Electronic Supplementary Material

Optimal design of extractive dividing-wall column using an efficient equation-oriented approach

Yingjie Ma[1], Nan Zhang[1], Jie Li (✉)[1], Cuiwen Cao[2]
1 Centre for Process Integration, Department of Chemical Engineering and Analytical Science, School of Engineering, The University of Manchester, Manchester M13 9PL, UK
2 Key Laboratory of Advanced Control and Optimization for Chemical Processes, Ministry of Education, East China University of Science and Technology, Shanghai 200237, China

E-mail: Jie.li-2@manchester.ac.uk

Appendix A: Steady-state distillation model with bypass efficiency

The MESH equations of steady-state distillation model is as eqs. (A1–A4).

Material balance equation is:

$$0 = V^{j+1}y_i^{j+1} + L^{j-1}x_i^{j-1} - V^{j,eq}y_i^{j,eq} - L^{j,eq}x_i^{j,eq} \quad i \in I, j \in J, \quad \text{(A1)}$$

where I and J are the sets of all components and stages respectively. The stages are numbered from top to bottom. V^{j+1} and y_i^{j+1} are the flow rate and molar composition of the vapor stream entering a stage j, while L^{j-1} and x_i^{j-1} are the flow rate and molar composition of the liquid stream entering the stage. $V^{j,eq}$, $y_i^{j,eq}$ and $L^{j,eq}$, $x_i^{j,eq}$ are flow rate and molar composition of vapor stream and liquid stream in phase equilibrium respectively.

Enthalpy balance equation is:

$$0 = V^{j+1}h_V^{j+1} + L^{j-1}h_L^{j-1} - V^{j,eq}h_V^{j,eq} - L^{j,eq}h_L^{j,eq} \quad j \in J, \quad \text{(A2)}$$

Here, h_V and h_L are vapor specific molar enthalpy and liquid specific molar enthalpy respectively.

Phase equilibrium equation is:

$$y_i^{j,eq} = k_i^j x_i^{j,eq} \quad i \in I, j \in J, \quad \text{(A3)}$$

where k_i^j is phase equilibrium constant, which is a function of temperature, pressure and vapor and liquid composition on stage j.

The summations of vapor and liquid molar fractions both need to be 1, leading to the summation equation:

$$\sum_{i \in I} x_i^j = 1, \quad \sum_{i \in I} y_i^j = 1 \quad j \in J. \quad \text{(A4)}$$

The vapor and liquid streams leaving a stage are got according to the bypass efficiency method [26], as shown in Fig. A1. In the model, a part of the inlet vapor (liquid) stream V^{j+1} (L^{j-1}) feeds to the stage, while the other part of the stream bypasses the stage. The streams entering into the stage j reach to phase equilibrium, getting $V^{j,eq}$ and $L^{j,eq}$. The vapor and liquid streams leaving the stage, V^j and L^j are the mixing of the bypass streams and equilibrium streams. The equations for bypass efficiency method are as Eqs. A5–A10.

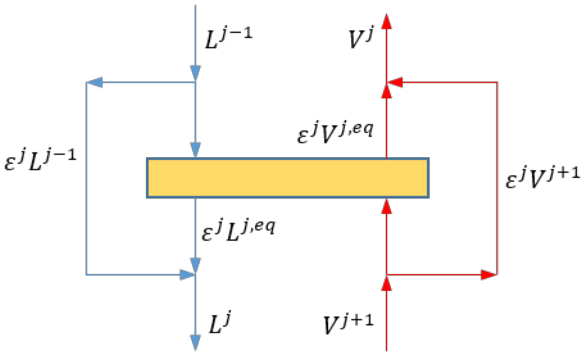

Fig. A1 Equilibrium stage applied with bypass efficiency method

$$V^{j} = \varepsilon^{j}V^{j,eq} + (1-\varepsilon^{j})V^{j+1} \qquad j \in J \ , \tag{A5}$$

$$L^{j} = \varepsilon^{j}L^{j,eq} + (1-\varepsilon^{j})L^{j-1} \qquad j \in J, \tag{A6}$$

$$y_i^{j,eq} = \varepsilon^{j}y_i^{j,eq} + (1-\varepsilon^{j})y_i^{j+1} \qquad i \in I, j \in J \ , \tag{A7}$$

$$x_i^{j,eq} = \varepsilon^{j}x_i^{j,eq} + (1-\varepsilon^{j})x_i^{j-1} \qquad i \in I, j \in J \ , \tag{A8}$$

$$h_V^{j} = \varepsilon^{j}h_V^{j,eq} + (1-\varepsilon^{j})h_V^{j+1} \qquad j \in J \ , \tag{A9}$$

$$h_L^{j} = \varepsilon^{j}h_L^{j,eq} + (1-\varepsilon^{j})h_L^{j-1} \qquad j \in J. \tag{A10}$$

where ε^{j} is the bypass efficiency on stage j, which is a continuous variable between 0 and 1.

Appendix B: Economic evaluation model and parameters

The *TAC* include capital cost (CAP_{cost}), energy cost (OPE_{cost}), as shown in Eq. (B1). All the costs are in the unit of \$ or \$·year^{-1}. The payback period is 3 years.

$$TAC = \frac{CAP_{cost}}{3} + OPE_{cost} \ , \tag{B1}$$

where CAP_{cost} is composed of column cost (COL_{cost}), heat exchanger cost (HX_{cost}) and compressor cost ($COMP_{cost}$) where COL_{cost} includes both column shell cost (SH_{cost}) and column tray cost ($TRAY_{cost}$).

$$CAP_{cost} = COL_{cost} + HX_{cost} + COMP_{cost} \ , \tag{B2}$$

$$COL_{cost} = SH_{cost} + TRAY_{cost} \ , \tag{B3}$$

The calculation of these costs are according to formulas in the book of Luyben [36], where SH_{cost} (\$) is:

$$\mathrm{SH_{cost}} = 17640 D^{1.066} H^{0.802} \ , \tag{B4}$$

Here, D (m) and H (m) are column diameter and column height respectively. H is calculated according to the total number of stages *NT*,

$$H = 1.2NT \cdot h_s \ , \tag{B5}$$

Here, h_s is the tray space, which is 0.61 m in this work. The column diameter is the maximum diameter among all the diameters of trays. A diameter of a tray d_j (m) is:

$$d_j = \sqrt{\frac{4 \cdot Vs_j}{\pi u_j}} \ , \tag{B6}$$

where Vs_j (m^3) and u_j (m·s^{-1}) are the volume flow rate and velocity of vapor stream leaving stage j respectively. Note that, the column diameter is usually determined by the diameter of one specific column section, while the diameter of a column section is usually determined by the diameter of the bottom tray. Thus, for the simplification, in example 1, the maximum tray diameter in column section 5 is taken as column diameter, whilst in examples 2 and 3, the column diameter is got from the quadratic mean diameter of the diameters of the last trays in column section 3 and 4. u_j is from

$$F = 0.8197 u_j \rho_j^{0.5} , \quad \text{(B7)}$$

where ρ_j (kg·m^{-3}) is the mass density of the vapor stream. F is the F factor, which is set to be 1 according to heuristic [35].

The column tray cost is:

$$TRAY_{cost} = 229 D^{1.55} NT \ , \quad \text{(B8)}$$

The heat exchanger cost is:

$$HX_{cost} = 7296 A^{0.65} \ , \quad \text{(B9)}$$

where A (m^2) is heat exchanger area got from

$$A = \frac{Q}{U \Delta T_m} \ , \quad \text{(B10)}$$

Here, Q (kW) is heat duty of heat exchanger, U (kW·m^{-2}·K^{-1}) is heat transfer coefficient and ΔT_m (°C) is logarithm mean temperature. The heat transfer coefficients for cooler and condenser are both 0.852 kW·m^{-2}·K^{-1}, while the U of reboiler is 0.568 kW·m^{-2}·K^{-1}. The heat transfer coefficient of process-process heat exchangers is 0.43 kW·m^{-2}·K^{-1}.

The centrifugal compressor is used, which is calculated from Eq. (B11) according to the work of Luo et al. [23].

$$COMP_{cost} = (1463.2/280)(664.1 W^{0.65}) \ . \quad \text{(B11)}$$

where W is the compressor power (kW). The prices of middle pressure steam and high pressure steam are 5.4 and 6.1 \$·GJ^{-1}, respectively and the price of cooling water is 0.54 \$·GJ^{-1}. The electricity price is assumed to be three times of the high pressure steam, so it is 18.3 \$·GJ^{-1}. The prices of entrainers DMSO and EG are 1557 and 1300 \$·ton^{-1} respectively.

Appendix C: PTC distillation model

The PTC distillation model is from the work of Ma et al. [17]. It is briefly described as followings.Material balance equation is:

$$\frac{dM_i^j}{dt} = V^{j+1} y_i^{j+1} + L^{j-1} x_i^{j-1} - V^{j,eq} y_i^{j,eq} - L^{j,eq} x_i^{j,eq} \qquad i \in I, j \in J \ , \quad \text{(C1)}$$

where M_i^j is component hold-up on stage j. The other notations in the equation have the same meaning as those in Appendix A.

Enthalpy balance equation is:

$$\frac{dH^j}{dt} = V^{j+1} h_V^{j+1} + L^{j-1} h_L^{j-1} - V^{j,eq} h_V^{j,eq} - L^{j,eq} h_L^{j,eq} \qquad j \in J \ , \quad \text{(C2)}$$

Here, H is the total hold-up enthalpy. The phase equilibrium equation and summation equations are the same as Eqs. (A3–A4). M_i^j and H^j are calculated from the following equations,

$$M_i^j = M_L^j x_i^{j,eq} + M_V^j y_i^{j,eq} \qquad i \in I, j \in J, \quad \text{(C3)}$$

$$H^j = M_L^j h_L^{j,eq} + M_V^j h_V^{j,eq} \qquad j \in J, \quad \text{(C4)}$$

Here, M_L^j, M_V^j are liquid molar hold-up and vapour molar hold-up on stage j respectively, which are calculated from the pseudo hydraulic correlation Eqs. B5–B6.

$$L^{j,eq} = C_L M_L^j \qquad j \in J, \quad \text{(C5)}$$

$$V^{j,eq} = C_V M_V^j \qquad j \in J. \quad \text{(C6)}$$

Here, C_L, C_V are two constant coefficients, which are both set to be 1800 h^{-1} according to our computational experience.The vapour and liquid streams leaving a stage are also got according to the bypass efficiency method [26] as with Eqs. (A5–A10).