

Separation Network Synthesis: Thermally Integrated Distillation Columns

1 Definition of Index Sets

1. $TASKS = \{t \mid t \text{ is a separation task}\}$
e.g. $TASKS = \{A/BC, AB/C, A/B, B/C\}$
2. $STATES = \{s \mid s \text{ is a state/mixture in the network}\}$
e.g. $STATES = \{ABC, AB, BC, A, B, C\}$
3. $FEED = \text{state that is the feed to the system}$
e.g. $FEED = \{ABC\}$
4. $FS_F = \{\text{columns whose feed is the initial mixture}\}$
e.g. $FS_F = \{A/BC, AB/C\}$
5. $TS_s = \{\text{tasks } t \text{ that state } s \text{ is able to produce}\}$
e.g. $TS_{ABC} = \{A/BC, AB/C\}$
6. $ST_s = \{\text{tasks } t \text{ that are able to produce state } s\}$
e.g. $ST_A = \{A/BC, A/B\}$
7. $PRE_i = \{\text{tasks } t \text{ that produce final product } i \text{ through a rectifying section}\}$
e.g. $PRE_B = \{B/C\}$
8. $PST_i = \{\text{tasks } t \text{ that produce final product } i \text{ through a stripping section}\}$
e.g. $PST_C = \{AB/C, B/C\}$
9. $COMP = \{i \mid i \text{ is a component in the mixture}\}$
e.g. $COMP = \{A, B, C\}$
10. $RECT_s = \{\text{tasks } t \text{ that produce state } s \text{ through a rectifying section}\}$
e.g. $RECT_B = \{B/C\}$
11. $STRIP_s = \{\text{tasks } t \text{ that produce state } s \text{ through a stripping section}\}$
e.g. $STRIP_C = \{AB/C, B/C\}$
12. $ISTATE = \{s \mid s \text{ is an intermediate state in the network}\}$
e.g. $ISTATE = \{AB, BC\}$
13. $IREC_s = \{\text{tasks } t \text{ that produce an intermediate state } s \text{ through a rectifying section}\}$
e.g. $IREC_{AB} = \{AB/C\}$
14. $ISTRIP_s = \{\text{tasks } t \text{ that produce an intermediate state } s \text{ through a stripping section}\}$
e.g. $ISTRIP_{BC} = \{A/BC\}$

15. $LK_t = \{i \mid i \text{ is the light key component in separation task } t\}$
e.g. $LK_{A/BC} = A$
16. $HK_t = \{i \mid i \text{ is the heavy key component in separation task } t\}$
e.g. $HK_{A/BC} = B$
17. $R = \{r \mid r \text{ is an Underwood root}\}$
note: a system with N components will have $N-1$ active Underwood roots
18. $RU A_t = \{\text{active Underwood roots for task } t\}$
e.g. $RU A_{AB/C} = \{r_1, r_2\}$

2 Variables

FT_t, BT_t, DT_t : Total molar flow rates of feed, bottoms, and distillate for task t in units [kmol/hr]

$F_{i,t}, B_{i,t}, D_{i,t}$: Component molar flow rates of feed, bottoms, and distillate for component i and task t in units [kmol/hr]

$V_{r,t}, L_{r,t}$: Total vapor and liquid molar flow rates for rectifying section in units [kmol/hr]

$V_{s,t}, L_{s,t}$: Total vapor and liquid molar flow rates for stripping section in units [kmol/hr]

$N_{min trays,t}$: Minimum number of trays for a separation task t

$Q_{reb,t}, Q_{cond,t}$: Reboiler and condenser heat duties for task t in units [kJ/hr]

$\phi_{r,t}$: Possible active Underwood root r in task t

Y_t : Boolean variable for existence of a separation task t

Z_s : Boolean variable for existence of a heat exchanger for an intermediate state s

W_i : Boolean variable for existence of a heat exchanger for a final state i

3 Parameters

$F_0, F_{i,0}$: Total and component inlet molar flows to system in units of [kmol/hr]

z_i : Molar fraction of component i in feed

α_i : Relative volatility of component i with respect to the least volatile component in the mixture

x_i : specified recovery of component i

λ_i : vaporization enthalpy for species i in units [kJ/mol]

C_{cw}, C_h : utility cost coefficients for cooling and heating

N : estimated life time of equipment in years

i : interest rate on capital

4 Global Constraints

$$\begin{aligned}
\min \quad TAC &= \frac{i(1+i)^N}{(1+i)^N - 1} [Capital\ Costs] + Operating\ Costs \\
s.t. \quad &\sum_{t \in FS_F} FT_k = F_0 \\
&\sum_{t \in FS_F} F_{i,t} = F_{0,i} \quad \forall i \in COMP \\
&\sum_{t \in TS_s} FT_t = \sum_{t \in RECT_s} DT_t + \sum_{t \in STRIP_s} BT_t \quad \forall s \in STATES \\
&\sum_{t \in TS_s} F_{i,t} = \sum_{t \in RECT_s} D_{i,t} + \sum_{t \in STRIP_s} B_{i,t} \quad \forall i \in COMP, \quad \forall s \in STATES \\
&\sum_{t \in TS_s} (V_{r,t} - V_{s,t}) - \sum_{t \in RECT_s} V_{r,t} + \sum_{t \in STRIP_s} V_{s,t} = 0 \quad \forall s \in STATES \\
&\sum_{t \in TS_s} (L_{r,t} - L_{s,t}) - \sum_{t \in RECT_s} L_{r,t} + \sum_{t \in STRIP_s} L_{s,t} = 0 \quad \forall s \in STATES
\end{aligned}$$

5 Column Disjuncts

$$\left[\begin{array}{l}
Y_t \\
FT_t = DT_t + BT_t \\
DT_t + L_{r,t} = V_{r,t} \\
BT_t + V_{s,t} = L_{s,t} \\
FT_t = \sum_{i \in COMP} F_{i,t} = 0 \\
DT_t = \sum_{i \in COMP} D_{i,t} = 0 \\
BT_t = \sum_{i \in COMP} B_{i,t} = 0 \\
\sum_{i \in COMP} \frac{\alpha_i F_{i,t}}{\alpha_i - \phi_r} - (V_{r,t} - V_{s,t}) = 0 \quad \forall r \in RU A_t \\
\sum_{i \in COMP} \frac{\alpha_i D_{i,t}}{\alpha_i - \phi_r} - V_{r,t} = 0 \quad \forall r \in RU A_t \\
\sum_{i \in COMP} \frac{\alpha_i B_{i,t}}{\alpha_i - \phi_r} + V_{s,t} = 0 \quad \forall r \in RU A_t \\
N_{trays,t} = 2 \cdot N_{min\ trays,t} \\
Height_t = f(Diameter, N_{trays}) \\
Area_t = g(\rho_L, \rho_V, V_{r,t}, V_{s,t}, \sigma) \\
Cost_t = h(Diameter, N_{trays}, P)
\end{array} \right] \quad \vee \quad \left[\begin{array}{l}
\neg Y_t \\
FT_t = BT_t = DT_t = 0 \\
F_{i,t} = B_{i,t} = D_{i,t} = 0 \quad \forall i \in COMP \\
V_{r,t} = V_{s,t} = 0 \\
L_{r,t} = L_{s,t} = 0 \\
Area_t = Height_t = N_{trays,t} = 0 \\
Cost_t = 0
\end{array} \right]$$

$\forall t \in TASKS$

6 Intermediate Product Heat Exchanger Disjuncts

$$\left[\begin{array}{l} Q_{cond,t}DT_t = V_{r,t} \sum_{i \in COMP}^{Z_s} \lambda_i D_{i,t} \quad \forall t \in IREC_s \\ Q_{reb,t}BT_t = V_{s,t} \sum_{i \in COMP} \lambda_i B_{i,t} \quad \forall t \in ISTRIP_s \\ Cost_s = f(Area_s, U, \Delta T_{lm}) \end{array} \right] \vee \left[\begin{array}{l} \sum_{t \in TS_s} (V_{r,t} - V_{s,t}) - \sum_{t \in RECT_s}^{Z_s} V_{r,t} + \sum_{t \in STRIP_s} V_{s,t} = 0 \\ \sum_{t \in TS_s} (L_{r,t} - L_{s,t}) - \sum_{t \in RECT_s} L_{r,t} + \sum_{t \in STRIP_s} L_{s,t} = 0 \\ Q_{cond,t} = 0 \quad \forall t \in IRECT_s \\ Q_{rec,t} = 0 \quad \forall t \in ISTRIP_s \\ Cost_s = 0 \end{array} \right]$$

$\forall s \in ISTATE$

7 Final Product Heat Exchanger Disjuncts

$$\left[\begin{array}{l} Q_{cond,t}DT = V_{r,t} \sum_{j \in COMP}^{W_i} \lambda_j D_{j,t} \quad \forall t \in PRE_i \\ Q_{reb,t}BT = V_{s,t} \sum_{j \in COMP} \lambda_j B_{j,t} \quad \forall t \in PST_i \\ Cost_i = f(Area_s, U, \Delta T_{lm}) \end{array} \right] \vee \left[\begin{array}{l} Q_{cond,t} = 0 \quad \forall t \in PRE_i \\ Q_{reb,t} = 0 \quad \forall t \in PST_i \\ Cost_i = 0 \end{array} \right]$$

$\forall i \in COMP$

8 Logical Relations

1. A given state s can give rise to at most one task (i.e. cannot split a stream into two different columns)

$$\sum_{t \in ST_s} Y_t \leq 1 \quad \forall t \in TASKS$$

2. A given state can be produced by at most two tasks; one must be from a rectifying section of a task and one must be from a stripping section of a task

$$\begin{aligned} \sum_{s \in RECT_s} Y_t &\leq 1 \quad \forall s \in STATES \\ \sum_{s \in STRIP_s} Y_t &\leq 1 \quad \forall s \in STATES \end{aligned}$$

3. All products must be produced by at least one task

$$\sum_{t \in (PRE_i \cup PST_i)} Y_t \geq 1 \quad \forall i \in COMP$$

4. Pure product i can only be produced by at most one rectifying section and one stripping section

$$\sum_{t \in PRE_i} Y_t \leq 1 \quad \forall i \in COMP$$

$$\sum_{t \in PST_i} Y_t \leq 1 \quad \forall i \in COMP$$

5. If a given final product is produced by exactly one task, the heat exchanger associated with the state must be selected

$$\left(\sum_{t \in PRE_i} Y_t = 1 \right) \implies W_i \quad \forall i \in COMP$$

$$\left(\sum_{t \in PST_i} Y_t = 1 \right) \implies W_i \quad \forall i \in COMP$$

6. If a given final state is produced by 2 tasks, then there is no heat exchanger associated with the state

$$\left(\bigvee_{t \in PRE_i} Y_t \right) \wedge \left(\bigvee_{t \in PST_i} Y_t \right) \implies \neg W_i \quad \forall i \in COMP$$

7. Cannot have a heat exchanger for an intermediate state if the state is not produced by a task

$$1 - Z_s + \sum_{t \in ST_s} Y_t \geq 1 \quad \forall s \in ISTATE$$

8. Connectivity relation 1 (e.g. the existence of task AB/C implies A/B)

$$Y_t \implies \bigvee_{k \in TS_s} Y_k \quad \forall t \in ST_s$$

9. Connectivity relation 2 (e.g. the existence of task A/B implies AB/C)

$$Y_t \implies \bigvee_{k \in ST_s} Y_k \quad \forall t \in TS_s$$

9 Explanation of Constraints

9.1 Global Constraints

$$1. \quad \sum_{t \in FS_F} FT_k = F_0$$

$$2. \quad \sum_{t \in FS_F} F_{i,t} = F_{0,i} \quad \forall i \in COMP$$

Total and component mass balance for system inlet stream to initial columns

3. $\sum_{t \in TS_s} FT_t = \sum_{t \in RECT_s} DT_t + \sum_{t \in STRIP_s} BT_t \quad \forall s \in STATES$
4. $\sum_{t \in TS_s} F_{i,t} = \sum_{t \in RECT_s} D_{i,t} + \sum_{t \in STRIP_s} B_{i,t} \quad \forall i \in COMP, \quad \forall s \in STATES$
Total and component mass balances on each separation task
(FEED = BOTTOMS + DISTILLATE)
5. $\sum_{t \in TS_s} (V_{r,t} - V_{s,t}) - \sum_{t \in RECT_s} V_{r,t} + \sum_{t \in STRIP_s} V_{s,t} = 0 \quad \forall s \in STATES$
6. $\sum_{t \in TS_s} (L_{r,t} - L_{s,t}) - \sum_{t \in RECT_s} L_{r,t} + \sum_{t \in STRIP_s} L_{s,t} = 0 \quad \forall s \in STATES$
Total mass balances on vapor and liquid flows for a separation task

9.2 Columns

1. $FT_t = DT_t + BT_t$
Total mass balance on column
2. $DT_t + L_{r,t} = V_{r,t}$
Total mass balance on rectifying section of a separation task
3. $BT_t + V_{s,t} = L_{s,t}$
Total mass balance on stripping section of a separation task
4. $FT_t = \sum_{i \in COMP} F_{i,t} = 0$
5. $DT_t = \sum_{i \in COMP} D_{i,t} = 0$
6. $BT_t = \sum_{i \in COMP} B_{i,t} = 0$
Constraints enforcing that component mass balances must sum to total for a given stream
7. $\sum_{i \in COMP} \frac{\alpha_i F_{i,t}}{\alpha_i - \phi_r} - (V_{r,t} - V_{s,t}) = 0 \quad \forall r \in RUA_t$
8. $\sum_{i \in COMP} \frac{\alpha_i D_{i,t}}{\alpha_i - \phi_r} - V_{r,t} = 0 \quad \forall r \in RUA_t$
9. $\sum_{i \in COMP} \frac{\alpha_i B_{i,t}}{\alpha_i - \phi_r} + V_{s,t} = 0 \quad \forall r \in RUA_t$
Underwood equations that act as a shortcut calculation to model column behavior

9.3 Intermediate Product Heat Exchanger

9.4 Final Product Heat Exchanger

1. $Q_{cond,t}DT = V_{r,t} \sum_{j \in COMP} \lambda_j D_{j,t} \quad \forall t \in PRE_i$
Heat duty of the condenser is a function of the vaporization enthalpy of a species (λ_j), the component molar flow of the species in the distillate ($D_{j,t}$), and the vapor flow rate in the rectifying section

$$2. Q_{reb,t}BT = V_{s,t} \sum_{j \in COMP} \lambda_j B_{j,t} \quad \forall t \in PST_i$$

Heat duty of the reboiler is a function of the vaporization enthalpy of a species (λ_j), the component molar flow of the species in the bottoms ($B_{j,t}$), and the vapor flow rate in the stripping section

10 Column Sizing

10.1 Column Area

Calculation procedure from Chapter 9.2 of: Stichlmair, J. G., Klein, H., & Rehfeldt, S. (2021). Distillation Principles and Practice. Newark American Institute Of Chemical Engineers Ann Arbor, Michigan Proquest.

Determination of the column area based on internal molar vapor flow rates, assumed physical properties of sieve tray column, and fixed pressure value for the column.

Input Variables

\dot{V} internal vapor flow rate of column in [kmol/sec]. If rectifying and stripping section vapor flow rates are different, use the greater of the two

\hat{M} molecular weight of input mixture [kg/kmol]

ρ_g density of gas [kg/m³]

ρ_L density of liquid [kg/m³]

σ surface tension [N/m]

Parameters

Assumed to be the same for all columns in the network

$\phi = 0.1$ relative free area of tray

$d_h = 8mm$ diameter of sieve holes in plate

$l_w/D_c = 0.7$ relative weir length

$g = 9.81m/s^2$ gravitational constant

Calculation Procedure:

(1) Maximum gas load: F_{max}

$$F_{max} = 2.5 \cdot (\phi^2 \cdot (\rho_L - \rho_g) \cdot g)^{1/4}$$

(2) Minimum gas load: F_{min}

Have to consider two criteria for minimum gas load in a column: non-uniform gas flow ($F_{min,1}$) and criterion for weeping ($F_{min,2}$). Take the maximum of the two values.

$$F_{min,1} = \phi \cdot \sqrt{2 \cdot \frac{\sigma}{d_h}}$$

$$F_{min,2} = \phi \cdot \sqrt{0.37 \cdot d_h \cdot g \frac{(\rho_L - \rho_G)^{1.25}}{\rho_g^{0.25}}}$$

(3) Column Cross-Sectional Area: A_c

Take the geometric mean of the minimum and the maximum gas load to determine F for the column.

$$u_G = \frac{F}{\sqrt{\rho_G}}$$

$$\dot{V} = \dot{G} \cdot \frac{\dot{M}}{\rho_G}$$

$$A_{ac} = \frac{\dot{V}}{u_G}$$

column cross section is given by:

$$A_c = A_{ac} + 2 \cdot A_d$$

area of the downcomer calculated by:

$$\frac{A_{ac}}{A_c} = 1 - \frac{2}{\pi} \cdot [\arcsin(\frac{l_w}{D_c} - \sqrt{(\frac{l_w}{D_c})^2 - (\frac{l_w}{D_c})^4}]$$

above equation allows calculation of the cross-sectional area $A_c [m^2]$

10.2 Tray Number and Height

The minimum number of trays needed for a separation task is determined using the Fenske equation based on the relative volatilities of the light key and heavy key components for that task. The actual number of trays used is twice the minimum tray number ($N_{trays} = 2 \cdot N_{trays,min}$). Empirical correlation for height per trays from Ch 4 of Ulrich, G. D., & Vasudevan, P. T. (2004). Chemical engineering process design and economics : a practical guide. Durham Process Publishing Cop.

Input Variables

x_i desired recovery fraction

α_i relative volatility for species i

D column diameter [m]

(1) Fenske Equation

$$N_{trays,min} = \frac{\log\left(\frac{x_i^2}{(1-x_i)^2}\right)}{\log\left(\frac{\sum_{i \in LK_k} \alpha_i}{\sum_{i \in HK_k} \alpha_i}\right)}$$

$$N_{trays} = 2 \cdot N_{trays,min}$$

(2) Column Height

$$\begin{aligned} \text{Height per tray: } H_t &= 0.5D^{0.3} \\ \text{Column Height: } Height &= H_t \cdot N_{trays} \end{aligned}$$

11 Calculation of Capital Cost

Calculation procedure from Chapter 7 of: Turton, R., & Al, E. (2009). Analysis, Synthesis, and Design of Chemical Processes. Prentice Hall.

11.1 Tower Capital Cost

Input Variables

D column diameter [m]

H column height [m]

P gauge pressure of the column [barg]

Parameters

Assumed to be the same for all columns in the network

$CI_{2004} = 444.2$ Cost index from the Chemical Engineering Plant Cost Index (CEPCI) for the year 2004 (year reference values were collected)

$CI_{2020} = 596.2$ CEPCI value for year 2020

K_1, K_2 empirical cost correlation parameters for tray and packed tower

$$K_1 = 5307$$

$$K_2 = 603.8$$

B_1, B_2 bare module factors vertical process vessels

$$B_1 = 2.25$$

$$B_2 = 1.72$$

$F_M = 1$ material factor for a carbon steel vertical vessel

$CA = 0.00315$ corrosion allowance value

$t_{min} = 0.0063$ minimum vessel thickness

Calculation Procedure:

(1) Cost correlation: C_p^0

$$C_p^0 = K_1 + K_2 A$$

A is the size factor of the equipment. For vertical process vessels (towers) use the vessel volume.

(2) Pressure factor: $F_{P,vessel}$

$$F_{P,vessel} = \frac{\frac{(P+1)D}{(2)(944)(0.9)-1.2(P+1)} + CA}{t_{min}}$$

(3) Bare Module Cost: C_{BM}

$$C_{BM} = C_p^0 F_{BM} = C_p^0 (B_1 + B_2 F_M F_P)$$

(4) Inflation Calculation: $C_{p,2020}$

$$C_{tower,2020} = \frac{CI_{2020}}{CI_{2004}} \cdot C_{BM}$$

11.2 Tray Capital Cost

Input Variables

N_{trays} number of trays in column

Parameters

Assumed to be the same for all columns in the network

$CI_{2004} = 444.2$ Cost index from the Chemical Engineering Plant Cost Index (CEPCI) for the year 2004 (year reference values were collected)

$CI_{2020} = 596.2$ CEPCI value for year 2020

K_1, K_2, K_3 empirical cost correlation parameters for sieve trays

$$K_1 = 571.1$$

$$K_2 = 406.8$$

$$K_3 = 38$$

$F_M = 1$ material factor for carbon steel sieve and valve trays

$f_q = 1$ quantity factor for trays for empirical relation

Calculation Procedure:

(1) Cost correlation: C_p^0

$$C_p^0 = K_1 + K_2 A + K_3 A^2$$

A is the size factor of the equipment. Use the area of the column for tray cost calculation.

(2) Bare Module Cost: C_{BM}

$$C_{BM} = C_p^0(N_{trays})(F_{BM})(f_q)$$

(3) Inflation Calculation: $C_{p,2020}$

$$C_{trays,2020} = \frac{CI_{2020}}{CI_{2004}} \cdot C_{BM}$$

11.3 Total Columns Capital Cost

$$Cost_{column} = Cost_{tower} + Cost_{trays}$$

12 Heat Exchanger Sizing and Costing

Calculation procedure from Chapter 4 of: Ulrich, G. D., & Vasudevan, P. T. (2004). Chemical engineering process design and economics. Durham Process Publishing Corp.

Determination of heat exchanger area based on required heat flow rate, overall heat transfer coefficient, and delta log mean temperature difference.

Values for overall heat transfer coefficient (U) from Ulrich table 4-15a.

Input Variables

$\dot{Q}_{reb/cond}$ Heat flow rate for exchanger (condenser or reboiler) in [kJ/sec]

$\Delta T_{LM} = \frac{\Delta T_h = \Delta T_c}{\ln(\frac{\Delta T_h}{\Delta T_c})}$ log mean temperature difference for the fluids in the exchanger

Parameters

$U_{reboiler} = 700 [J/m^2 sec K]$ overall heat transfer coefficient for hot side fluid of condensing steam and cold side fluid of low viscosity liquid hydrocarbons

$U_{condenser} = 150 [J/m^2 sec K]$ overall heat transfer coefficient for hot side fluid of hydrocarbon gases and cold side fluid of liquid water

$F_m = 1$ material factor for carbon steel construction heat exchanger

$F_p = 1$ pressure factor for exchanger operating below a pressure of 10 barg

$C_{reboiler}^0 = \$20,000$ base purchase price for kettle reboiler with $100 m^2$ exchange area with CEPCI = 400

$C_{condenser}^0 = \$15,000$ base purchase price for floating head shell and tube heat exchanger with $100 m^2$ exchange area with CEPCI = 400

$n = 0.6$ scaling exponent for equipment

Calculation Procedure:

(1) Area of exchanger

$$\begin{aligned} \text{Unit conversion to [J/sec]: } \dot{Q}_{reb/cond} &= \dot{Q}_{reb/cond} \cdot 1000 \\ \text{Area} &= \frac{\dot{Q}}{U \Delta T_{LM}} \quad [m^2] \end{aligned}$$

(2) Cost of exchanger

Determine K values for reboiler and condenser based on given data (Ulrich 5.36) for a carbon steel exchanger with $100 m^2$ of exchange area

$$K_{reboiler} = \frac{C_{reboiler}^0}{(100 m^2)^n}$$

$$K_{condenser} = \frac{C_{condenser}^0}{(100 m^2)^n}$$

Cost for each exchanger(reboiler / condenser) is then determined by:

$$Cost_{reboiler} = \frac{CI_{2020}}{CI_{2004}} (K_{reboiler} Area^n)$$

$$Cost_{condenser} = \frac{CI_{2020}}{CI_{2004}} (K_{condenser} Area^n)$$

13 System Capital Costs

$$\begin{aligned} CAPEX &= \sum_{t \in TASKS} Cost_{Column_t} + \sum_{i \in COMP} Cost_{Final\ Heat\ Exchangers_i} \\ &\quad + \sum_{s \in ISTATE} Cost_{Intermediate\ Heat\ Exchangers_s} \end{aligned}$$

14 Operating Costs

Input Variables

$Q_{reb,t}$ reboiler heat duty

$Q_{cond,t}$ condenser heat duty

Parameters

C_{cw} Cost coefficient for cooling utility (cooling water) [\$/kJ]

C_H Cost coefficient for heating utility (steam) [\$/kJ]

$$OPEX = \sum_{t \in TASKS} C_{cw} Q_{cond,t} + C_h Q_{reb,t}$$