9
C ₃	<u>4.1</u>	<u>87.8</u>	<u>91.9</u>	0.486	<u>189.1</u>
	60.8	275.3	336.1		348

close enough

INTERNAL REFLUX

Assume $H_{V2} = H_{V1}$; with V_1 and R compositions known along with their temperatures, the molal enthalpies can be determined. Thus internal reflux can be computed.

Internal Reflux



$$L_1 = 275.3 \times \frac{8500 - 3300}{8500 - 4950} = 402.0$$

Example of Tray-to-Tray Calculation

- Deethanizer, constant internal reflux
- Top section, $L = 402.0$, $V = 462.8$

	Net Overhead Gas V_0	External Reflux L_0	$V_0 + L_0$ $= V_1$	K 315 psia 60°F	V_1/K	L_1	$V_0 + L_1$ $= V_2$	K 315 psia 90°F	V_2/K
H ₂	14.2	0.9	15.1	63.9	0.2	0.2	14.4	59.2	0.2
C ₁	12.4	14.1	26.5	5.5	4.8	5.5	17.9	6.75	2.6
C ₂	30.1	172.5	202.6	1.32	153.9	177.8	207.9	1.52	137.0
C ₃	4.1	87.8	91.9	0.486	189.1	218.5	222.6	0.65	342.5
	60.8	275.3	336.1		348.0	402.0	462.8		482.3

C₂/C₃

7.34

1.96

$L1 = (402/348.0)(V1/K)$
0.815

Close
enough

Example of Tray-to-Tray Calculation

- Deethanizer, constant internal reflux
- Top section, $L = 402.0$, $V = 462.8$

	L_2	$V_0 + L_2 = V_3$	K 315 psia 105°F	V_3/K	L_3	$V_0 + L_3 = V_4$	K 315 psia 115°F	V_4/K	L_4
H ₂	0.2	14.4	57.0	0.3	0.3	14.5	55.5	0.3	0.3
C ₁	2.2	14.6	7.25	2.0	1.7	14.1	7.61	1.9	1.6
C ₂	114.1	144.2	1.77	81.5	69.3	99.4	1.85	53.7	46.0
C ₃	285.5	289.6	0.745	388.7	330.7	334.8	0.81	413.3	354.1
	402.0	462.8		472.5	402.0	462.8		469.2	402.0

C₂/C₃ 0.400

0.210

0.130

Example of Tray-to-Tray Calculation

- Deethanizer, constant internal reflux
- Top section, $L = 402.0$, $V = 462.8$

Comparisons to this point.

	Feed	Feed Vapor	Feed Liquid	L_0	L_1	L_2	L_3	L_4
C_2/C_3	0.264	0.534	0.231	1.96	0.815	0.400	0.210	0.130
Temp °F				0	60	90	105	115

Example of Tray-to-Tray Calculation

■ Deethanizer – Bottom Section

$$L_n = L_F + \text{Internal Reflux} = 337.5 + 402.0 \text{ mol/h} = 739.5 \text{ mol/h}$$

$$V_B = L_n - L_B = 739.5 - 321.9 = 417.6 \text{ mol/h}$$

	Bottoms B	K 315 psia 230°	KL_B	V_B	$L_n =$ $V_B + L_B$	K 315 psia 200°F	KL_n	V_n
C ₂	1.0	3.56	3.6	4.3	5.3	3.04	15.9	9.1
C ₃	113.4	1.64	186.0	224.3	337.7	1.35	455.9	262.4
iC ₄	44.9	1.03	46.2	55.7	100.6	0.870	87.5	50.3
nC ₄	69.5	0.895	62.2	75.0	144.5	0.732	105.8	60.8
iC ₅	50.9	0.570	29.0	35.0	85.9	0.444	38.1	21.9
nC ₅	32.4	0.500	16.2	19.5	51.9	0.380	19.7	11.3
iC ₆	9.8	0.332	3.2	3.8	13.6	0.236	3.2	1.8
	321.9		346.4	417.6	739.5		726.1	417.6

C₂/C₃ 0.0088

0.0157

Example of Tray-to-Tray Calculation

■ Deethanizer - Bottom Section

	$L_{n-1} =$ $V_n + L_B$	K 315 psia 190°F			$L_{n-2} =$ $V_{n-1} + L_B$	K(*) 315 psia 190°F		
			KL_{n-1}	V_{n-1}			KL_{n-2}	V_{n-2}
C_2	10.1	2.88	29.1	16.7	17.7	2.88	51.0	28.2
C_3	375.8	1.29	484.8	278.2	391.6	1.29	505.2	279.1
iC_4	95.2	0.819	78.0	44.8	89.7	0.819	73.5	40.6
nC_4	130.3	0.682	88.9	51.0	120.5	0.682	82.2	45.4
iC_5	72.8	0.405	29.5	16.9	67.8	0.405	27.5	15.2
nC_5	43.7	0.344	15.0	8.6	41.0	0.344	14.1	7.8
iC_6	11.6	0.210	2.4	1.4	11.2	0.210	2.4	1.3
	739.5		727.7	417.6	739.5		755.9	417.6

C_2/C_3 0.0269

0.0452

(*) Note that, when T changes but little per tray, using the same K as for previous tray gives a satisfactory result

Example of Tray-to-Tray Calculation

■ Deethanizer - Bottom Section

	$L_{n-3} =$ $V_{n-2} + L_B$	K 315 psia 180°F			$L_{n-4} =$ $V_{n-3} + L_B$	K(*) 315 psia 170°F		
			KL_{n-3}	V_{n-3}			KL_{n-4}	V_{n-4}
C_2	29.2	2.72	79.4	44.4	45.4	2.58	117.1	67.6
C_3	392.5	1.23	482.8	270.3	383.7	1.17	448.9	259.3
iC_4	85.5	0.762	65.2	36.5	81.4	0.71	57.8	33.4
nC_4	114.9	0.631	72.5	40.6	110.1	0.58	63.8	36.8
iC_5	86.1	0.367	31.6	17.7	68.6	0.332	22.8	13.2
nC_5	40.2	0.309	12.4	6.9	39.3	0.277	10.9	6.3
iC_6	11.1	0.186	2.1	1.2	11.0	0.164	1.8	1.0
	739.5		746.0	417.6	739.5		723.1	417.6
C_2/C_3	0.074				0.118			

Example of Tray-to-Tray Calculation

■ Deethanizer - Bottom Section

	$L_{n-5} = V_{n-4} + L_B$	K 315 psia 170°	KL_{n-5}	V_{n-5}	$L_{n-6} = V_{n-5} + L_B$
C ₂	68.6	2.58	177.0	96.7	97.7
C ₃	372.7	1.17	436.1	238.4	351.8
iC ₄	78.3	0.71	55.6	30.4	75.3
nC ₄	106.3	0.58	61.6	33.7	103.2
iC ₅	64.1	0.332	21.3	11.6	62.5
nC ₅	38.7	0.277	10.7	5.8	38.2
iC ₆	10.8	0.164	1.8	1.0	10.8
	739.5		764.1	417.6	739.5

C₂/C₃ 0.184

0.277

(end of calculation)
(C₂/C₃ in feed liquid = 0.231)

Summary

External R/F = 0.719

Internal R/F = 1.050

Number of theoretical trays in column

Top 3

Bottom 7

Note: Reboiler and condenser are each a theoretical stage.

Aspen Problem No. 3

DeEthanizer

- **Open DeEthanizer0.bkp**
- **Add a RadFrac column**
- **Connect feed (stream 1) and add distillate vapor and bottoms streams**
- **Open column**
 - **20 Stages**
 - **Partial vapor condenser**
 - **61 lb-mol/h distillate**
 - **300 lb-mol/h reflux**
 - **Feed above tray 10**

Aspen Problem No. 3

DeEthanizer

- 314.7 psia condenser pressure
- 8 psi condenser pressure drop
- 0.15 stage pressure drop
- Start calculation
- Review the results in:
 - Results summary folder
 - Profile folder
 - Stream results folder

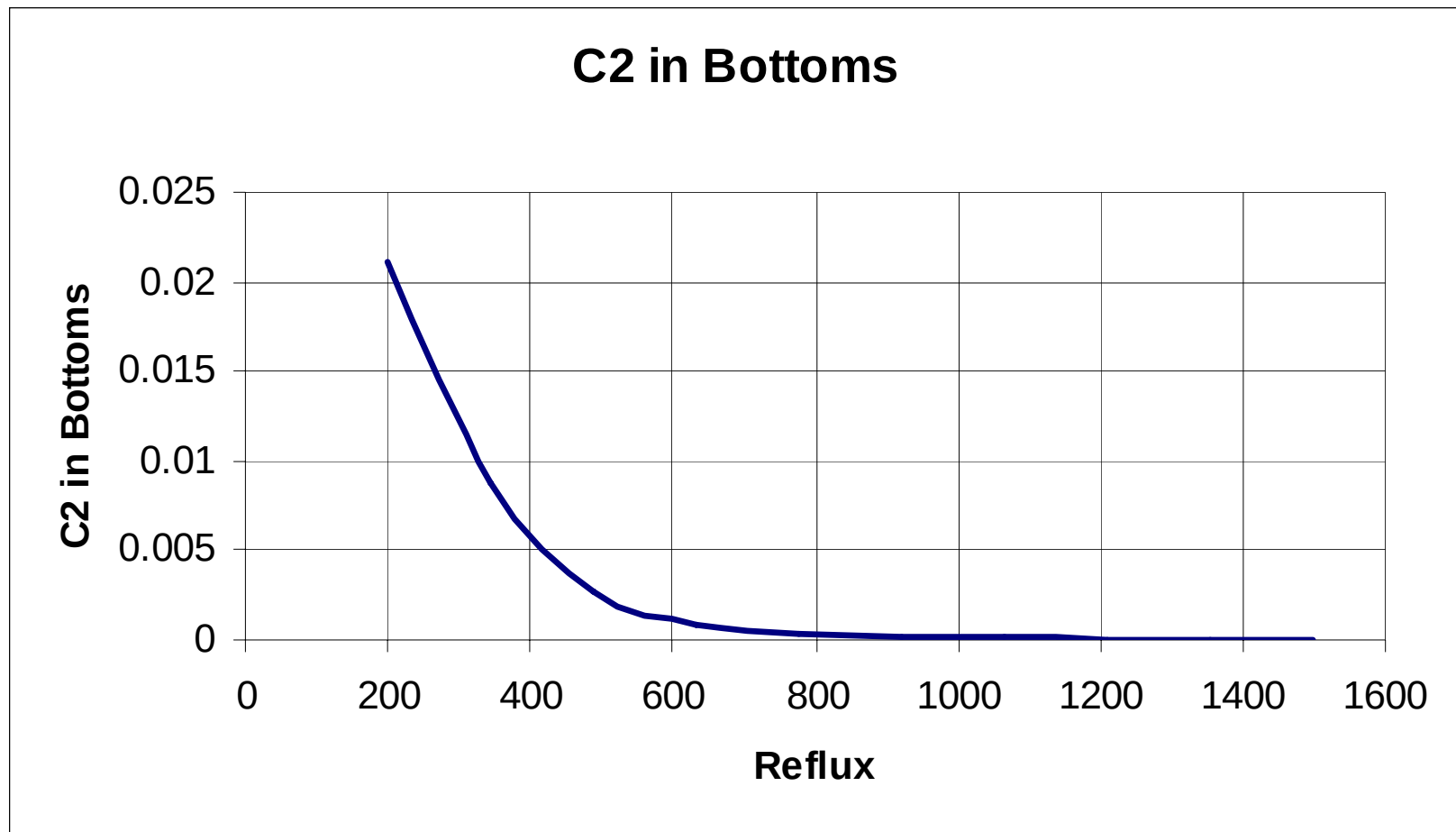
Aspen Problem No. 3

DeEthanizer

- **Add design spec**
 - 0 F, stage 1
- **Add varies**
 - **Distillate rate**
 - 0 lb-mol/h lower bound
 - 500 lb-mol/h upper bound
- **Start calculations**
- **Review concentrations of C2 in bottoms and C3 in distillate**
- **Vary reflux from 200 to 1500 lb-mol/h and tabulate/graph the concentrations of C2 in bottoms and C3 in distillate**

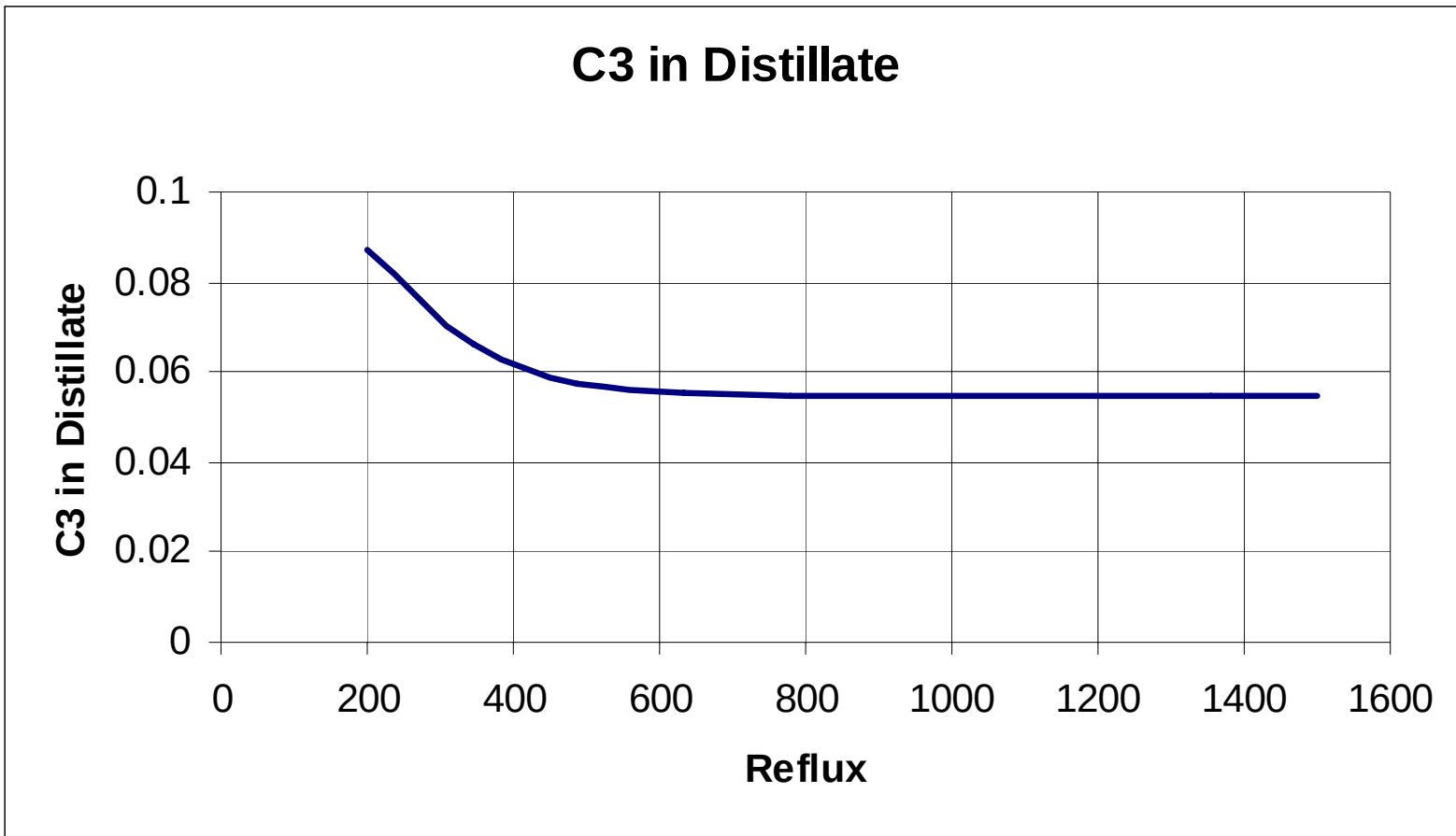
Aspen Problem No. 3

DeEthanizer



Aspen Problem No. 3

DeEthanizer



Aspen Problem No. 3

DeEthanizer

- **Add design spec**
 - 1 lb-mol/h C2 in bottoms
- **Add varies**
 - **Reflux rate**
 - 0 lb-mol/h lower bound
 - 1000 lb-mol/h upper bound
- **Start calculations**
- **Reflux rate should be 575 lb-mol/h**
- **Reflux to feed is 1.5**

Aspen Problem No. 4

DeEthanizer

- **Replace RadFrac with DSTWU**
- **20 Stages**
- **C2 recovery to distillate 0.968**
- **C3 recovery to distillate 0.035**
- **314.7 psi condenser**
- **325.7 psi reboiler**
- **Partial condenser with all vapor distillate**
- **Start calculations**
- **Review results**

Aspen Problem No. 4

DeEthanizer

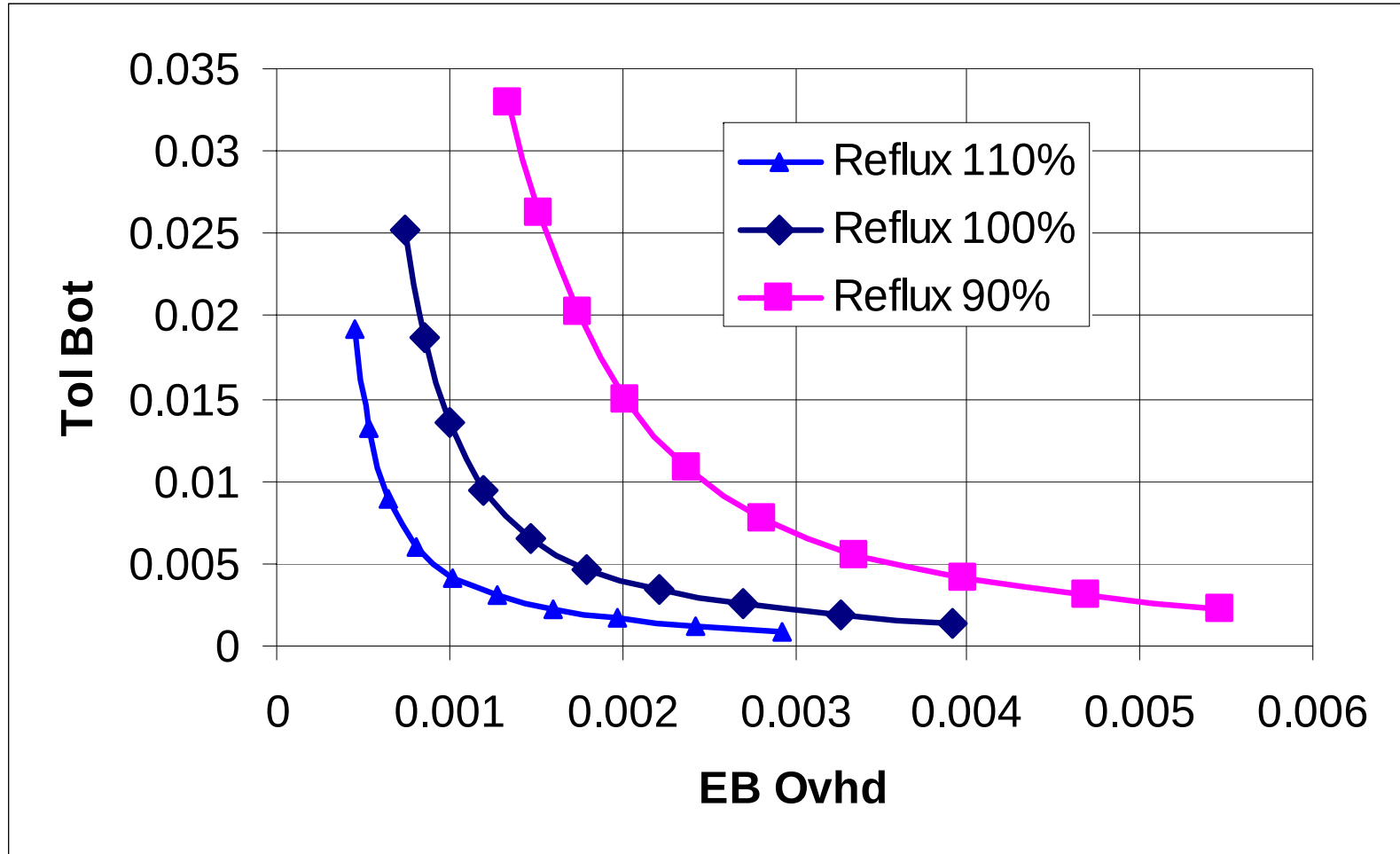
Minimum reflux ratio:	7.781	
Actual reflux ratio:	8.465	
Minimum number of stages:	8.3	
Number of actual stages:	20	
Feed stage:	10.3	
Number of actual stages above feed:	9.3	
Reboiler heating required:	2.30	MMBtu/hr
Condenser cooling required:	1.91	MMBtu/hr
Distillate temperature:	4	F
Bottom temperature:	222	F
Distillate to feed fraction:	0.077	

Aspen Problem No. 4

DeEthanizer

Reflux/Feed	0.601
Reflux/Min Reflux	1.088
Stages/Min Stages	2.409

Operating Chart



Operating Chart

- **Increasing the distillate rate increases the heavies in the distillate**
- **Increasing the reflux rate produces much higher purities**

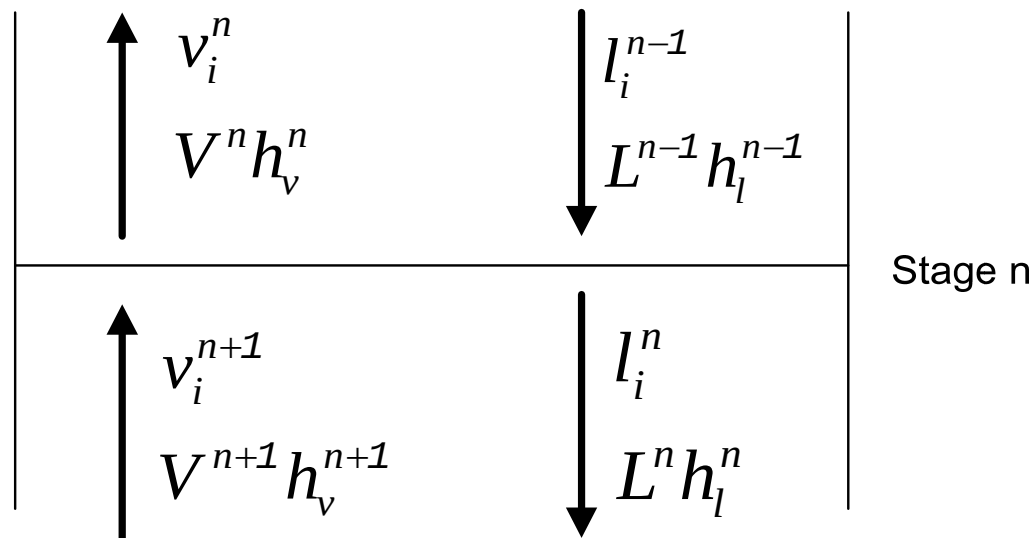
Assumes fixed feed rate and constant tray efficiency

Tray Efficiency

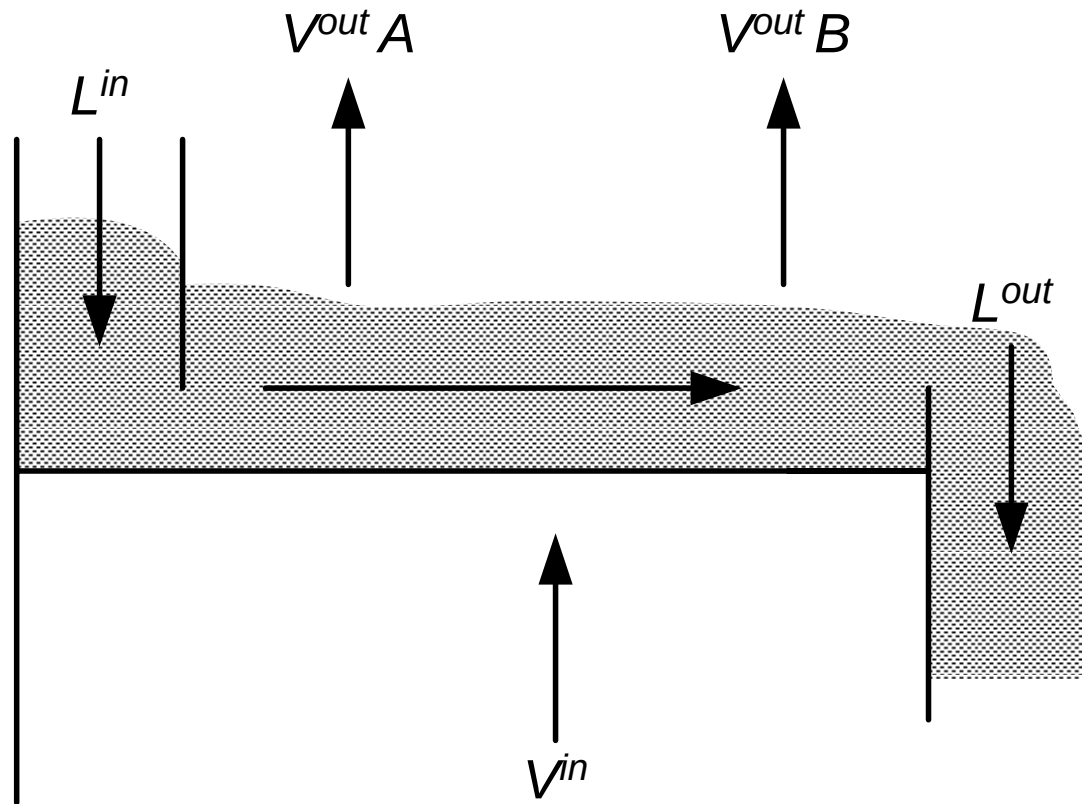
- **Definition**
- **Calculation**
- **Application**

Equilibrium Stage

- How most calculation methods see a tray



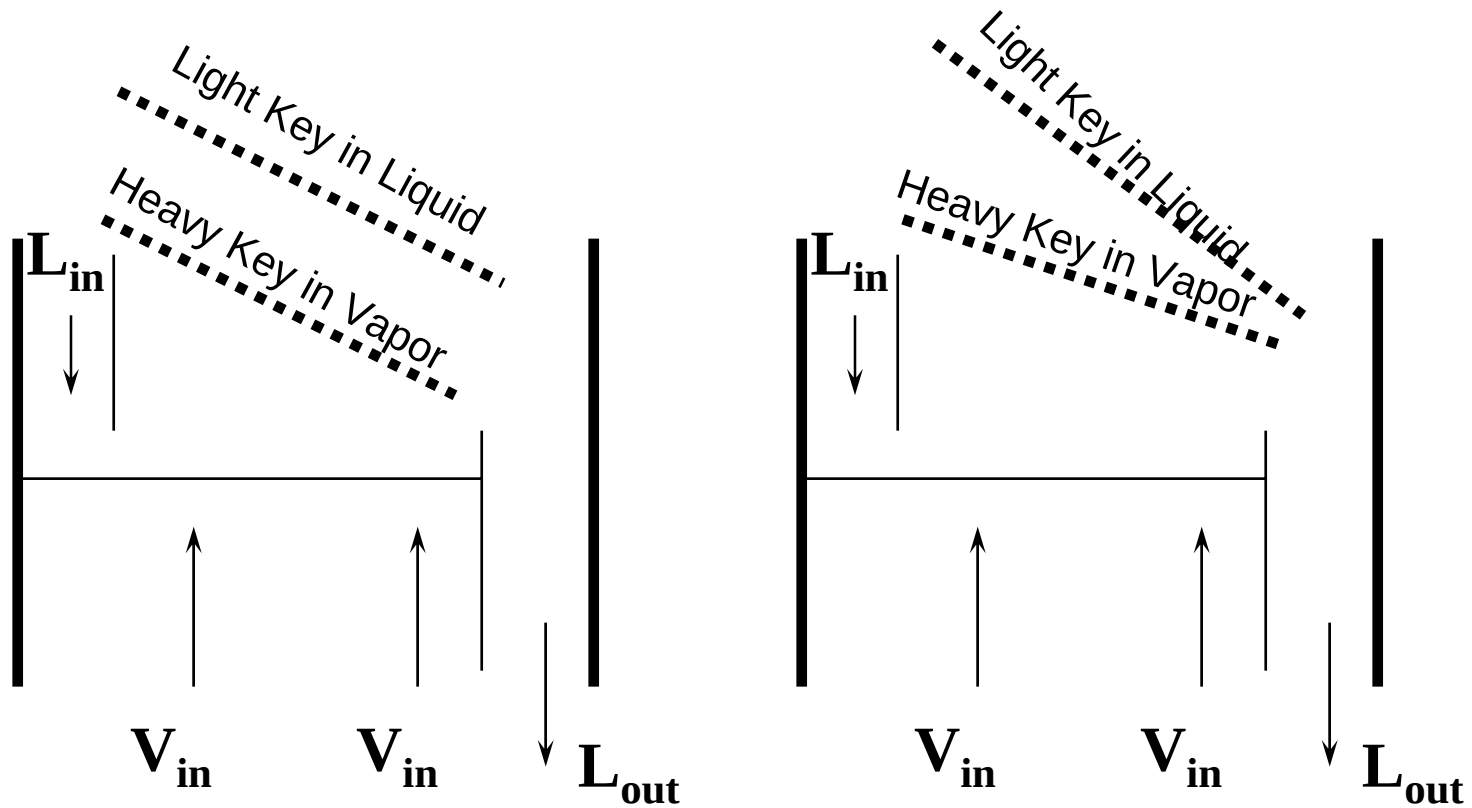
Conventional Tray



Real Life Seldom Meets Criteria for Theoretical Stage

1. V^{out} “A” in equilibrium with inlet liquid
2. V^{out} “B” in equilibrium with outlet liquid
3. What about liquid weeping to tray below?

Tray Efficiency



Tray Efficiency

- Deviation from ideal

$$\text{efficiency} = N_{\text{ideal}} / N_{\text{actual}} \quad \text{Real Stages} = \frac{\text{Theoretical Stages}}{\text{Tray Efficiency}}$$

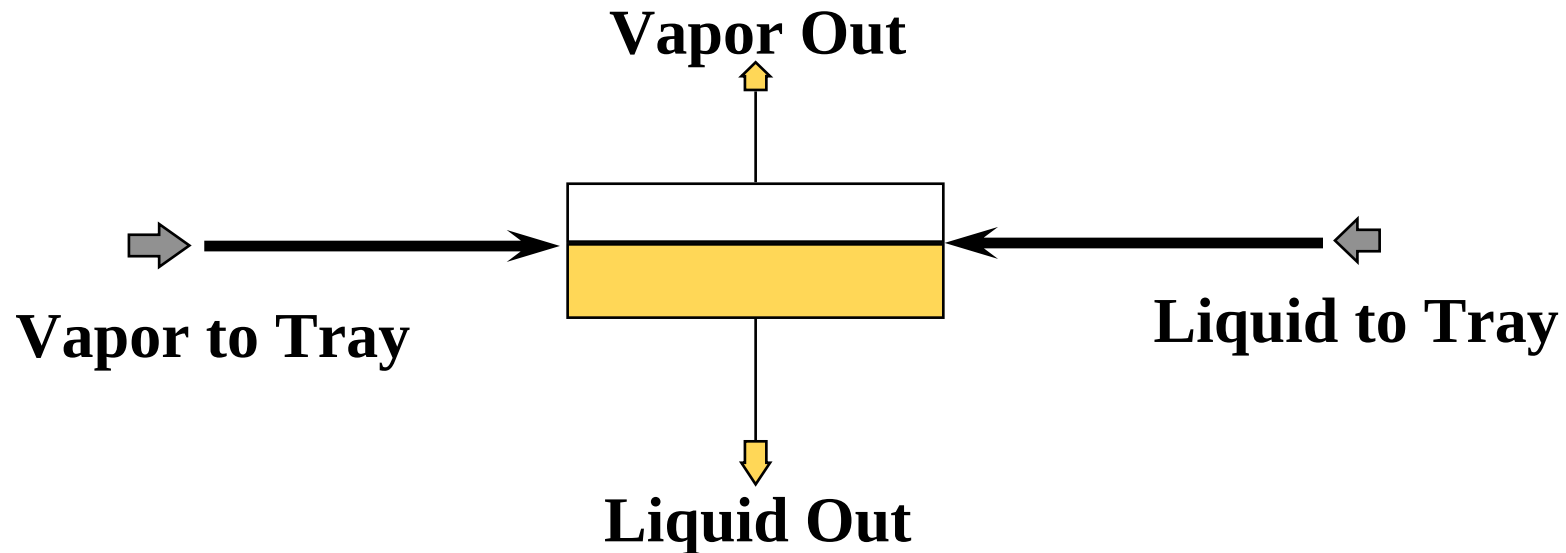
- Tray efficiency obtained from:
- Experience
- Judgment
- Rules of Thumb
- Calculation Methods

Tray Efficiency

**What can lower tray efficiency in operating columns?
(anything that prevents thorough mixing and
equilibrium) Some of these can be under our control.**

- **Tray Bypassing**
 - Liquid weeping
 - Vapor channeling
- **Liquid Flow not Uniform**
 - Tray not level
 - Tray hardware missing

Tray Efficiency – Real Trays vs. Theoretical (Equilibrium) Stages

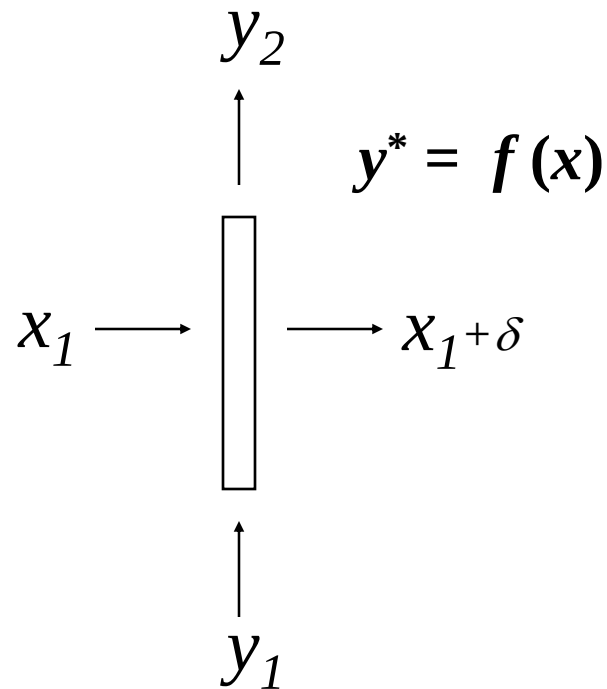


Criteria for Theoretical Stage

- 1. Steady state operation**
- 2. Vapor and liquid to tray thoroughly mixes**
- 3. Vapor and liquid in equilibrium**

Tray Efficiency

Murphree Point Efficiency

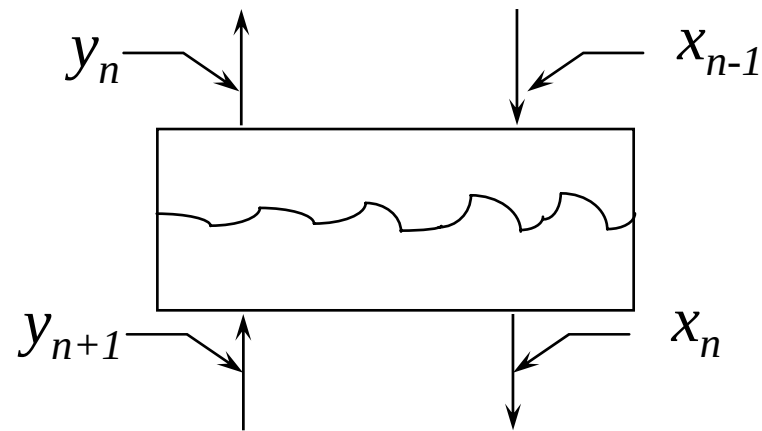


$$E_{OG} \equiv \left(\frac{y_2 - y_1}{y^* - y_1} \right)$$

Tray Efficiency

Murphree Tray Efficiency

$$y_n^* = f(x_n)$$



$$E_{mv} = \left(\frac{y_n - y_{n+1}}{y_n^* - y_{n+1}} \right)$$

Point Efficiency

Assuming

- Vapor flows in plug flow through froth
- Liquid is completely mixed in vertical direction

$$\int_0^{h_f} \frac{K_{OG} a(dh_f)}{u_b} = -\ln \left(\frac{y^* - y_2}{y^* - y_1} \right)$$

$$N_{og} \equiv \int_0^{h_f} \frac{K_{OG} a(dh_f)}{u_b}$$

Tray Efficiency

Point Efficiency

$$E_{OG} = 1 - e^{-N_{OG}}$$

Tray Efficiency

Two Film Theory

- Values for NOG are usually calculated using a Two Film Theory model
- Typical input values for these models include
 - Fluid properties and rates
 - Vapor orifice parameters and number
 - Bubbling area and froth height

Tray Efficiency

- **The point efficiency is used with a model for the vapor and liquid flow across the whole tray**
- **The Murphree tray efficiency is normally the most convenient to calculate**
- **If the liquid plus flows across the tray there is and enhancement to the efficiency**
- **Lewis analyzed three idealized cases**

Typical Observed Tray Efficiency

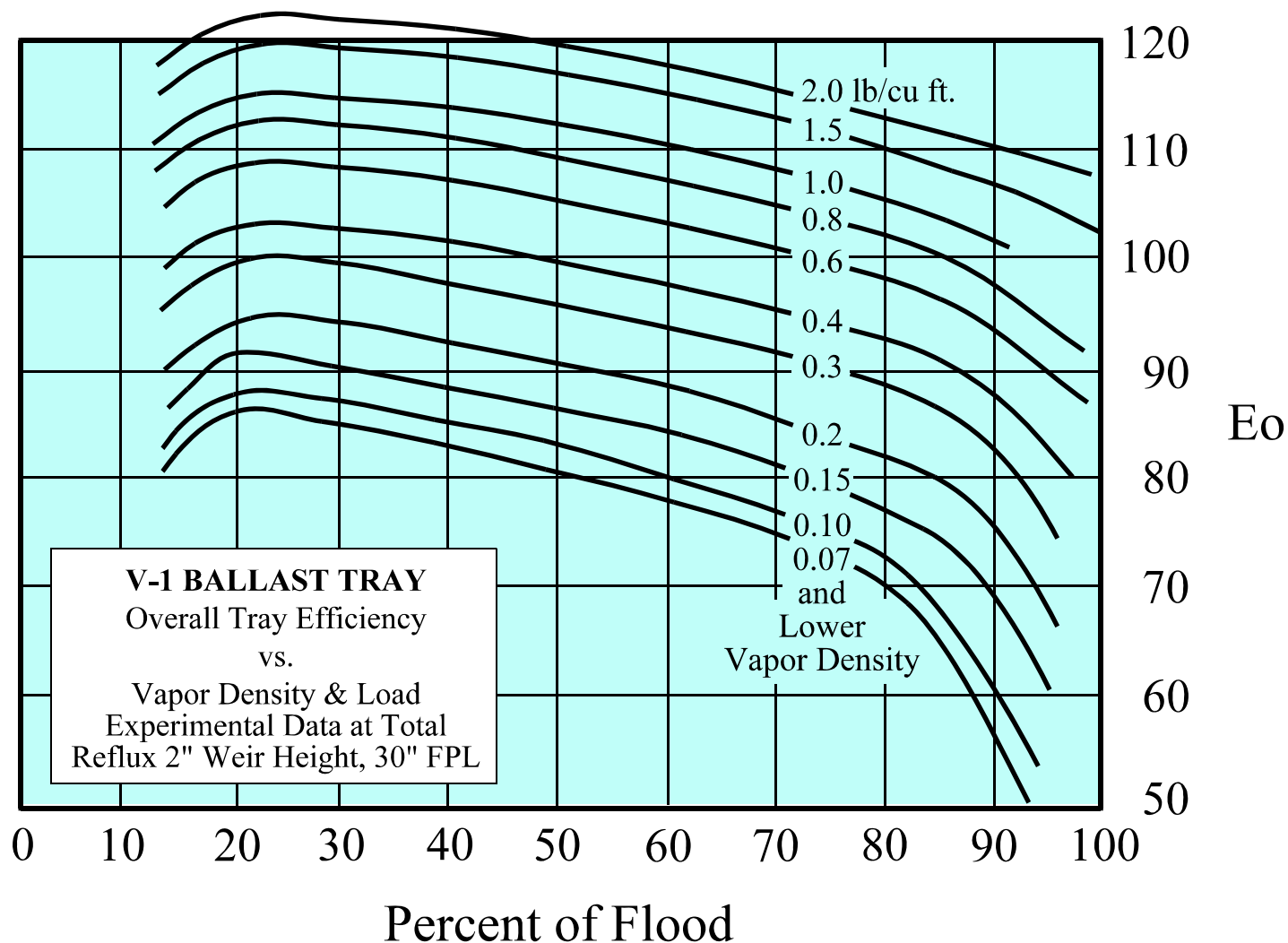
(Simplistic Overall)

Xylene Isomer Fractionators	80-100
Deisopentanizers/Deisobutanizers	80-100
Benzene/Toluene/Xylene	75-80
Depropanizers/Debutanizers	75-80
Naphtha Fractionators	65-85
High Pressure Deethanizers	50-60
Low Pressure Drop Columns	40-60
Distillation Dryers	15
Gas Strippers	7-10
Gas Con Absorbers	
Primary	30-35
Sponge	20-25

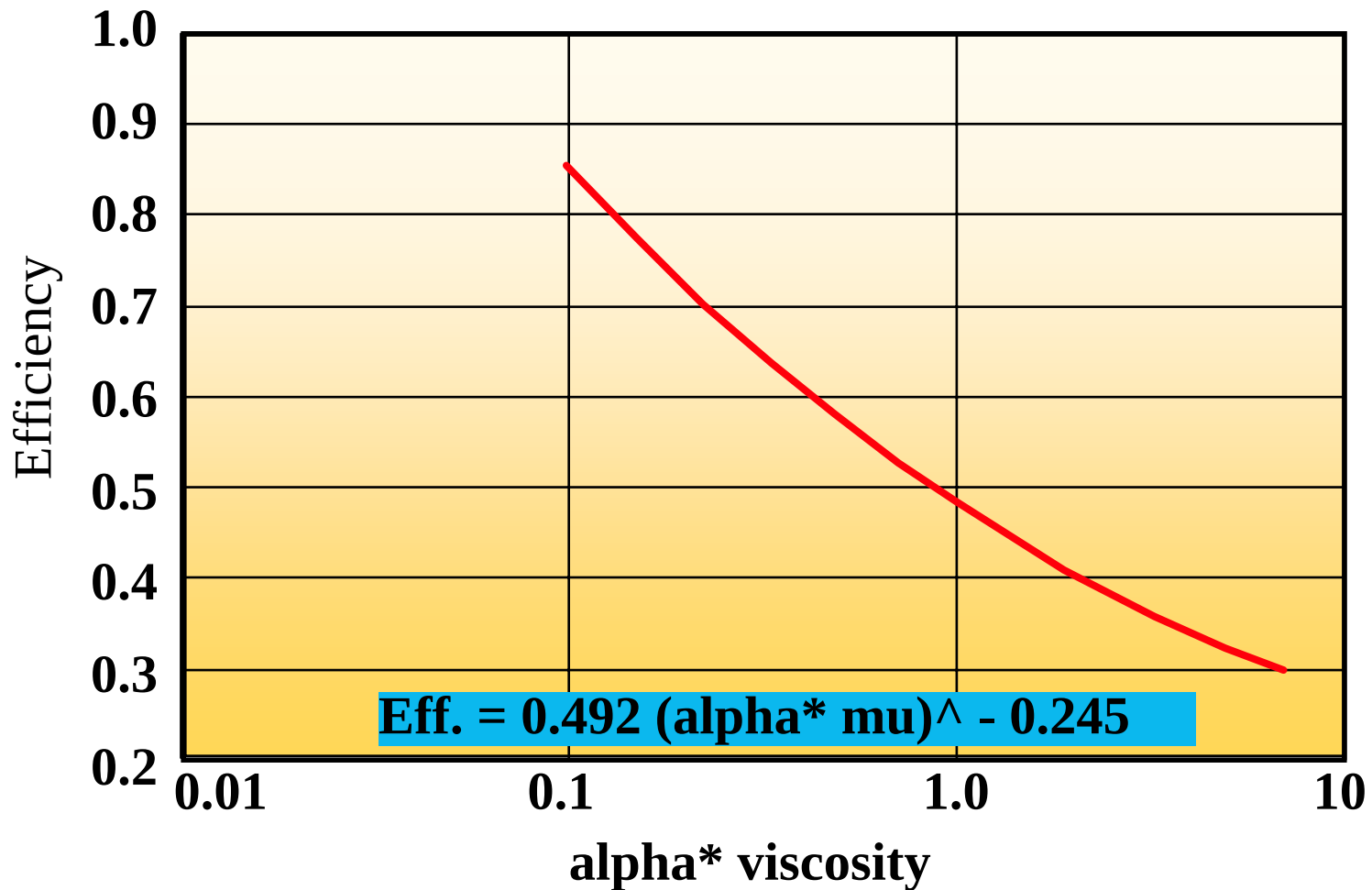
General Guide for Tray Efficiency as Function of α Alone

<u>Alpha</u>	<u>Tray Efficiency</u>
1.2	90
2.0	70
3.0	50
5.0	20
15.0	10

Tray Efficiency



O'Connell Efficiency Correlation



Tray Efficiency

Lewis Tray Efficiency Enhancements

- **All Cases Assume Plug Flow Liquid**
- **Lewis Case 1 (Middle Efficiency)**
 - Vapor is well mixed

Tray Efficiency

Lewis Tray Efficiency Enhancements

- **Lewis Case 2 (Best Efficiency)**
 - Vapor is not radially mixed
 - Liquid flows in same direction on all trays

- **Lewis Case 3 (Worst Efficiency)**
 - Vapor is not radially mixed
 - Liquid flows in alternate direction on alternate trays

Tray Efficiency

**For Lewis Case 1
Murphree Tray Efficiency**

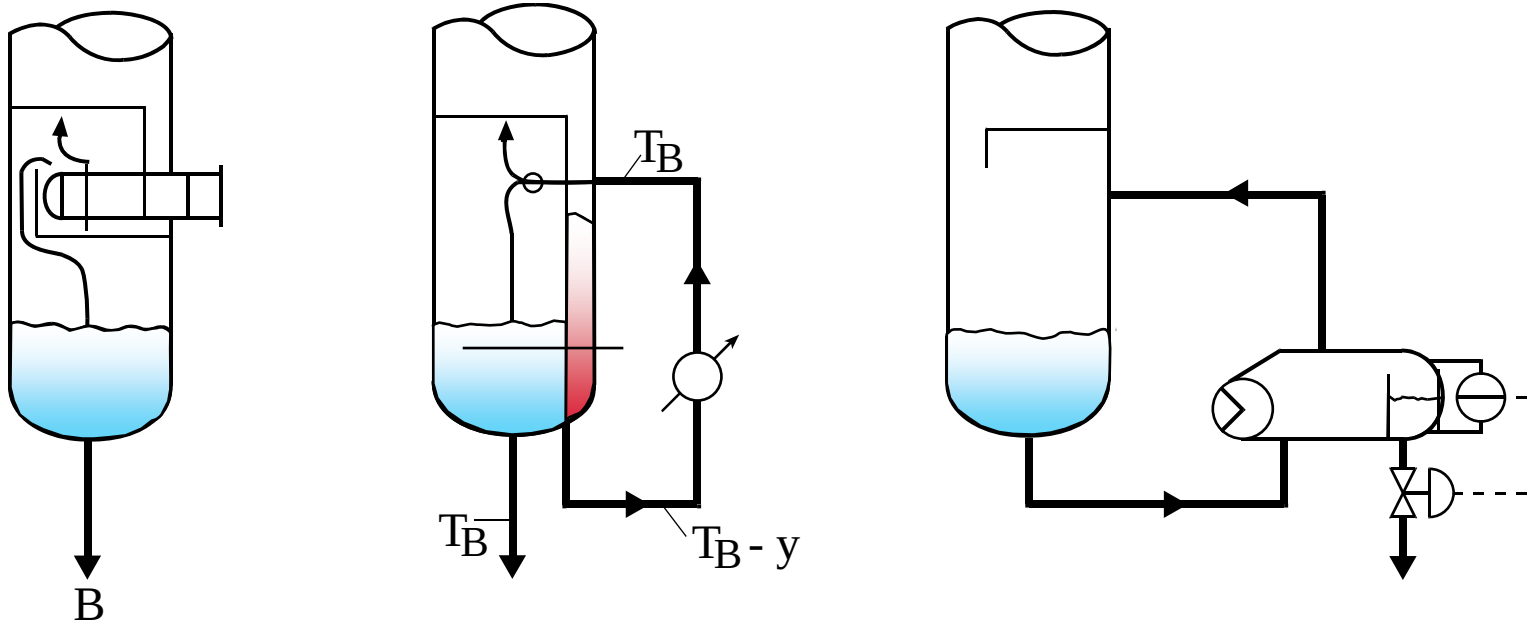
$$E_{MG} = \frac{\exp(\lambda E_{OG}) - 1}{\lambda}$$

Tray Efficiency

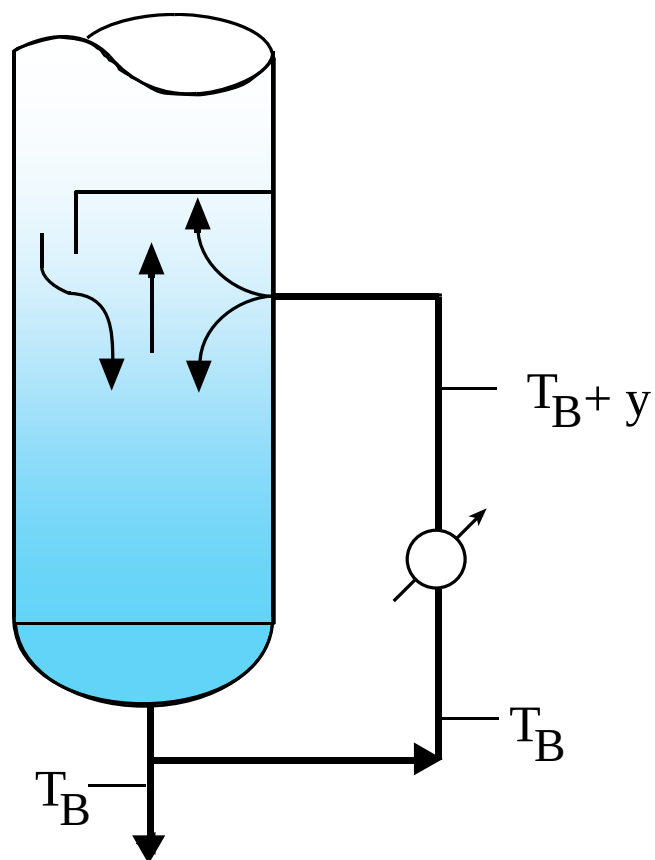
If E_{MG} is constant, then the over all column efficiency can be calculated via

$$E_O = \frac{\log[1 + E_{MG}(\lambda - 1)]}{\log(\lambda)}$$

Once Through Reboilers



Recirculating Reboiler



Types of Reboilers

- **Once Through Reboilers**
 - Colder temperature
 - One theoretical stage
 - Lower loading

- **Recirculating Reboiler**
 - Simple
 - 1/3 theoretical stage

Column Design and Optimization



A Honeywell Company

Performance Goals/Specifications

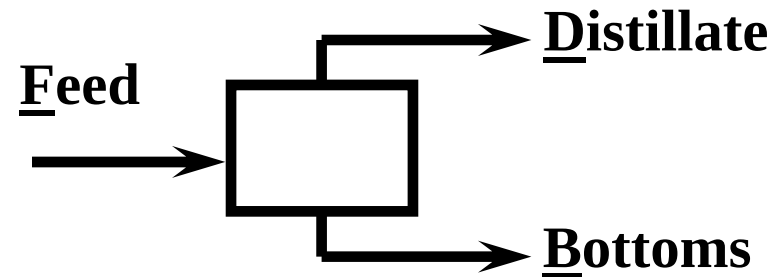
Measure the performance of a fractionator

Performance goals – in a computer program:

- **Performance Specifications**

- Recovery (or loss)
- Purity (or impurity)
- Product qualities – end point, vapor pressure, etc.
- Capacity

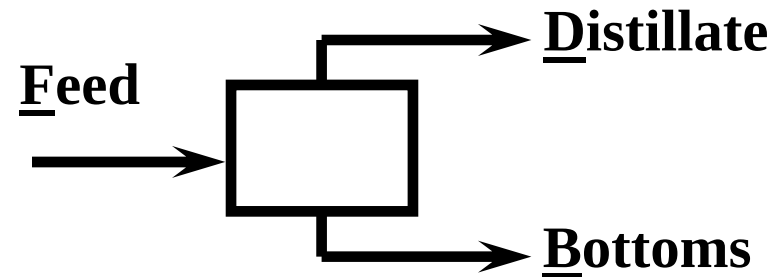
Performance Goals



Purity and/or Recovery – For this typical two cut fractionator, there is a light key component purity specified for the distillate and a heavy key component purity specified for the bottoms. An alternative goal would have the light key purity specified and the light key recovery specified.

Capacity – Normally the feed rate is specified. Sometimes the bottoms or distillate flow is specified instead of feed.

Performance Goals



Purity and/or Recovery – For example a debutanizer, the overhead liquid product can contain 0.5 mol% C5+, while the bottoms product can contain 0.5 mol% C4-

Capacity – For example, the design feedrate is 46,450 kg/hr with 1.80 m³/sec of overhead vapor product, 1530 kg/hr of overhead liquid product, and 44,590 kg/hr of bottoms product with the product purities specified above

Performance Goals

What independent variables are available to the process engineer to make operational changes?

Fixed by Design

Reflux (Partial)

Trays

Feed Tray

Available for Control

Reflux, 50-115% design

Overhead Composition

Bottom Composition

or

Reflux

Overhead Composition

Recovery of Light Key

Can one show graphically the relationship of the operating variables? (Yes, McCabe-Thiele Diagram)

Designing a Column

- **Define Feed**
- **Define Product Specification**
- **Set Column Pressure**
- **Optimize Column Design**
- **Calculate Tray Loads**
- **Size Trays**
- **Set Composition Control**

Define Feed

- **Composition**
- **Flow Rate**
- **Temperature**
- **Pressure**
- **Enthalpy**
- **Key components and contaminants**
- **Feed cases**
 - **Controlling case or cases**
 - **Non-controlling may influence heat media, tray type**

Define Product Specifications

- **Receiver temperature**
- **Top Tray Vapor Temperature**
- **Product purities and recoveries**
- **Zero purity spec is not acceptable**
- **Get a good definition of the desired purities and recoveries from any project definition (or the customer)**
- **Consult with specialist and project definition for streams internal to unit or complex**
- **Determine the highest purities that the column ever has to produce**

Set Column Pressure

- **Maximize alpha value**
- **Minimize column cost**
- **Keep flare material out of overhead**
- **Totally condense overhead products**
- **Prevent need for net gas compression**
- **Use cheaper heat source (MP Steam or HP Steam?)**

Set Column Pressure (continued)

- **Minimize net overhead vapor**
- **Use condenser as heat source**
- **Use bottoms as hot oil**
- **Limit bottom temperature**
 - **Cracking**
 - **Polymerization**
 - **Approach to critical**

Other Design Considerations

■ **Reboiler:**

- **Thermosyphon or forced circulation**
- **Vertical or horizontal**
- **Fired heater**
- **Integrated**
- **Number of Reboilers (in parallel) – May be determined by level of steam**
- **Fouling Service**

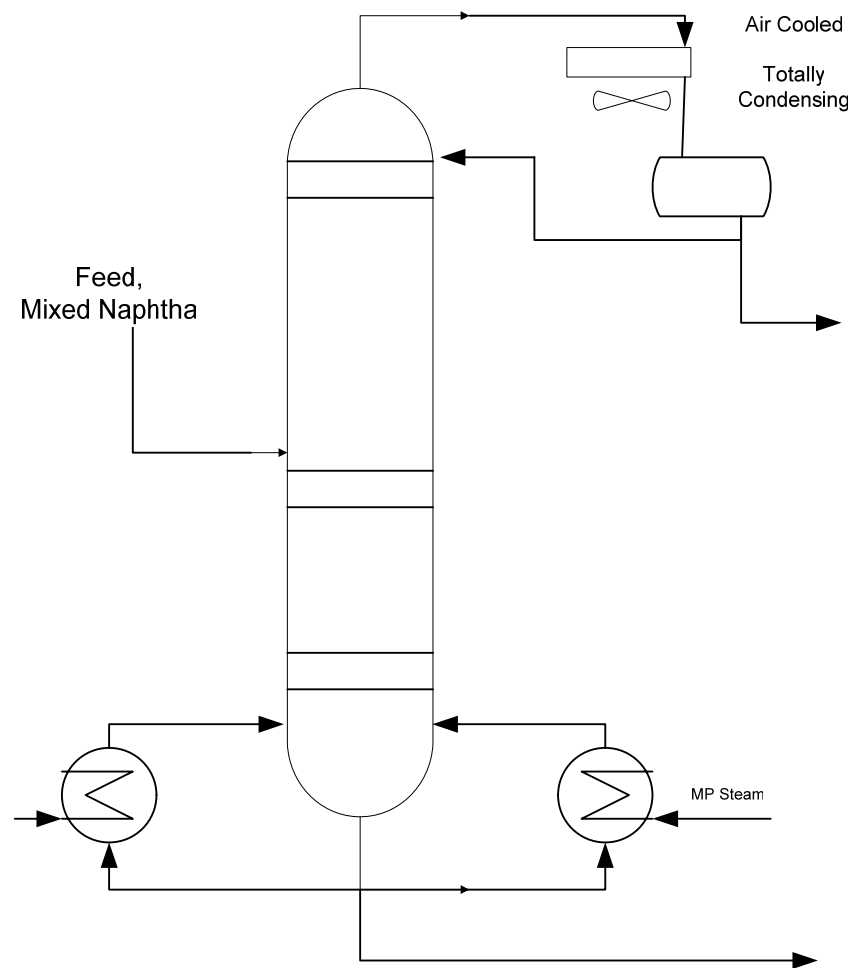
Other Design Considerations

- **Condenser Type and Cooling Medium**
 - **Operating Pressure vs. Condenser Size vs. Column Cost vs. Process Needs**
 - **Consider using condensing duty to reboiler another column**
 - **Air cooling or water cooling only**
 - **Air followed by water**
 - **Receiver temperature limits to prevent water forming**

Other Design Considerations

- **Select and Design Internals**
 - **Conventional Trays**
 - **Sieve vs Valve**
 - **High Capacity Trays**
 - **Packing**

Column Pressure Case Study



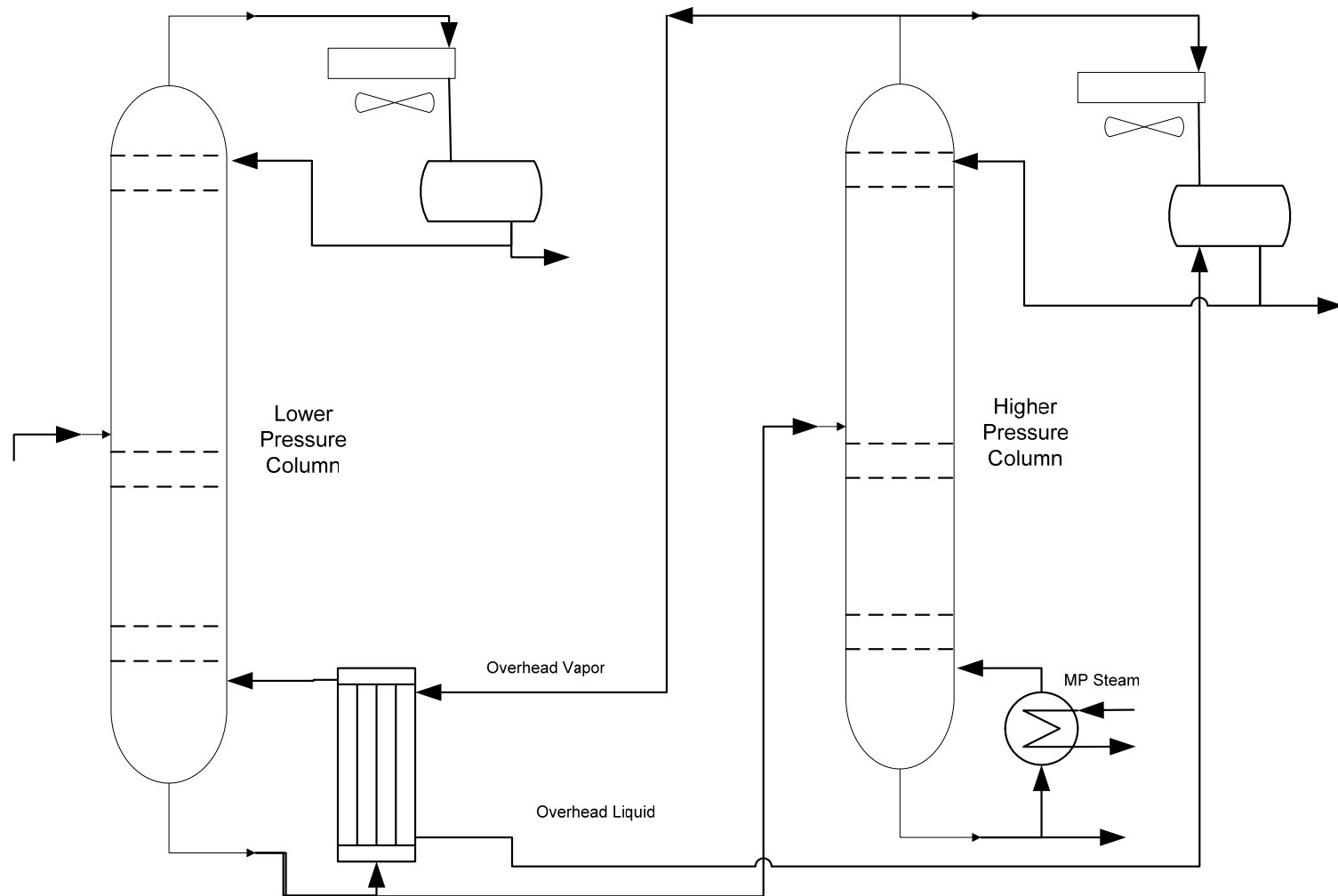
Column Pressure Case Study

- **Three feed cases with differences in the boiling ranges and composition of the naphtha.**
- **Reboiler duty:**
 - Case 1: 17.0 mmkcal/hr
 - Case 2: 16.9 mmkcal/hr
 - Case 3: 17.7 mmkcal/hr
- **Which controls reboiler design?**

Column Pressure Case Study

- **Three feed cases with differences in the boiling ranges of the naphtha.**
- **Reboiler duty and approach:**
 - **Case 1: 17.0 mmkcal/hr, 10 C**
 - **Case 2: 16.9 mmkcal/hr, 9 C**
 - **Case 3: 17.7 mmkcal/hr, 18 C**
- **Which controls reboiler design?**

Column Pressure Case Study



Column Pressure Profile

- **Need to set receiver, top tray, reboiler at minimum – use pressure drops of equipment**
- **Condenser/Receiver**
 - Air Condenser, 3 to 5 psi
 - Water Condenser, same or a little higher
- **Examples of Typical Tray Pressure Drops**
 - Allow 0.05 to 0.2 psi Per Tray
 - 0.12 psi Per Real Tray is Typical
 - Most Simulators Use Theoretical Trays,
 - To adjust, divide actual tray drop by efficiency for theoretical trays
- **No pressure drop needed for reboiler**

Optimize Column Design

- **Best trays versus reboiler duty**
- **Best feed tray location**
- **Feed preheat**

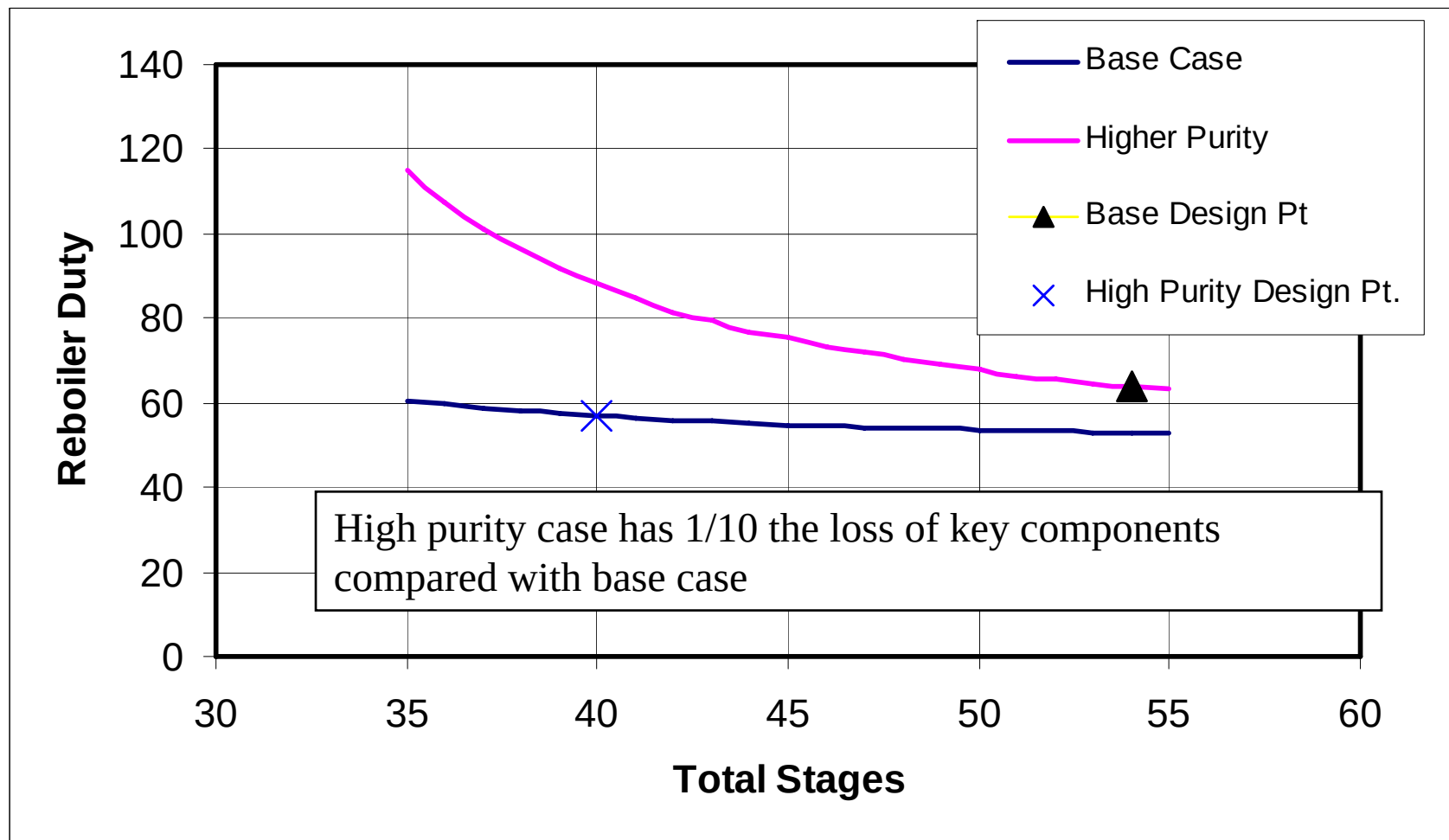
Trays vs. Reboiler Duty

(Constant Product Specs)

- **More trays – smaller reboiler and condenser**
- **More capital – smaller utility cost**
- **Economic analysis with help from simple guidelines**

Trays vs. Reboiler Duty

(Constant Product Specs)



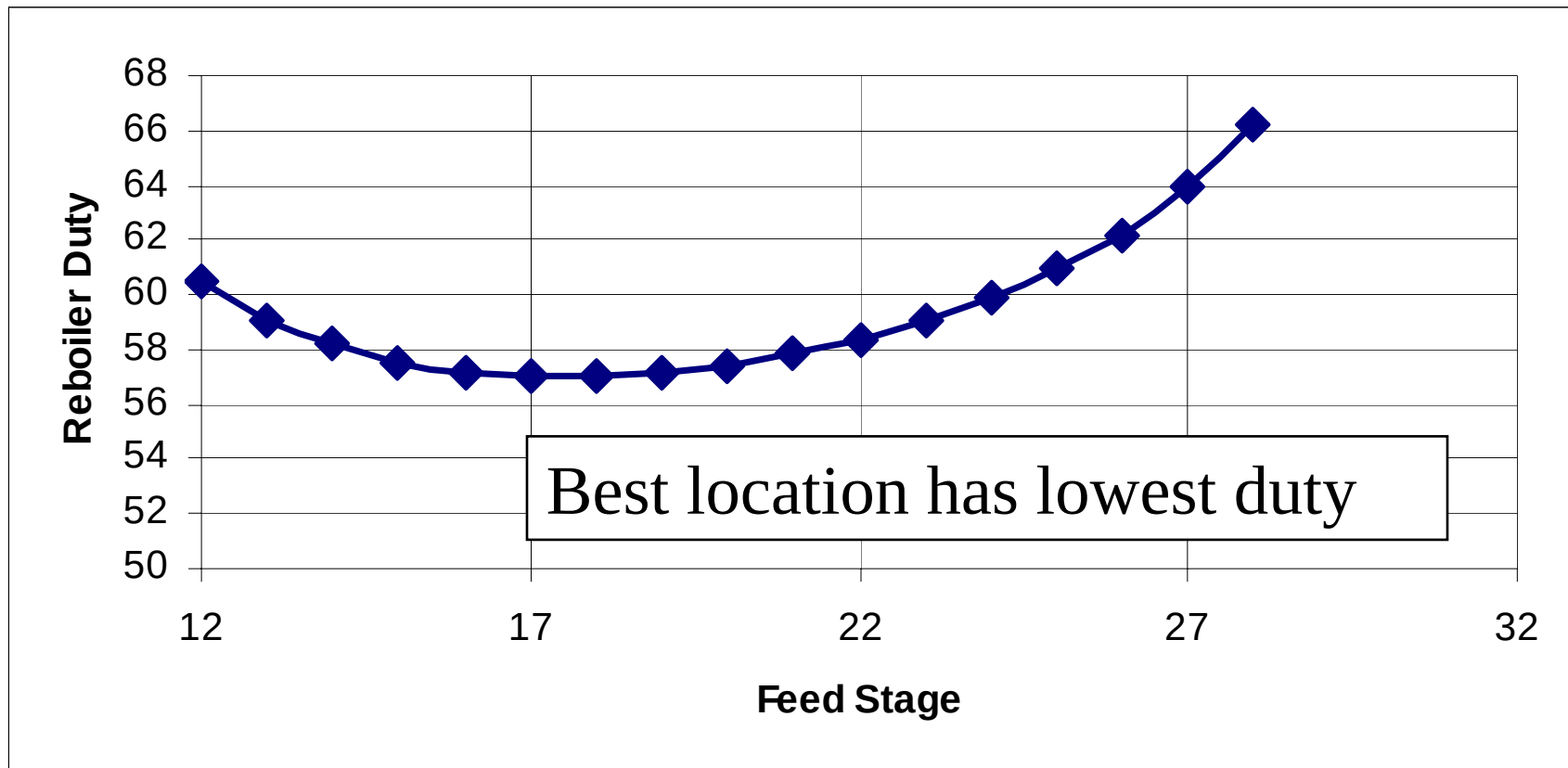
Trays Versus Reboiler Duty Selection

C_3/C_4 Splitter

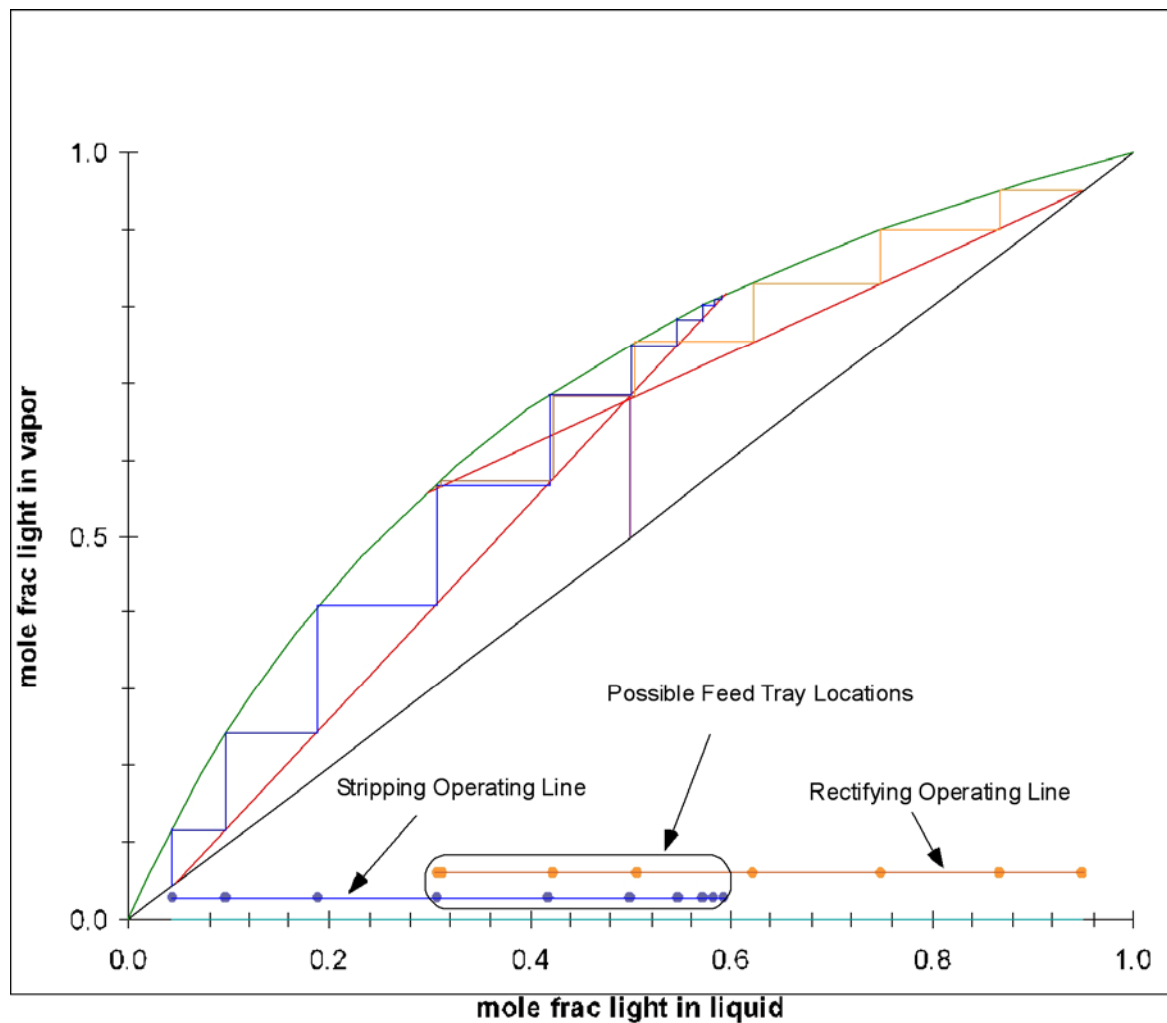
Feed Stage	Total Stages	Reboiler 1E6 BTU/h	% Delta Reboiler Theo Tray	Feed Stage	Total Stages	Reboiler 1E6 Btu/h	% Delta Reboiler Theo Tray
25	50	7.58	0.18	15	30	8.69	2.38
24	48	7.61	0.21	14	28	9.109	3.28
23	46	7.64	0.31	13	26	9.70	4.74
22	44	7.69	0.36	12	24	10.6	7.17
21	42	7.74	0.43	11	22	12.1	11.7
20	40	7.81	0.61	10	20	15.0	22.7
19	38	7.91	0.77	9	18	21.8	72.9
18	36	8.03	0.99	8	16	53.58	771
17	34	8.19	1.28	7	15	466	
16	32	8.40	1.74	7	14	Will Not Solve	

Feed Tray Location vs. Reboiler Duty

(Constant Product Specs)

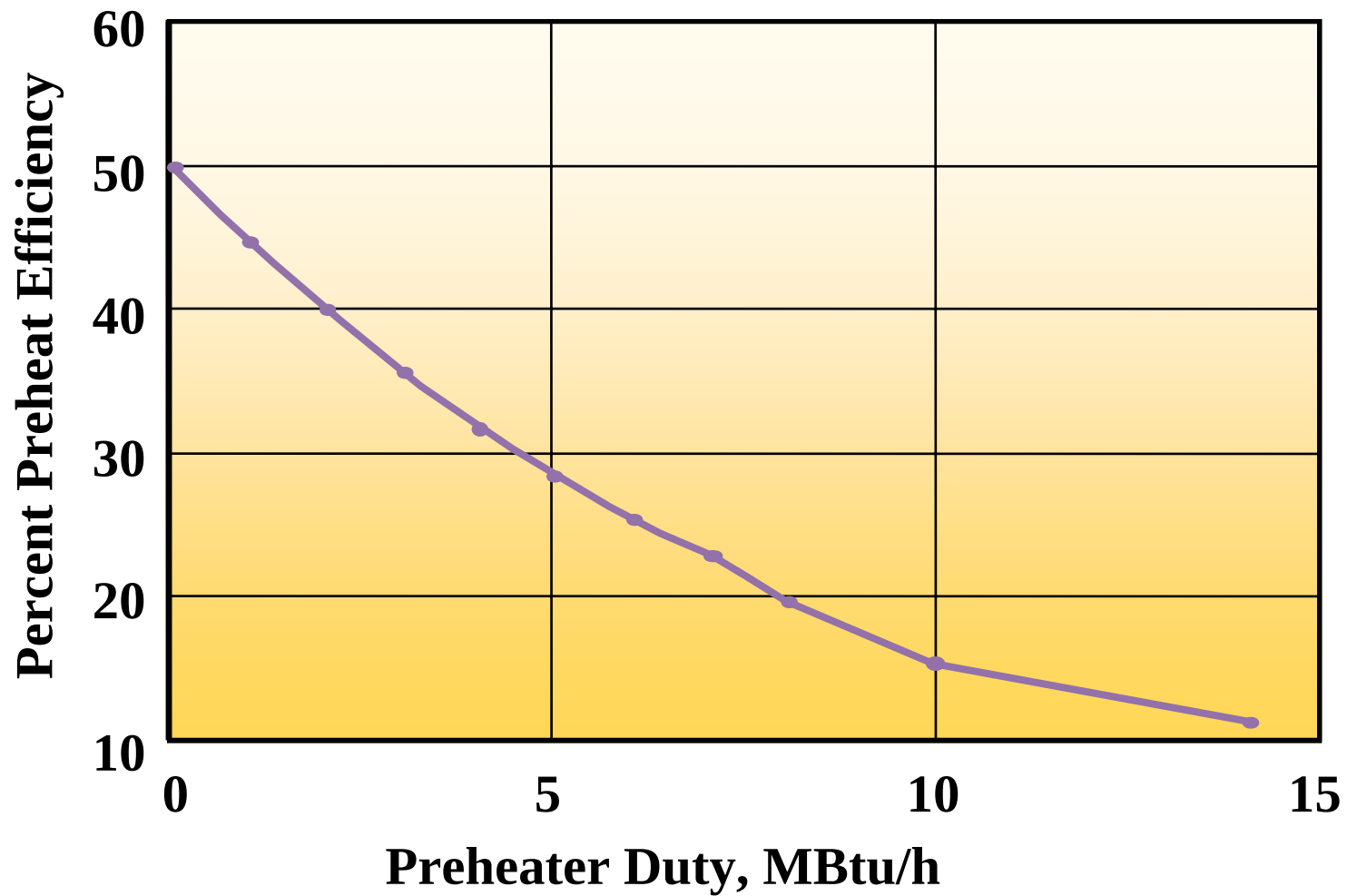


Feed Tray Location



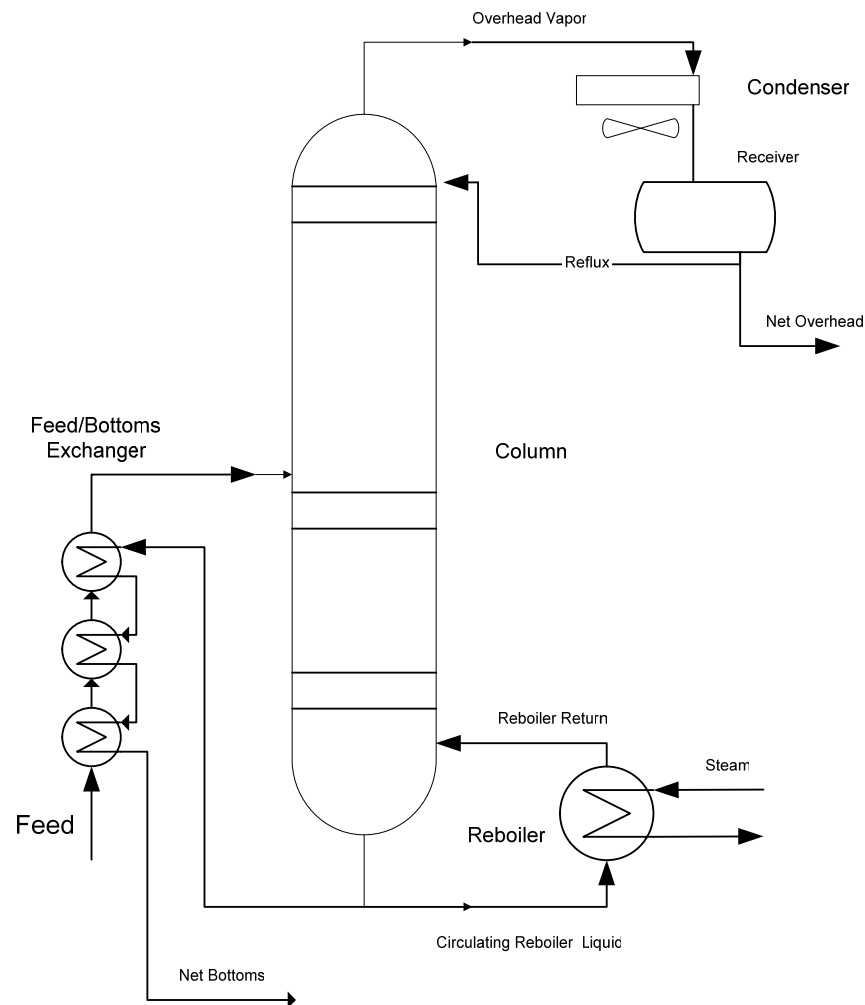
■ Rooks, R.E., Chemical Processing, May 2006

Feed Preheat Efficiency



Feed Preheat

- **Best source of feed preheat is from the column itself**
- **Becomes both a process study and an economic study**
- **Take advantage of possible feed-bottoms temperature cross with countercurrent flow and more than one shell**
- **Payback is incremental reboiler duty saved per additional shell**



Multicomponent Distillation Naphtha Stripper – Preheat Efficiency

Preheat efficiency is the delta reboiler duty divided by the delta feed enthalpy.

Multicomponent Distillation

Naphtha Stripper – Preheat Efficiency

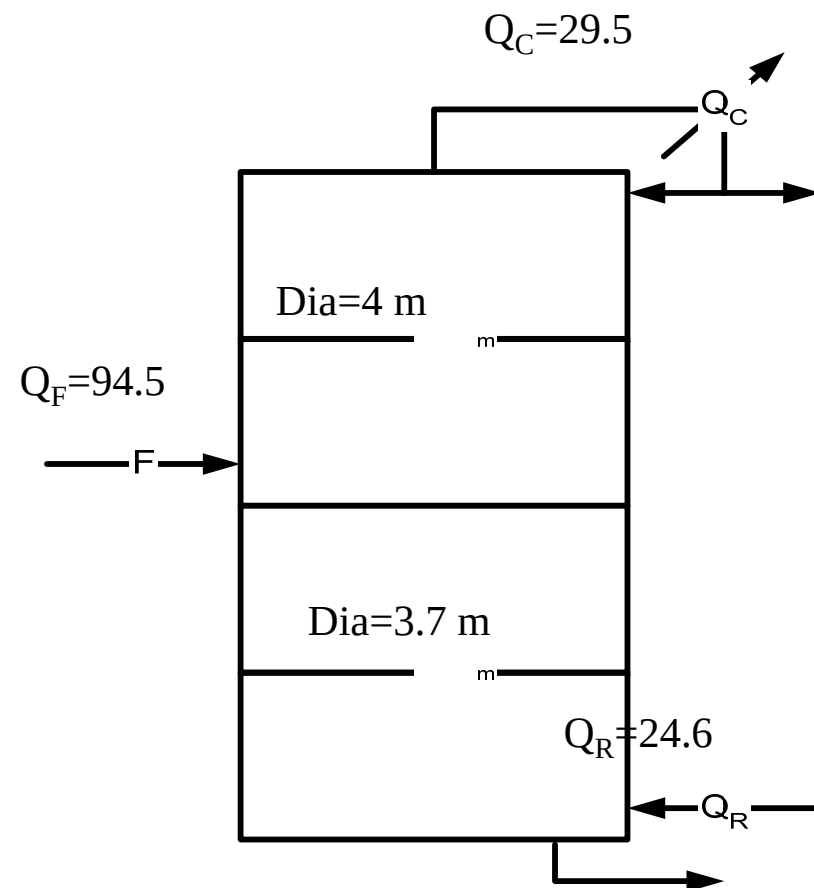
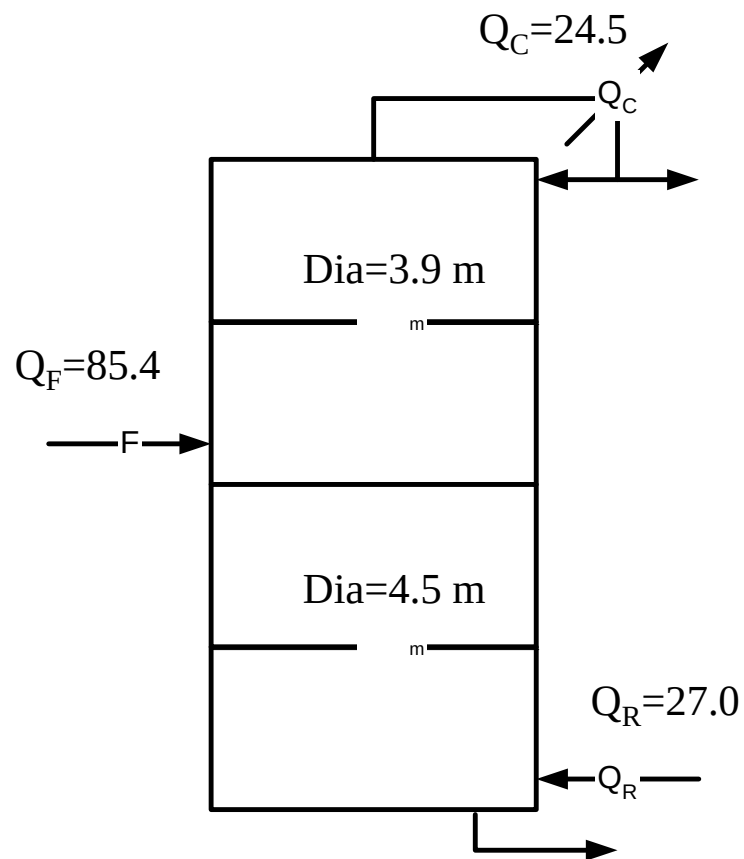
<u>Delta Temp</u>	<u>Preheat Eff. %</u>
340->350	37.4
350->360	34.8
360->370	34.1
370->380	31.1

Multicomponent Distillation

Naphtha Splitter – Preheat Efficiency

Delta Temp	Preheat Eff. %
275->285	47.3
285->305	38.7
305->315	28.2

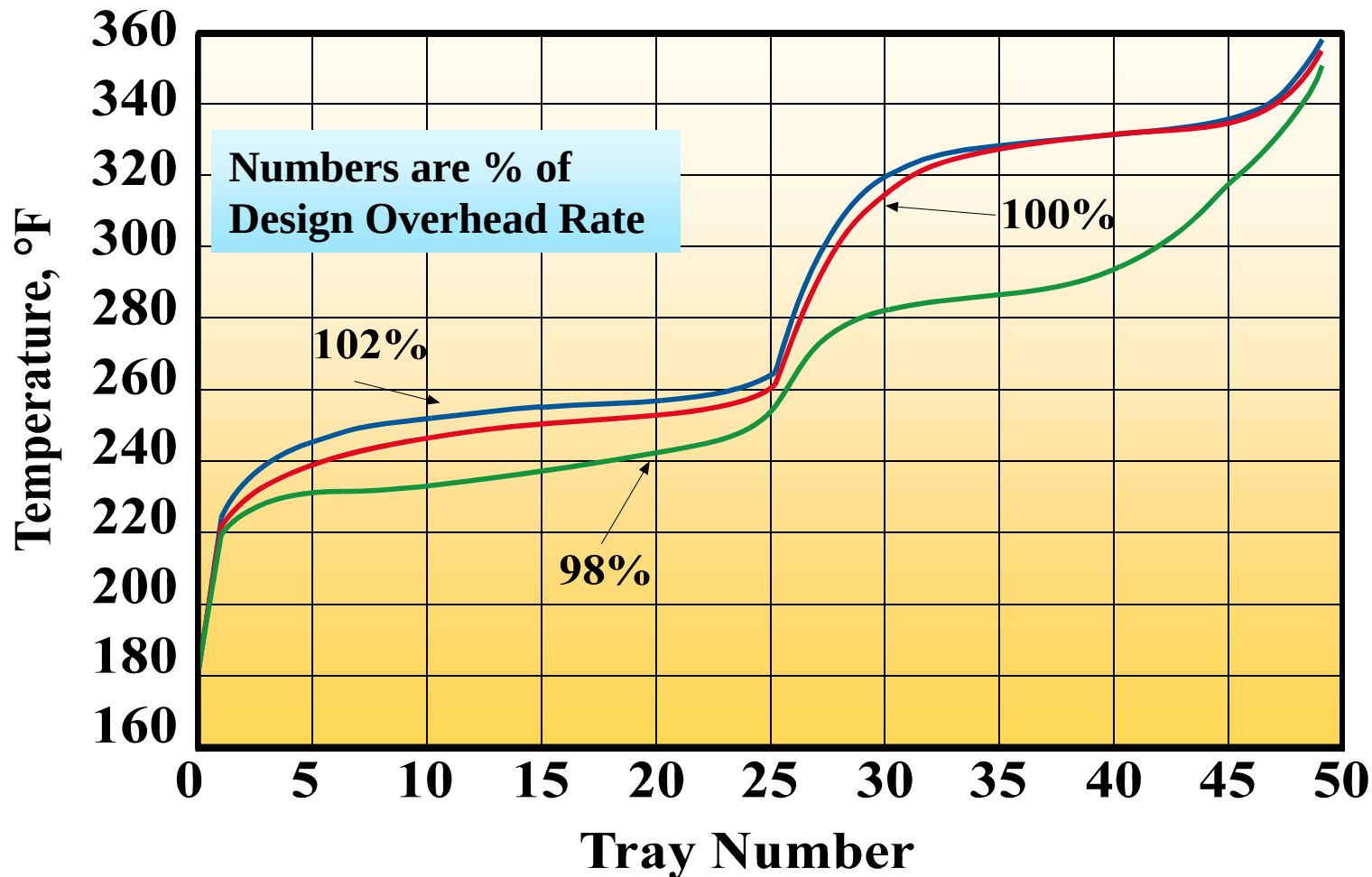
Column Feed Heat Example



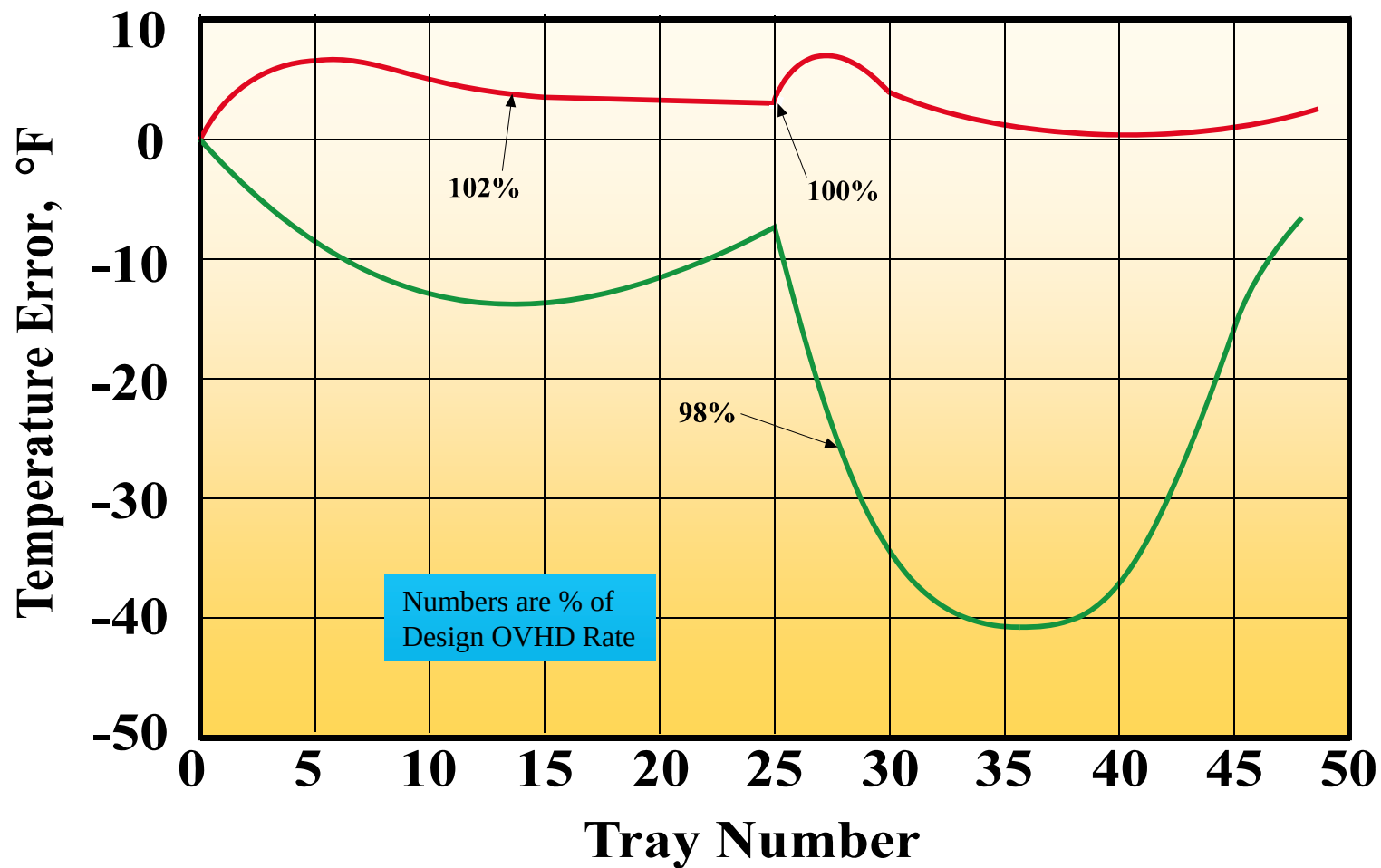
Setting Control Recommendations

- **If the goal is purity or recovery control:**
 - **Find the tray or trays that will serve as indicators of deviations from product purity**
 - **Perturb product composition**
 - **Plot simulation runs and pick trays that have the widest range in deviation from design**

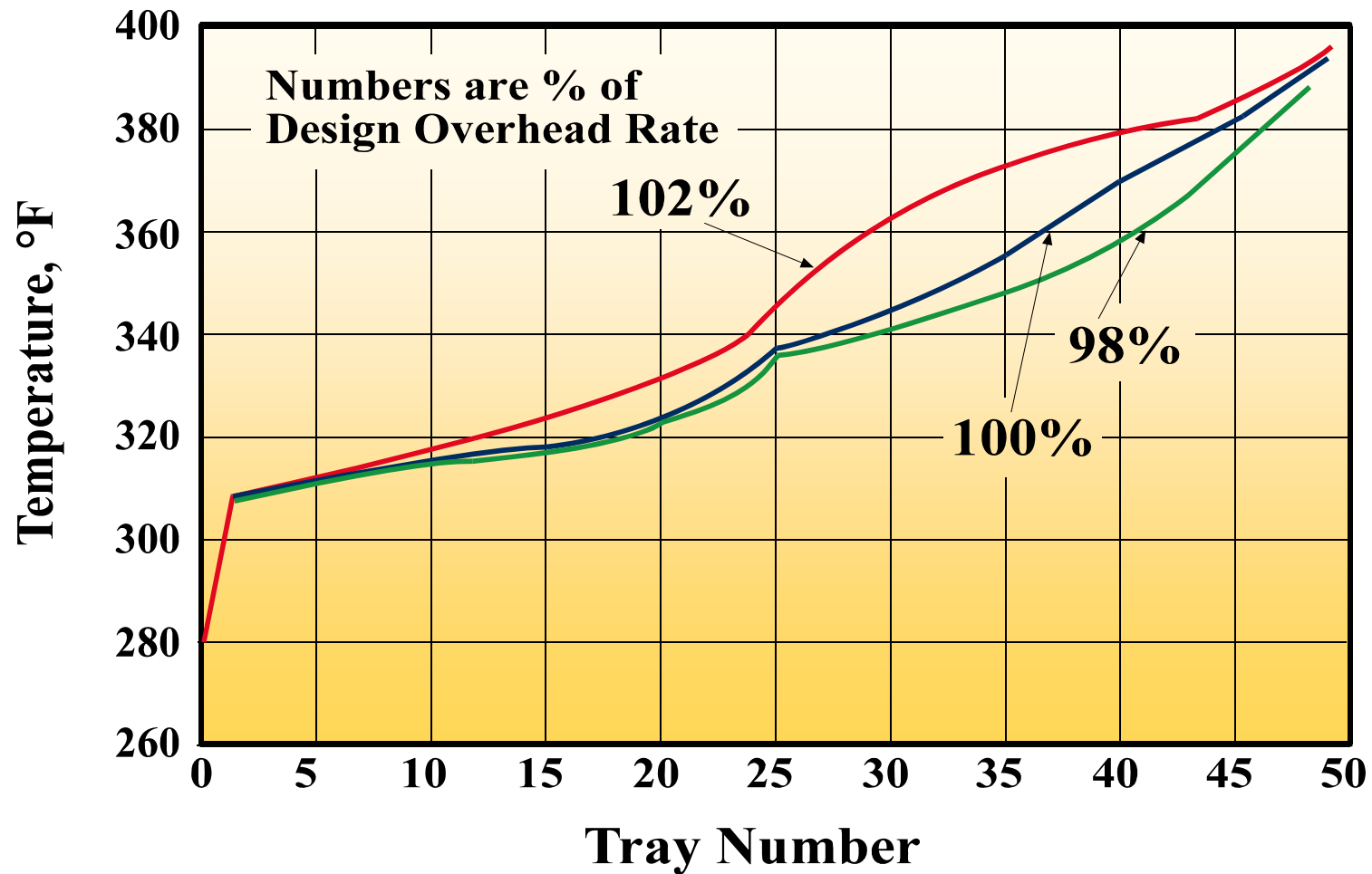
Predistillation Column



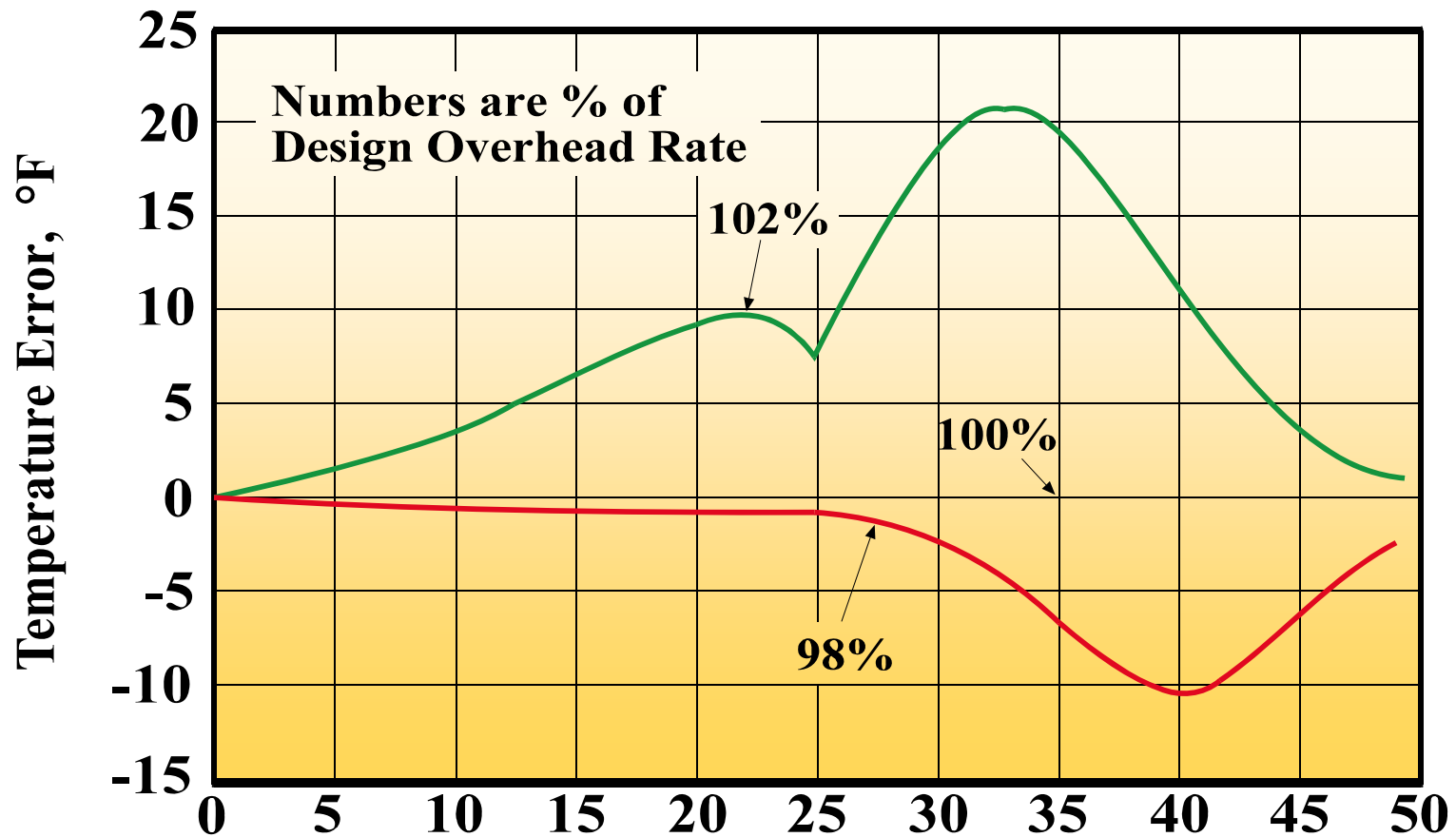
Predistillation Column



Xylene Column



Xylene Column



Choice of Column Internals

- **Sieve Tray**
 - UOP default
 - 2 to 1 operating range
 - Check customer preference and desired and expected turndown
- **Valve Tray**
 - Cost about 20% more than sieve tray
 - 5 to 1 operating range

Choice of Column Internals

(continued)

- **Packing**
 - Cost may be 5 times sieve tray
 - Pressure drop may be 1/5 that of sieve tray
- **Bubble Cap Trays**
 - Cost may be 3 times valve tray
 - Good if no weeping is critical
- **Grid**
 - Highest capacity
 - Lowest efficiency

Mass Transfer Devices

(continued)

Tray Problems

- **Flooding**
 - Vapor or jet flood (massive entrainment)
 - Liquid or downcomer backup flood
- **Dry Trays**
 - Insufficient liquid
 - Excessive boilup
- **Damaged Trays**
- **Foaming**

Mass Transfer Devices

(continued)

Packing Problems

- **Support Grid**
 - Migration of packing
- **Hold Down Grid**
 - Migration of packing
- **Vapor Distribution**
- **Liquid Distribution**
 - Typically the key to packing performance is good liquid distribution
- **“Build with trays, revamp with packing (or specialty trays)”**

Suggestions on Using a Fractionation Simulator

Getting Started

- **Look at what you are trying to accomplish**
- **Product quality or purity, stabilize products, split across a mixture for later processing**
- **Plan a little with pencil and paper if needed – map rates and profiles (material balance)**
- **Get to know the system and what we are separating – what components go where**
- **Get to know the feed, get a feel for the equilibrium**
- **Start simple and then move to more difficult product conditions**
- **There may be a composition or recovery goal but let float what the operator might turn to meet the goal such as duty or reflux**

Estimates

- **Some systems require better estimates than common hydrocarbon mixtures**
- **Presence of water – especially if the K-value method allows greater mixing of water to the hydrocarbon other than minor solubility**
- **Non-ideal systems such as Alcohol/Hydrocarbon**
- **The more complex the column – exchangers, side equipment, side products, more than one feed – the more the estimates required**
- **The wider the boiling mixture, the greater the need for estimates – temperatures and heat effects in the column mean shifts in flows**
- **Narrow split between key components but with the presence of light components and non-condensables**

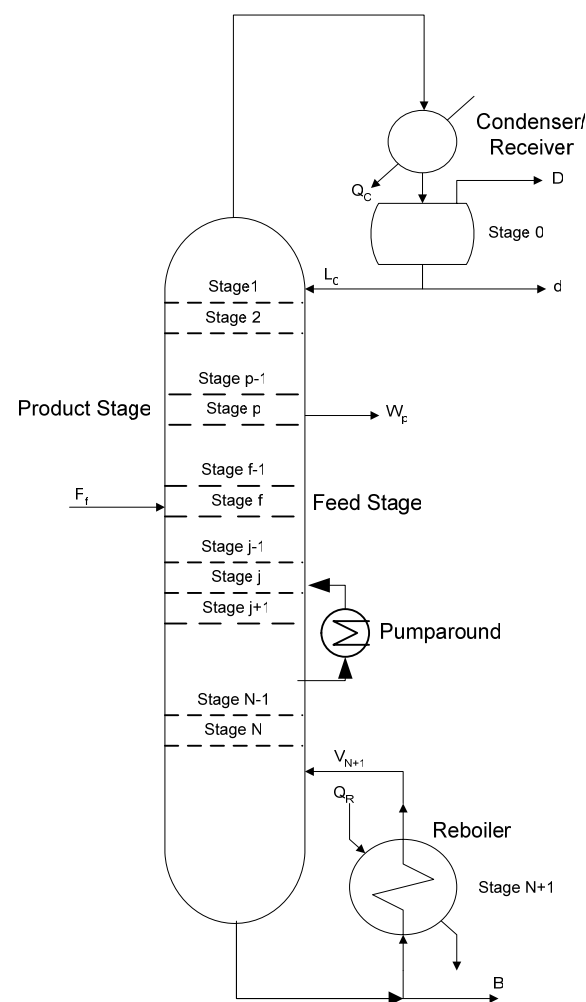
Product Flow Estimates – Debutanizer

- If we let the program default, the net overhead vapor and liquid estimates would be 1/3rd the feed = 659.43 lbmole/hr
- Product distribution and ratio of top L/V is far off from final
- Because of the low interaction between the non-condensables in the vapor and the liquid phase, the program will have a hard time moving toward a solution
- Do a perfect split estimate to initialize net overhead products
- R/D and R/F will also be high

H2	3.73	Net overhead vapor estimate = 23 lbmole/hr
C1	0.96	
C2	4.75	
C3	14.57	
IC4	10.99	Net overhead liquid estimate = 31 lbmole/hr
NC4	20.65	
IC5	43.94	
NC5	37.17	
C6+ Plat cut 1	401.68	
C6+ Plat cut 2	371.24	
C6+ Plat cut 3	376.85	
C6+ Plat cut 4	366.72	
C6+ Plat cut 5	325.03	
	1978.29	

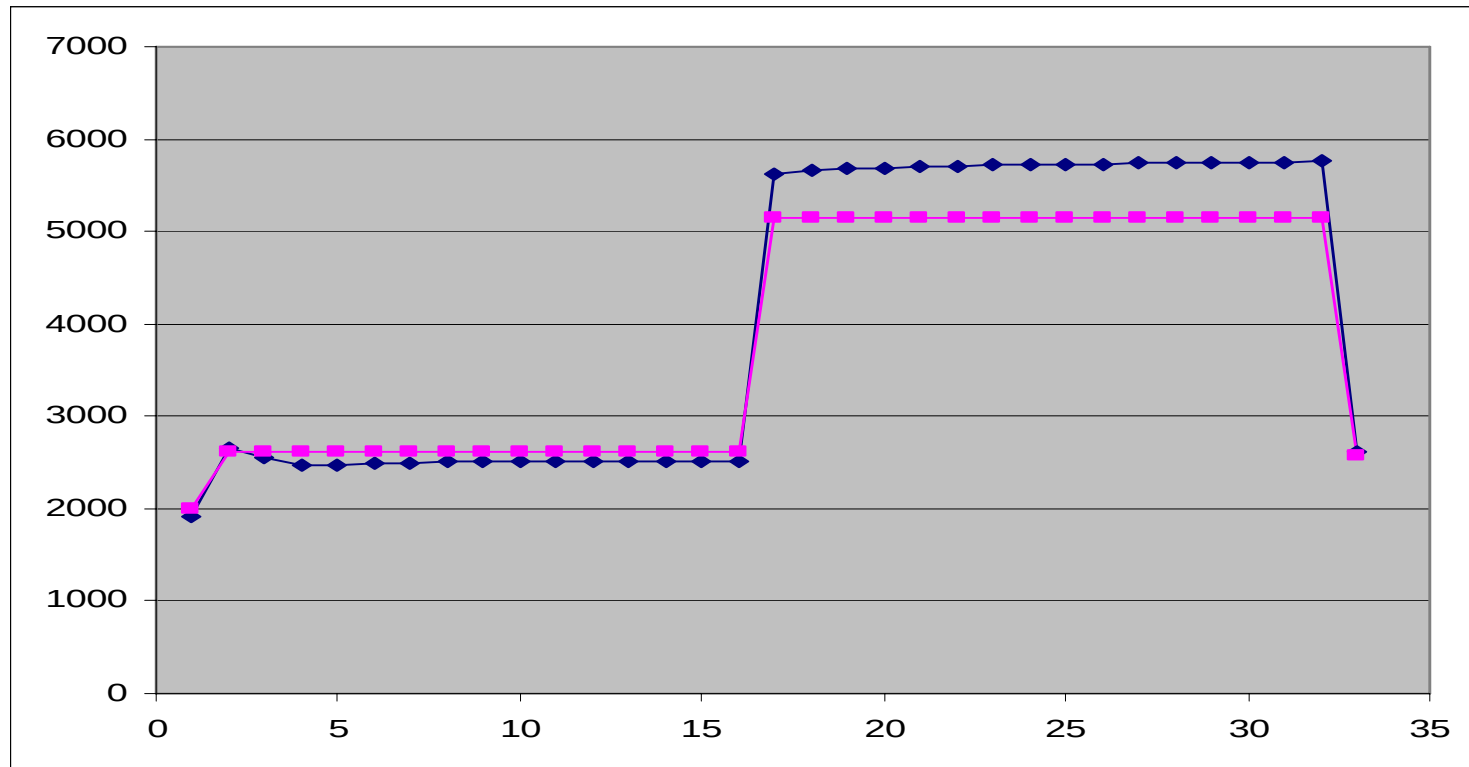
Flow Estimates

- Program should infer from the product and reflux estimates
- May need help on a very cold feed or where heat is added or taken out in the middle of the column such as with interheaters or intercoolers or pumparounds
- Most programs should handle the internal traffic at vapor or liquid side products or pumparounds but you should enter estimates for those flows



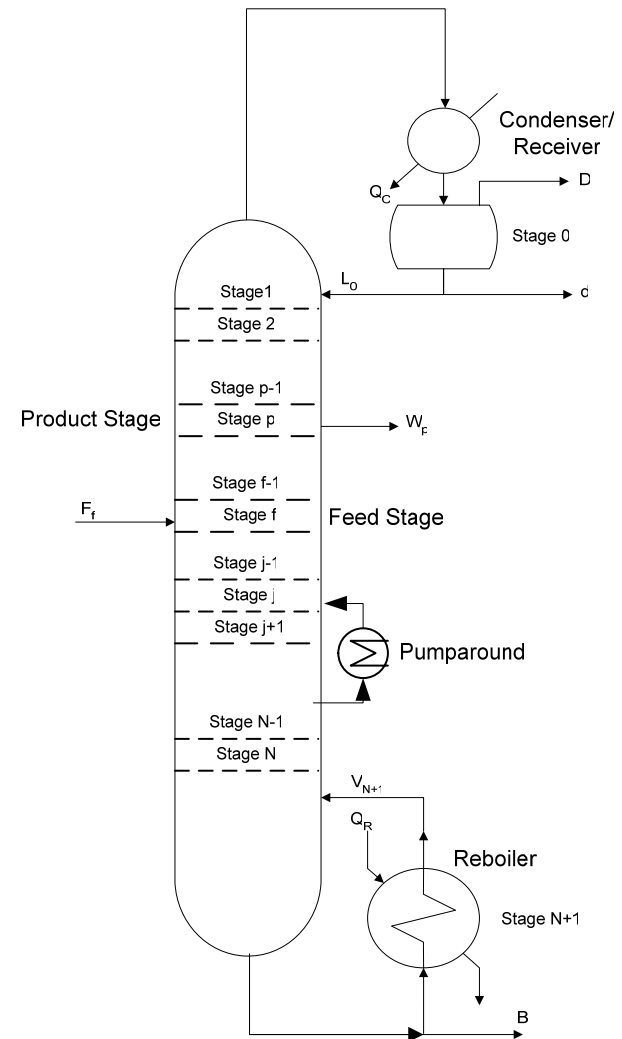
Flow Estimates

- Black-Flow estimates profile
- Red-converged flow profile



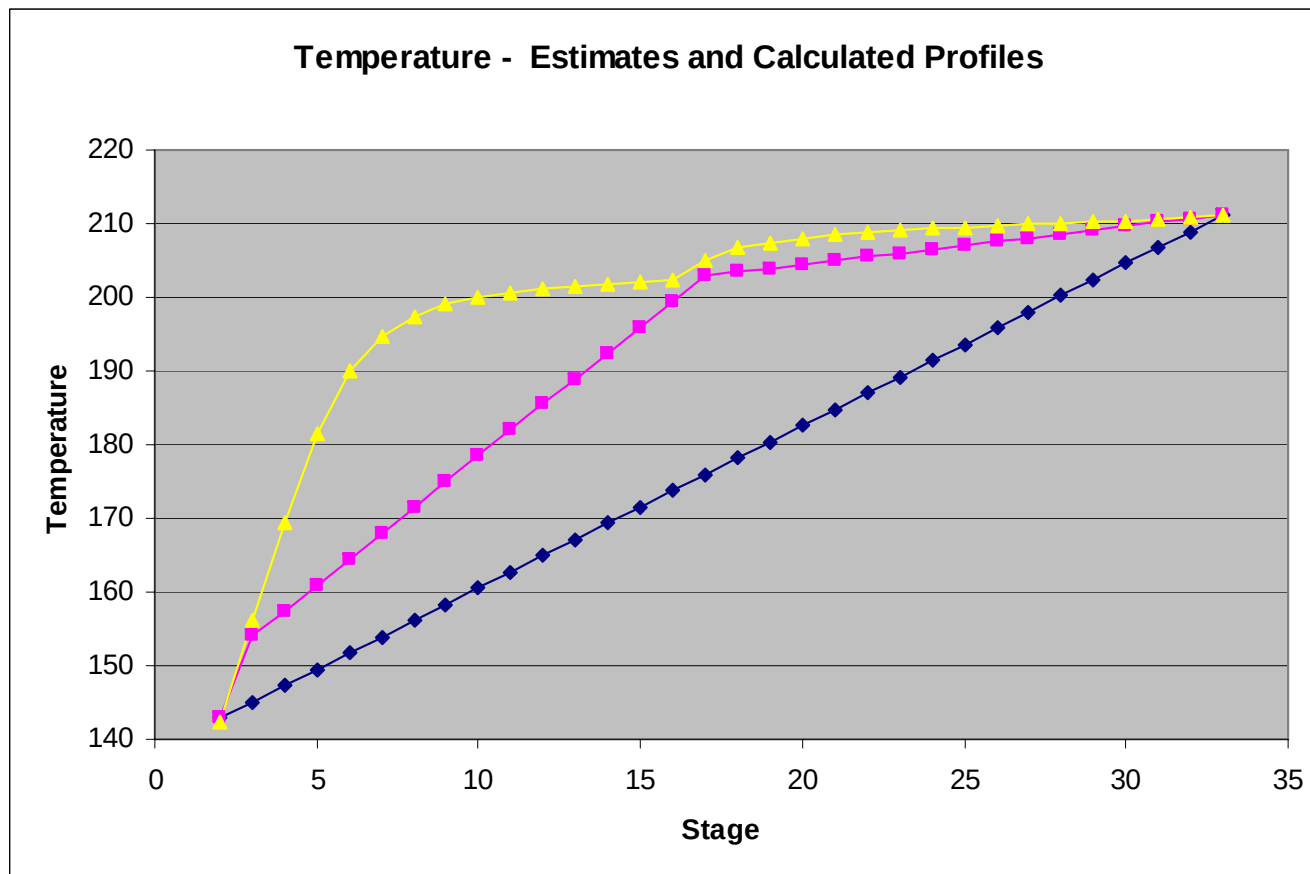
Temperature Estimates

- Good idea for wide boiling feeds such as splitters, de-ethanizers, de-butanizers, etc – great temperature range across the column
- Receiver/Condenser
- Top tray, especially when there is a large overhead vapor product or a subcooled reflux where there will be a large difference between the receiver and top tray
- Feed tray temperature on wide boiler and many light ends leaving top
- If you do the top estimates, you will need to do a bottom/reboiler temperature estimate



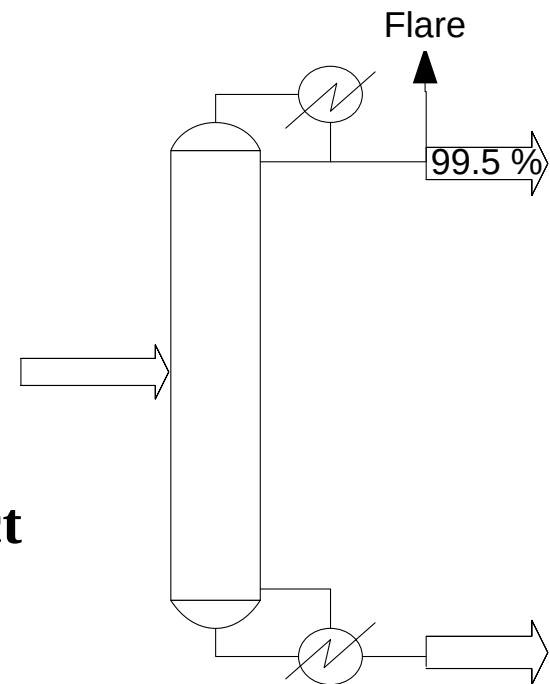
Temperature Estimates

- **Black**-Initial guess with only top and bottom trays estimated
- **Red** – added a guess for the feed tray near that of a slightly vapor feed
- **Yellow** – converged temperature profile



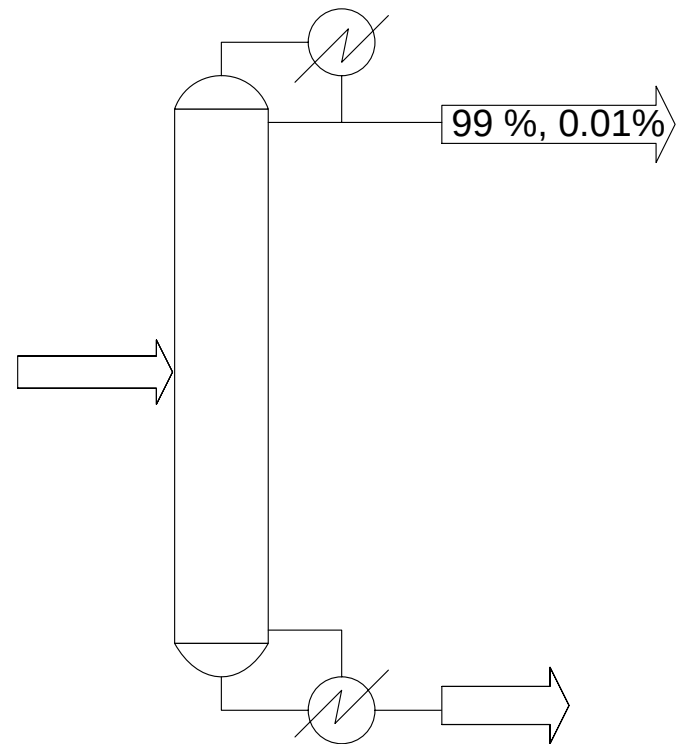
Insensitive to Temperature Specification

- Fixed bubble point temperature on receiver
- High purity overhead in finishing column
- Receiver rides on flare (atmospheric)
- Just like in the field, top temperature is set by the system pressure with a nearly pure component in overhead
- Little freedom of movement in column compositions and rates
- Slight changes in impurities have little effect on temperature
- Can still do sub-cooled reflux which eliminates pure component effect
- Do a recovery or total product flow



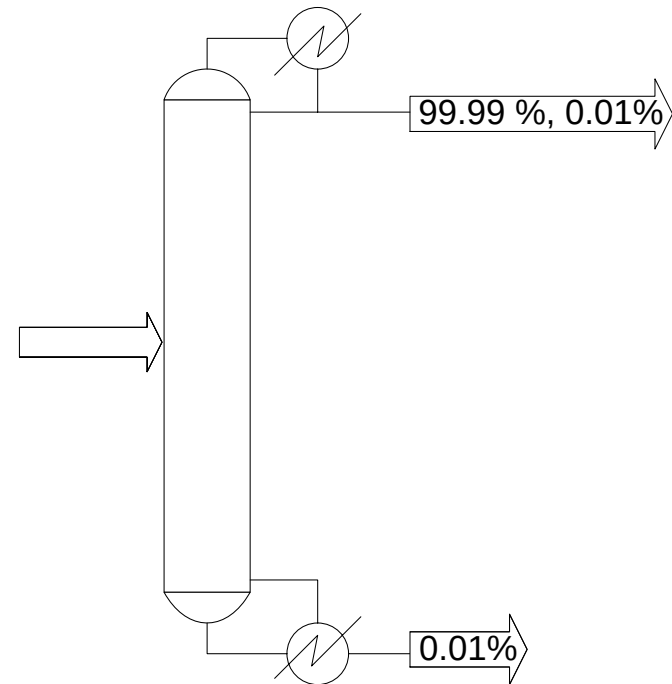
2 Composition Specifications on same product, or same component, different products

- Recovery of a desired component or an undesired to the overhead plus-
- Purity or impurity in the overhead
- Both flow and purity in overhead
- It may meet one spec but miss the other
- Try another combination to the bottom product but avoid using the same component top and bottom to give the program freedom of movement
- Problems are worse with binary splits or split of 2 major components and only a few impurities



Very High Purity or Recovery

- **99.9% of recovery or purity**
- **Freedom of movement in the math is plus of minus 0.05%**
- **Math could lock on 100% of a component during convergence and not move off**
- **Loss of 0.1% in opposite product or impurity of other components may give math more freedom**
- **Avoid impurity of high relative volatility components in overhead with respect to light key**
- **More true if few components, finishing column or sharp split, less for broad mixture**
- **Unrepresentative non-key compounds**



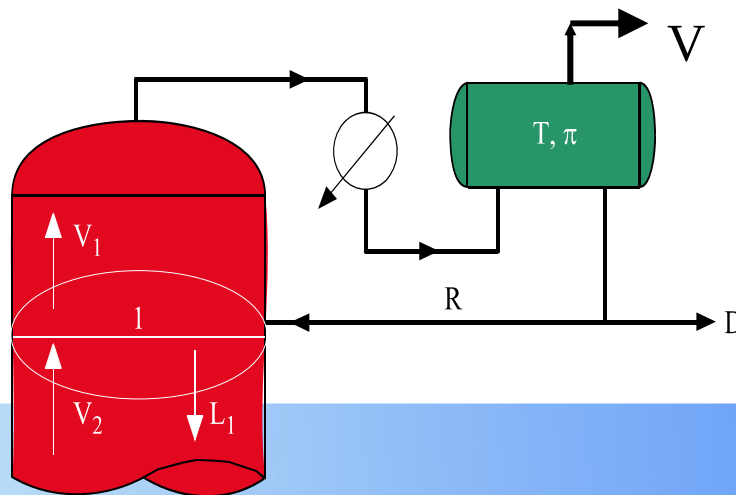
Component Selection

■ Representative Non-Key Component

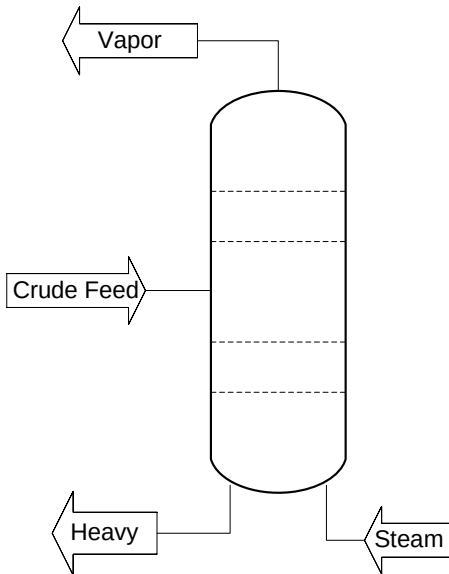
Toluene	231.13 F	65 mole/hr
1,1,2 Trimethylcyclopentane	220.81	Or 200 mole/hr??
1,1,3 Trimethylcyclopentane	236.71	Or 200 mole/hr??
Trans-1,4 Dimethylcyclohexane	246.85	
1,1 Dimethylcyclohexane	247.19	
Cis-1,3 Dimethylcyclohexane	248.16	
1-Methyl-2-ethylcyclopentane	250.74	
Trans-1,2 Dimethylcyclohexane	254.17	
Cis-1,4 Dimethylcyclohexane	255.78	
Isopropylcyclopentane	259.57	
Trans-1,3 Dimethylcyclohexane	265.03	
Cis-1,2 Dimethylcyclohexane	265.62	
Ethylcyclohexane	269.23	Or 200 mole/hr??
Ethylbenzene	277.16	945
Para-xylene	281.05	1015
Meta-xylene	282.42	2550
Ortho-xylene	291.97	1190

Bubble Point Receiver Temperature

- Bubble point receiver but temperature is not specified
- Upper limit on pressure to save on equipment cost
- Given a receiver pressure, a few but significant amount of lights can make for a cold receiver
- Fix a vent rate or limit lights in liquid to get temperature to meet cooling media limits – when vapor & liquid mix well
- At same time, do not fix net vapor rate when little interaction with liquid like in de-_____tanizer



Specifications Insensitive to System



- Specify water purity in the overhead or bottoms

$$K_w = \frac{(1 - X_{hw})P^o}{X_{wh}\pi}$$

- Water K set by partial pressure and solubility
- Little freedom of movement –water is set by the system – nothing to vary to meet a spec on water in the overhead or bottom
- Try a property of the hydrocarbon in the overhead or bottoms

Other Specifications to Avoid

- **Duties and reflux together – energy and internal flows directly effect each other – energy balance has a big affect on rates**
- **Both temperature and product on a stage – only a narrow range of operation – exception is when there is a sub-cooled reflux**
- **Tray temperature specification when goal is product purity – control system may use the tray temperature – works for dynamic system but not steady state simulator – temperature has to be sensitive to composition (and not controlled by pressure)**

Checking Results

- Assume nothing is correct until proven so
- Check the heat balances – feeds, products, duties
- Check the material balances – both mole and mass.
- Make sure products are what you need – trace heavies in the overhead may mean need more stages – or if the mass balance and not number of trays determines impurities in products, may need to try a change in flow sheet
- Re-check input – it may have done what you told it to
- Check profiles – if internal flows are negative, may need to check initialization
- Did not move from initialization – may be insensitive to specifications try something simple such as reflux and product rates

Checking Results

- Check profiles – if rates are huge, may be starting or specified below minimum trays – reflux runs to infinity
- If there is a purity spec, and rates are large, may need to add trays
- If a section has extremely large rates in column with non-condensables, they may be bottled up because the overhead rate is set too low
- Check profiles – if trays dry up, may be starting or specified below minimum reflux – or a composition pinch
- May take away trays, move feed, warm feed, cool feed
- Flat spot in temperature profiles, move feed in that direction

Books

- **Distillation Operation, Henry Z. Kister, McGraw-Hill, 1989, ISBN 0-07-034910-X**
- **Distillation Design, Henry Z. Kister, McGraw-Hill, 1992, ISBN 0-07-034909-6**
- **Distillation Troubleshooting, Henry Z. Kister, Wiley, 1989, ISBN 0-471-46744-8**
- **Distillation Design and Control Using Aspen Simulation, William L. Luyben, Wiley, 2006, ISBN 0-471-77888-5**
- **Equilibrium Stage Separations, Phillip C. Wankat, Elsevier, 1988, ISBN 0-444-01255-9**

Q&A

Questions?
Special topics?