Lecture 13.
# Approximate Multicomponent Methods (1)
[Ch. 9]

- Approximate Methods

- Fenske–Underwood–Gilliland (FUG) Method

- Selection of Two Key Components

- Column Operating Pressure

- Fenske Equation for Minimum Equilibrium Stages

- Distribution of Nonkey Components at Total Reflux

Approximate Methods for Multicomponent Separation

- Use of approximate methods
  - Preliminary design
  - Parametric studies : establish optimal design conditions
  - Process synthesis studies : determine optimal separation sequence
  - Obtaining an initial approximation for a rigorous method

- Fenske-Underwood-Gilliland (FUG) method
  - Approximate method for simple distillation
  - Manual calculation : if physical properties are independent of composition
  - Computer-aided calculation : included in most process design programs
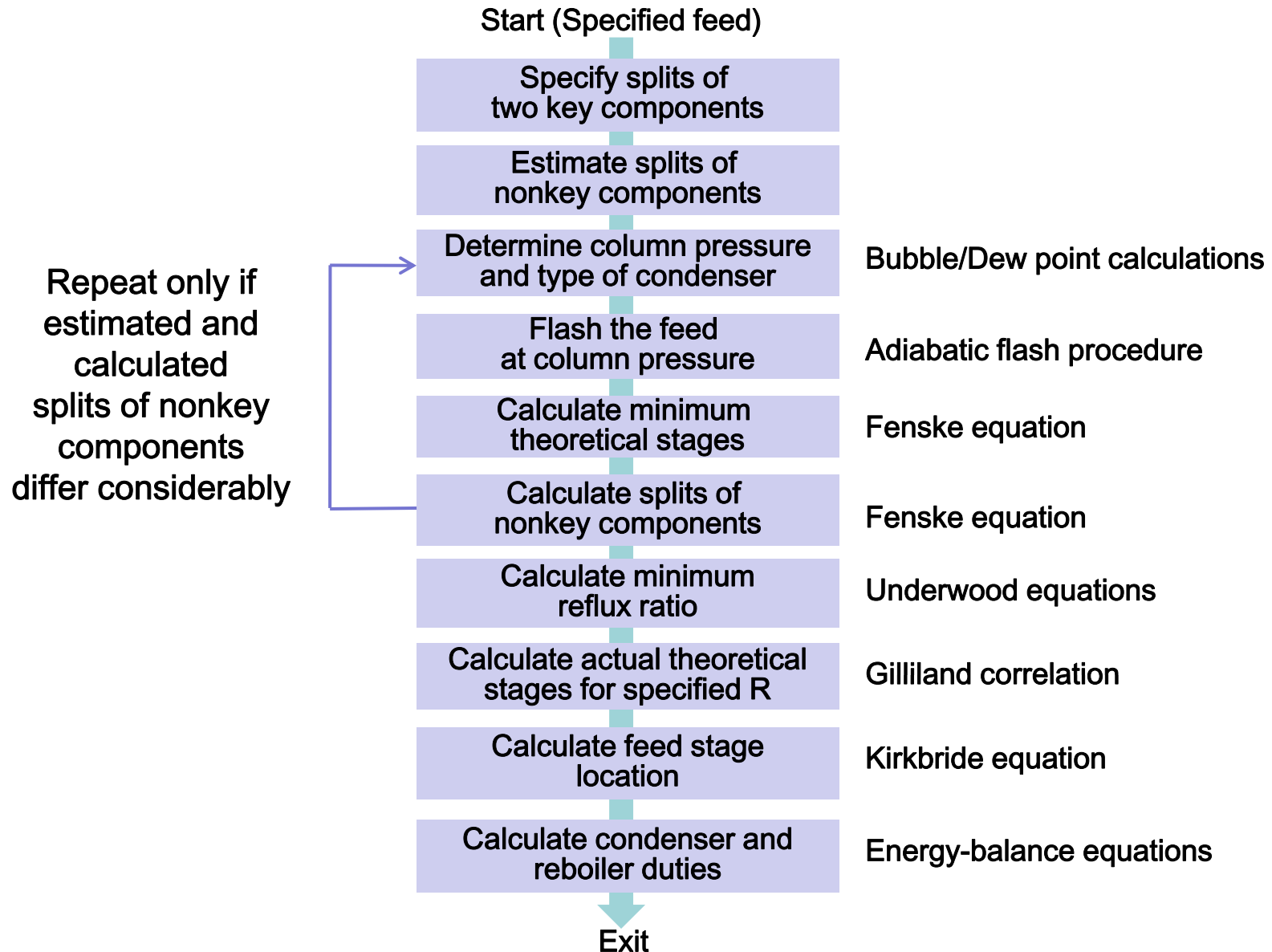
Variable Specification for Distillation

- Distillation with one inlet stream, total condenser, and partial reboiler

No. of specifications
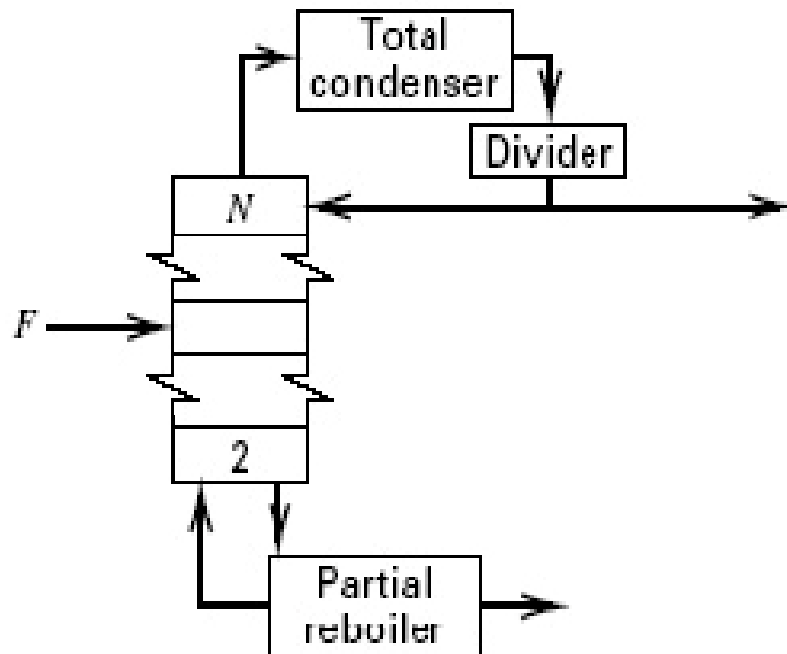
	No. of specifications
Feed flow rate	1
Feed mole fractions	C-1
Feed temperature	1
Feed pressure	1
Adiabatic stages (excluding reboiler)	N-1
Stage pressures (including reboiler)	N
Split of light key component	1
Split of heavy key component	1
Feed stage location	1
Reflux ratio (as multiple of R_{min})	1
Reflux temperature	1
Adiabatic reflux divider	1
Pressure of total condenser	1
Pressure at reflux divider	1
	2N+C+9

Algorithm for FUG Method

Start (Specified feed)

Specify splits of
two key components

Estimate splits of
nonkey components

Repeat only if
estimated and
calculated
splits of nonkey
components
differ considerably

Determine column pressure
and type of condenser — Bubble/Dew point calculations

Flash the feed
at column pressure — Adiabatic flash procedure

Calculate minimum
theoretical stages — Fenske equation

Calculate splits of
nonkey components — Fenske equation

Calculate minimum
reflux ratio — Underwood equations

Calculate actual theoretical
stages for specified R — Gilliland correlation

Calculate feed stage
location — Kirkbride equation

Calculate condenser and
reboiler duties — Energy-balance equations

Exit

Selection of Two Key Components

Isobutane recycle

Component	lbmol/h
nC_4	25

Alkylation reactor effluent → Distillation process

n-Butane product

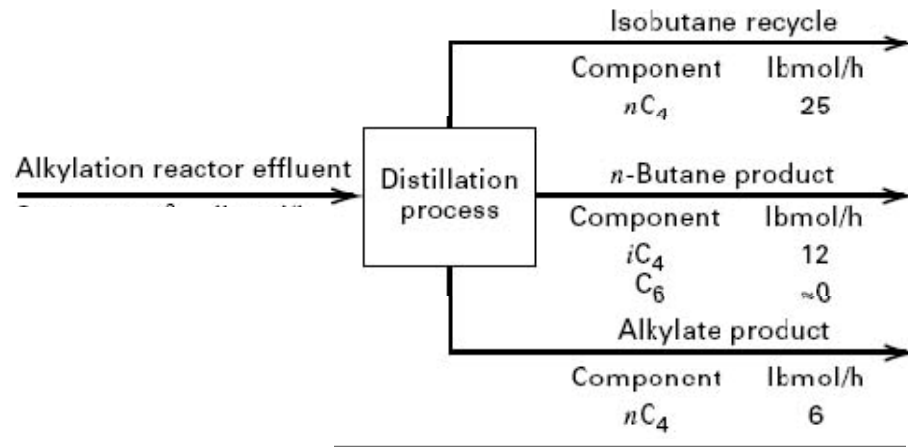| Component	lbmol/h
iC_4	12
C_6	≈0

Alkylate product

Component	lbmol/h
nC_4	6

Selection of distillation columns including a deisobutanizer and a debutanizer

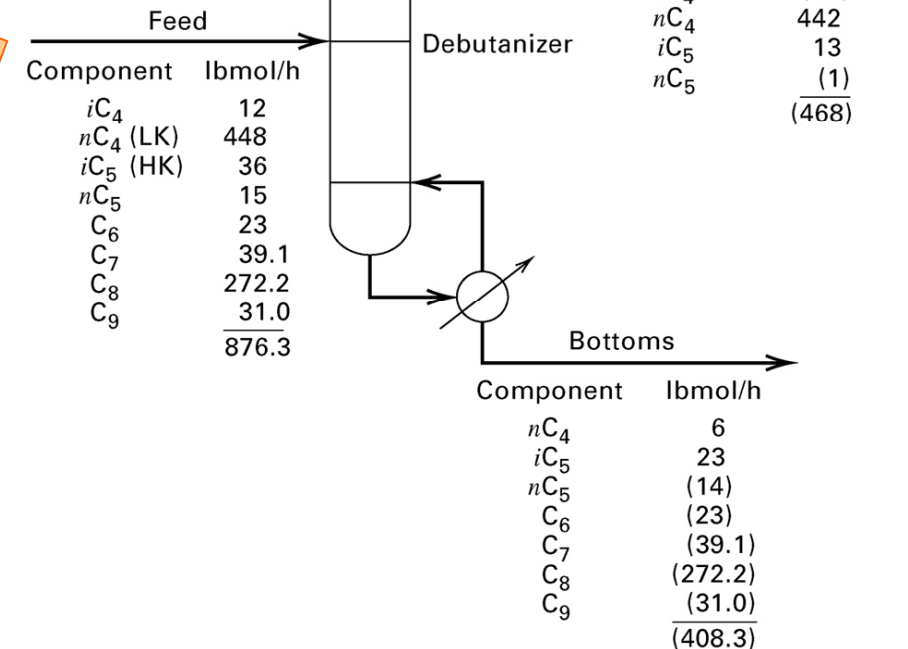| Component	Feed, lbmol/h	Case 1, Deisobutanizer Column First, lbmol/h		Case 2, Debutanizer Column First (iC_5 is HK), lbmol/h		Case 3, Debutanizer Column First (C_6 is HK), lbmol/h	
		Distillate	Bottoms	Distillate	Bottoms	Distillate	Bottoms
C_3	30.7	(30.7)	(0)	(30.7)	(0)	(30.7)	(0)
iC_4	380	368[a]	12[b]	(380.0)	(0)	(380.0)	(0)
nC_4	473	25[b]	448[a]	467[a]	6[b]	467[a]	6[b]
iC_5	36	(0)	(36)	13[b]	23[a]	(13)	(23)
nC_5	15	(0)	(15)	(1)	(14)	(1)	(14)
C_6	23	(0)	(23)	(0)	(23)	0.01[b]	22.99[a]
C_7	39.1	(0)	(39.1)	(0)	(39.1)	(0)	(39.1)
C_8	272.2	(0)	(272.2)	(0)	(272.2)	(0)	(272.2)
C_9	31.0	(0)	(31.0)	(0)	(31.0)	(0)	(31.0)
	1,300.0	423.7	876.3	891.7	408.3	891.71	408.29

Component Splits for Alkylation Reactor Effluent

In practice, the deisobutanizer is usually placed first

Isobutane recycle

Component	lbmol/h
nC_4	25

n-Butane product

Component	lbmol/h
iC_4	12
C_6	≈0

Alkylate product

Component	lbmol/h
nC_4	6

Component	Feed, lbmol/h	Case 1, Deisobutanizer Column First, lbmol/h	
		Distillate	Bottoms
C_3	30.7	(30.7)	(0)
iC_4	380	368[a]	12[b]
nC_4	473	25[b]	448[a]
iC_5	36	(0)	(36)
nC_5	15	(0)	(15)
C_6	23	(0)	(23)
C_7	39.1	(0)	(39.1)
C_8	272.2	(0)	(272.2)
C_9	31.0	(0)	(31.0)
	1,300.0	423.7	876.3

Feed

Component	lbmol/h
iC_4	12
nC_4 (LK)	448
iC_5 (HK)	36
nC_5	15
C_6	23
C_7	39.1
C_8	272.2
C_9	31.0
	876.3

Debutanizer

Distillate

Component	lbmol/h
iC_4	(12)
nC_4	442
iC_5	13
nC_5	(1)
	(468)

Bottoms

Component	lbmol/h
nC_4	6
iC_5	23
nC_5	(14)
C_6	(23)
C_7	(39.1)
C_8	(272.2)
C_9	(31.0)
	(408.3)

Column Operating Pressure

- Factors to determine column pressure

    - Condition of condenser
        - If distillate temperature is less than 120°F (49℃), a refrigerant, rather than cooling water, is used
        - Reflux drum pressure
            - To 215 psia (1.48 MPa): total condenser is recommended
            - 215 psia–365 psia (2.52 MPa): partial condenser is appropriate

    - Condition of reboiler
        - Column bottom temperature should not exceed decomposition or near-critical conditions

    - Pressure drops
        - Condenser: 0–2 psia
        - Column: 5 psia or 0.1 psi/tray

Fenske Equation for Minimum Equilibrium Stages (1)

- Distillation column operation at total reflux

- For steady−state operation without heat loss

(heat input to reboiler)=(heat output from condenser)

- From material balance

$$V_{N-1} = L_N$$

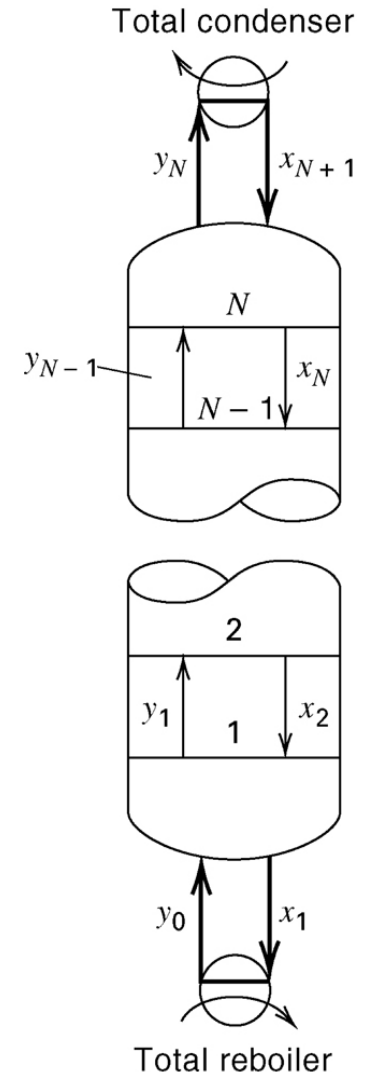$$y_{i,N-1} = x_{i,N}$$

- Equilibrium relations for stage 1

$$y_{i,1} = K_{i,1}x_{i,1}$$

$$x_{i,2} = K_{i,1}x_{i,1}$$

$$y_{i,1} = x_{i,2}$$

- Equilibrium relations for stage 2

$$y_{i,2} = K_{i,2}x_{i,2} = K_{i,2}K_{i,1}x_{i,1}$$

Total condenser

y_N x_{N+1}

N

y_{N-1} x_N

$N-1$

2

y_1 x_2

1

y_0 x_1

Total reboiler

Fenske Equation for Minimum Equilibrium Stages (2)

- Equilibrium relations for stage N

$$y_{i,N} = K_{i,N} K_{i,N-1} \cdots K_{i,2} K_{i,1} x_{i,1}$$

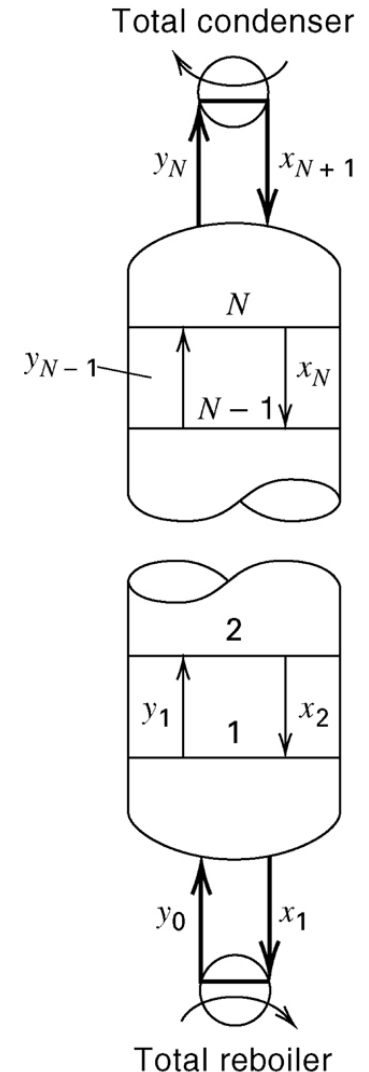$$y_{j,N} = K_{j,N} K_{j,N-1} \cdots K_{j,2} K_{j,1} x_{j,1}$$

$$\frac{y_{i,N}}{y_{j,N}} = \alpha_N \alpha_{N-1} \cdots \alpha_2 \alpha_1 \left(\frac{x_{i,1}}{x_{j,1}} \right)$$

$$y_{i,N} = x_{i,N+1}$$

$$y_{j,N} = x_{j,N+1}$$

$$\left(\frac{x_{i,N+1}}{x_{i,1}} \right) \left(\frac{x_{j,1}}{x_{j,N+1}} \right) = \prod_{k=1}^{N_{\min}} \alpha_k$$

Relative enrichments of any two components i and j over a cascade of N theoretical stages

Fenske Equation for Minimum Equilibrium Stages (3)

- If an average relative volatility is used

$$\left(\frac{x_{i,N+1}}{x_{i,1}}\right)\left(\frac{x_{j,1}}{x_{j,N+1}}\right) = \alpha^N$$

$$N_{min} = \frac{\log\left[\left(\dfrac{x_{i,N+1}}{x_{i,1}}\right)\left(\dfrac{x_{j,1}}{x_{j,N+1}}\right)\right]}{\log \alpha_{i,j}}$$

Fenske equation

- More convenient form using distillate and bottoms flow rates (d and b)

Geometric mean

$$N_{min} = \frac{\log\left[(d_i/d_j)(b_j/b_i)\right]}{\log \alpha_m}$$

$$\alpha_m = \left[(\alpha_{i,j})_N (\alpha_{i,j})_1\right]^{1/2}$$

The Fenske equation is exact only if (1) α does not vary and/or (2) the mixture forms ideal solutions

Distribution of Nonkey Components at Total Reflux

- Once N_{min} is known, the Fenske equation can be used to calculate molar flow rates d and b for nonkey components

$$\left(\frac{d_i}{b_i}\right) = \left(\frac{d_r}{b_r}\right)(\alpha_{i,r})_m^{N_{min}}$$

i : a nonkey component
r : the reference component (or the heavy key component)

$$f_i = d_i + b_i$$

$$\begin{cases} b_i = \dfrac{f_i}{1 + (d_r/b_r)(\alpha_{i,r})_m^{N_{min}}} \\[4mm] d_i = \dfrac{f_i(d_r/b_r)(\alpha_{i,r})_m^{N_{min}}}{1 + (d_r/b_r)(\alpha_{i,r})_m^{N_{min}}} \end{cases}$$