Supporting information for

From batch to continuous sustainable production of 3-methyl-3-penten-2-one for synthetic ketone fragrances

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Details about TAC calculation

TAC includes TCC and TOC. The TCC estimation follows the procedure of Douglas [1]. To calculate TCC, the equipment size should be known.

1. Equipment size

1.1 Condenser heat-transfer area (A_C)

$$A_C = \frac{Q_C}{U_C \times \Delta T_C}$$

Q_C (kW) is the condenser heat duty. The overall heat-transfer coefficient U_C is set as 0.852 kW/K·m^2. ΔT_C (K) is the temperature difference in the condenser. The inlet and outlet temperatures of cooling water are set as 298 K and 308 K, respectively.

1.2 Reboiler heat-transfer area (A_R)

$$A_R = \frac{Q_R}{U_R \times \Delta T_R}$$

Q_R (kW) is the reboiler heat duty. The overall heat-transfer coefficient U_R is set as 0.568 kW/K·m^2. ΔT_R (K) is the temperature difference in the reboiler, which is heated by water vapor.

1.3 Column diameter (D)

In this work, the column diameter is calculated by using the tray sizing tool in Aspen Plus.

1.4 Column length (L)

$$L = 0.609 N_T + 3$$

Total number of stage N_T is necessary for the calculation of L (m). 0.609 m is the tray spacing, and 3 is the height for distributor et al.

2. Equipment TCC ($)

All equipment materials are carbon steel. The TCC of each piece of equipment is calculated as follows.

2.1 Column shell cost

$$\text{Shell cost} = \left(\frac{M\&S}{280}\right)\times\left(101.9\times D^{1.066}\times L^{0.802}\right)\times\left(2.18+F_C\right)=15642.5\times D^{1.066}\times L^{0.802}$$

Marshall & Swift index ($M\&S$) of 1468.8 in 2019 is used in the calculation. F_C = $F_M F_P$, where F_M and F_P are the equipment material and pressure coefficients, respectively. Since the carbon steel is chosen as equipment material, F_M = 1. All the columns is operated at atmosphere pressure, so F_P = 1.

2.2 Column tray cost

$$\text{Tray cost} = \left(\frac{M\&S}{280}\right)\times\left(4.7\times D^{1.55}\times L\times F_C\right)=510.2\times D^{1.55}\times L$$

$F_C = F_S + F_T + F_M$, where F_S = 1, F_T = 0, and F_M = 0 are the tray spacing, tray type and equipment material coefficients, respectively.

2.3 Heat exchanger cost

$$\text{HX cost} = \left(\frac{M\&S}{280}\right)\times\left(101.3\left(A_R^{0.65}+A_C^{0.65}\right)\right)\times\left(2.29+F_C\right)=9064.1\times\left(A_R^{0.65}+A_C^{0.65}\right)$$

$F_C = (F_D + F_P)F_M$, where reboiler type coefficient F_D is 1.35 when the Kettle reboiler is used. F_M = 1, and F_P = 0.

2.4 Reactor or tank cost

$$\text{Reactor cost} = \left(\frac{M\,\&\,S}{280}\right) \times \left(101.9 \times D^{1.066} \times L^{0.802}\right) \times \left(2.18 + F_C\right) = 15642.5 \times D^{1.066} \times L^{0.802}$$

$F_C = F_M F_P$

3. TOC ($/year)

TOC consists of steam cost, cooling water cost and electricity cost:

$$TOC = \left(Q_R \cdot C_S + Q_C \cdot C_{CW} + Q_E \cdot C_E\right) \times 8000$$

Q_R and Q_C represent the reboiler and condenser heat duties with the unit of GJ/h, respectively. The electricity consumption for the stirrer of BSTR is calculated by:

$$Q_E = \frac{N_P \rho N_i^3 D^5}{277.78}$$

where, N_P = 0.35, ρ (kg/m^3) is liquid density, N_i (s^{-1}) is the stirring speed, and coefficient 277.78 is to change the unit from kw to GJ/h. 8000 (h/year) is the annual working hour. The prices of heating stream, cooling water, and electricity C_S, C_C, and C_E are listed as follows:

Low pressure stream (433 K): $7.78 per GJ;

Middle pressure stream (457 K): $8.22 per GJ;

High pressure stream (527 K): $9.88 per GJ;

Cool water (298.15 K): $0.354 per GJ;

Electricity: $ 16.8 per GJ;

REFERENCE

[1] Douglas, JM. Conceptual Design of Chemical Process, New York: McGraw-Hill; 1988.