Electronic Supplementary Material

A novel method for generating distillation configurations

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The total annual cost (TAC) is used as the objective function in the optimization. It was calculated by applying Eq. (A-1):

$$\mathrm{TAC} = \frac{C_{cap}}{Y_{back}} + C_{energy} \tag{A-1}$$

In Eq. (A-1), C_{cap} is the total capital cost and C_{energy} is the energy cost. Y_{back} represents the payback period. The capital cost is the sum of the capital cost of the columns, condensers, and reboilers in the configurations, as represented by Eq. (A-2).

$$C_{cap} = C_{col,cap} + C_{hx,cap} \tag{A-2}$$

For the column capital cost, we only consider the vessel cost. All the capital costs were calculated according to Eqs. (A-3)−(A-8) from Luyben's book [25].

$$C_{cap} = C_{col,cap} + C_{hx,cap} \tag{A-2}$$

$$C_{col,cap} = 17{,}640\, D^{1.066} L^{0.802} \tag{A-3}$$

$$C_{hx,cap} = 7296\, A^{0.65} \tag{A-4}$$

$$\mathrm{A} = \frac{Q}{U \Delta T_{mean}} \tag{A-5}$$

$$\mathrm{D} = \max\left(\sqrt{\frac{V_{g,1}}{\frac{\pi}{4} u_1}}, \sqrt{\frac{V_{g,2}}{\frac{\pi}{4} u_2}}, \dots, \sqrt{\frac{V_{g,j}}{\frac{\pi}{4} u_j}}, \dots, \sqrt{\frac{V_{g,Ns}}{\frac{\pi}{4} u_{Ns}}} \right) \quad j = 1,2,\dots,Ns \tag{A-6}$$

$$\mathrm{L} = 1.2 \times 0.61\mathrm{Ns} \tag{A-7}$$

$$\mathrm{F} = 0.8197 u_j \sqrt{\rho_{v_j}} \qquad \mathrm{j} = 1,2,\dots,\mathrm{Ns} \tag{A-8}$$

In Eqs. (A-3)−(A-8), A and U are the heat exchanger area and heat transfer coefficient of the condensers and reboilers, respectively. D, L, and Ns represent the diameter, height, and total stage number of the columns, respectively. $V_{g,j}$, u_j, and ρ_{v_j} refer to the vapor volume flow rate, maximum vapor velocity, and vapor mass density at each stage, respectively. To calculate the

maximum vapor velocity in Eq. (A-8), the F factor is used; F is set to 1 $kg^{0.5}\cdot m^{0.5}$ s, according to the approximate heuristic. The variable ΔT_{mean} is used to estimate the logarithmic mean temperature difference to avoid numerical difficulty. The relevant equations is represented by Eq. (A-9).

$$\Delta T_{mean} = \left[\frac{(T_{hot}^{in} - T_{cold}^{out})(T_{hot}^{out} - T_{cold}^{in})(T_{hot}^{in} - T_{cold}^{out} + T_{hot}^{out} - T_{cold}^{in})}{2}\right]^{\frac{1}{3}} \quad \text{(A-9)}$$

For all the variables in Eqs. (A-3)−(A-9), SI units are used.