Additional Material

“Thermodynamic Equations and Calculation Method for Techno-economic Analysis”

Purification of 2,3-Butanediol from Fermentation Broth: Process Development and Techno-economic Analysis

Gregorius Rionugroho Harvianto¹#, Junaid Haider¹#, Jimin Hong¹, Nguyen Van Duc Long¹, Jae-Jin Shim¹, Moo Hwan Cho¹, Woo Kyoung Kim¹, Moonyong Lee¹*

¹School of Chemical Engineering, Yeungnam University, Gyeongsan 712-749, Republic of Korea

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*Correspondence concerning this article should be addressed to:

Prof. Moonyong Lee
Address: School of Chemical Engineering, Yeungnam University, Dae-dong 214-1, Gyeongsan 38541, Republic of Korea
Email: mynlee@yu.ac.kr
Telephone: +82 53 810 3241
A. NRTL and UNIQUAC equations

1. NRTL equation:

\[
\ln \gamma_i = \frac{\sum x_j \tau_{ij} G_{ij}}{\sum_k x_k G_{ki}} + \sum_j \frac{x_j G_{ij}}{x_k G_{kj}} \left( \tau_{ij} - \frac{\sum_m x_m \tau_{mj} G_{mj}}{\sum_k x_k G_{kj}} \right) \quad (A.1)
\]

\[G_{ij} = \exp(-\alpha_{ij} \tau_{ij}) \quad (A.2)\]

\[\tau_{ij} = a_{ij} + \frac{b_{ij}}{T} \quad (A.3)\]

\[\alpha_{ij} = c_{ij} + d_{ij} T \quad (A.4)\]

\[\tau_{ii} = 0 \quad (A.5)\]

\[G_{ii} = 1 \quad (A.6)\]

\(\gamma_i\) is the activity coefficient of molecule i, \(x\) is the mole fraction, \(\tau_{ij}(\neq \tau_{ji})\) is the interaction parameter between groups i and j, \(G_{ij}\) is as defined in equation 2, \(m\) is the measured data, \(k\) is Boltzmann’s constant, \(\alpha_{ij}\) is the non-randomness constant for binary ij interactions. \(a_{ij}, b_{ij},\) and \(c_{ij}\) are binary interactions of \(a, b,\) and \(c\) between a pair of groups i and j, respectively.

2. UNIQUAC equation:

\[
\ln \gamma_i = \frac{\ln \frac{\Phi_i}{x_i} + \frac{z}{2} q_i \ln \frac{\Phi_i}{\theta_i} - q_i' \ln t_i' - q_i' \sum_j \theta_j' \tau_{ij}}{t_i' + l_i + q_i' - \frac{\Phi_i}{x_i} \sum_j x_j l_j} \quad (A.7)
\]
\[ \theta_i = \frac{q_i x_i}{q_r}; q_r = \sum_k q_k x_k \]  \hspace{1cm} (A.8)

\[ \theta_i' = \frac{q_i' x_i}{q_r'}; q_r' = \sum_k q_k' x_k \]  \hspace{1cm} (A.9)

\[ \Phi_i = \frac{r_i x_i}{r_r}; r_r = \sum_k r_k x_k \]  \hspace{1cm} (A.10)

\[ l_i = \frac{z}{2} (r_i - q_i) + 1 - r_i \]  \hspace{1cm} (A.11)

\[ t_i' = \sum_k \theta_k' \tau_{ki} \]  \hspace{1cm} (A.12)

\[ \tau_{ij} = \exp \left( a_{ij} + \frac{b_{ij}}{T} + c_{ij} \ln T \right) \]  \hspace{1cm} (A.13)

\( \Phi \) is the segment fraction, \( \theta \) is the area fraction, \( r \) and \( q \) are respectively pure component relative volume and surface area parameters, \( \tau_{ij} (\neq \tau_{ji}) \) is the interaction parameter, and \( z \) is the lattice coordination number (equal to 10). The \( r \) and \( q \) values are obtained from the Aspen Plus databank.

B. Economic Evaluation of Proposed Configurations

1. Sizing the distillation column

A distillation column was determined to have a sieve tray with 0.61 m tray spacing. The column diameter was determined by the column flooding condition that fixes the upper limit of the vapor velocity. The operating velocity is usually between 70 and 90% of the flooding velocity \([1, 2]\); in this study, 80% of the flooding
velocity was used as the default. Column analysis in Aspen Plus®V9 was used to calculate the diameter of the column and ensure the satisfaction of hydraulic flow inside of the column.

2. Sizing the extraction column

Due to the number of stages required for the extraction column, an agitated extraction column was used in this work. The column diameter and height were determined from the methods provided by Todd [3]. The diameter of the column will be evaluated so that the column operates at 75% of the flood point.

3. Capital cost (CC)

Guthrie’s modular method was applied [4]. In this study, the Chemical Engineering Plant Cost Index (CEPCI) 576.1 (2014) was used for cost updating.

\[ CC = BMC \text{ column} + BMC \text{ wall} + BMC \text{ tray stack} + BMC \text{ condenser} + BMC \text{ reboiler} \]  

\[ \text{Updated bare module cost (BMC)} = UF \times BC \times (MPF + MF - 1) \]  

where \( UF \) is the update factor: \( UF = \frac{\text{present cost index}}{\text{bare cost index}} \)

\[ BC = BC_0 \times \left(\frac{A}{A_0}\right)^\alpha \]  

where MPF is the material and pressure factor; MF is the module factor (a typical value), which is affected by the base cost.

Area of the heat exchanger, \( A = \frac{Q}{U \Delta T} \)

Material and pressure factor: \( MPF = F_m + F_p + F_d \)

where \( F_m, F_p, \text{ and } F_d \) are the construction material, pressure variation, and design variation factors, respectively.

Particularly for the HED configuration, the vacuum pump cost \( (C_{VP}) \) was calculated according to Ji et al. [5] and is presented in the following equations.
\[ C_{VP} = 4200 \frac{CEPCI\ 2014}{CEPCI\ 1994} \left( \frac{60g_TRT_0}{3600P_0} \right)^{0.55} \] (B.7)

where \( g_T \) is the total feed flow (kmol/h), \( R \) is the gas constant (0.0831 m\(^3\)/kmol K), \( T_0 \) is the temperature at the standard condition (273.15 K), and \( P_0 \) is the pressure at the standard condition (1.013 bar).

4. Operating cost (OC):

**Table A.1.** Utilities cost data [6].

| Utility               | Price ($/GJ) |
|-----------------------|--------------|
| Cooling Water         | 0.35         |
| Steam (High Pressure) | 17.7         |
| Electricity           | 16.80        |

\[ OC = C_{HPS} + C_{CW} + C_E + C_{NG} \] (B.8)

where \( C_{HPS} \) is the cost of the high-pressure steam; \( C_{CW} \) is the cost of cooling water; and \( C_E \) is the cost of electricity.

The power consumption of the vacuum pump \( W_{VP} \) and the condenser in the HED configuration were calculated according to Ji et al. [5] using the following equation, which involves the total feed flow. Because the distillate stream is condensed before the vacuum pump, the power consumption \( W_{VP} \) is over-predicted (but the influence of this on the total cost is small).

\[ W_{VP} = 10\% \frac{g_T}{3600} RT_{intake} \frac{kr}{kr-1} \left( \frac{P_{DIS}}{P_{OP}} \right)^{(\frac{kr-1}{kr})} - 1 \] (B.9)
where $W_{VP}$ is in kW, $g_T$ is the total feed flow (kmol/h), $T_{intake}$ is the absolute temperature of vapor at the intake conditions (298 K), $kr$ is the heat capacity ratio (1.33), $P_{DIS}$ is the discharge pressure (1.013 bar), and $P_{OP}$ is the condenser operating pressure in bar.

In addition, the price of oleyl alcohol (solvent) was 3,517 USD / ton, obtained from the MOLBASE database [7].

5. Total annual cost (TAC):

The total annual cost includes the annual capital cost (ACC) and the annual operating cost (AOC). The annual investment cost was obtained from the literature and refers to the annual payments over the life of the project [8].

$$ACC = CC \left[ \frac{i(1+i)^n}{(1+i)^n - 1} \right] \quad (B.10)$$

where $i$ is the interest rate per year (8%), and $n$ is the project duration (10 years).

$$TAC = ACC + AOC \quad (B.11)$$

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