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Batch Distillation: Thermodynamic Efficiency

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1. Introduction

The batch distillation is a separation processes that requires great amounts of energy. Due to high energy costs, the study of energy consumption is of great interest in this process (Zavala et al. 2007). According to Luyben (1990), the energy consumption increases when operation occurs in a batch manner. Determining how efficient is the heat transfer under specific conditions and to modify them in order to find how efficient the heat is used, is an important task.

The analysis of thermodynamic efficiency in a batch distillation column has been presented by Kim and Diwekar (2000), Zavala-Loría (2004), Zavala et al. (2007), Zavala & Coronado (2008) and Zavala et al. (2011). The first work only developed expressions to calculate thermodynamic efficiency while the rest of the works developed expressions to calculate thermodynamic efficiency and have applied them to a new problem of optimal control: Maximum thermodynamic efficiency.

2. Description of the process

For this study we used a conventional batch distillation column consisting of:

- Reboiler
- Tray column
- Condenser
- Reflux drum
- Receiver

Figure 1 Shows a conventional batch column like the one used for this study.

Mass balances resulting from the process shown in Figure 1, allow us to obtain the mathematical model in Table 1. The model considers the following elements:

- Theoretical stages
- Total condenser
- Neglible pressure drop
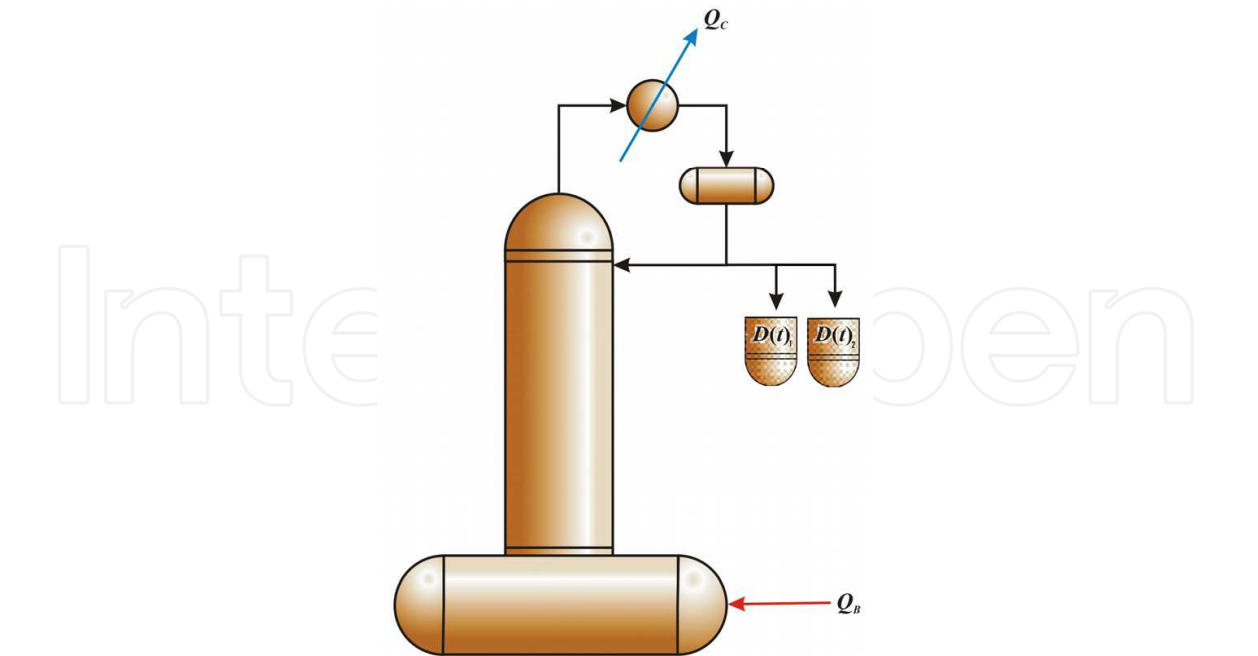
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Fig. 1. Conventional batch distillation column.

- Constant flows:
  - Vapor
  - Liquid.
- Constant liquid holdup:
  - Stages
  - Condenser-Reflux drum.
- Adiabatic column

$$\frac{dB}{dt} = -D_t = -\frac{V}{R_t + 1} \tag{1}$$

$$\frac{dx_B^{(i)}}{dt} = \left(\frac{V}{B}\right)\left\{x_B^{(i)} - y_B^{(i)} + \left(\frac{L}{V}\right)\left[x_1^{(i)} - x_B^{(i)}\right]\right\} \; ; \; i = 1,\ldots,n \tag{2}$$

$$\frac{dx_j^{(i)}}{dt} = \left(\frac{V}{H_j}\right)\left\{y_{j-1}^{(i)} - y_j^{(i)} + \left(\frac{L}{V}\right)\left[x_{j+1}^{(i)} - x_j^{(i)}\right]\right\} \; ; \; i = 1,\ldots,n \; ; \; j = 1,\ldots,N \tag{3}$$

$$\frac{dx_D^{(i)}}{dt} = \left(\frac{V}{H_D}\right)\left[y_n^{(i)} - x_D^{(i)}\right] \; ; \; i = 1,\ldots,n \tag{4}$$

$$\sum_{i=1}^{n} y_j^{(i)} = \sum_{i=1}^{n} K_j^{(i)} x_j^{(i)} = 1 \quad ; i = 1,\ldots,n \; ; \; j = 1,\ldots,N \tag{5}$$

Table 1. Mathematical model of a batch distillation column (*n*=number of components and *N*=number of equilibrium stages).

Considering ideal mixtures, the vapor-liquid equilibrium (VLE) can be obtained from Raoult's law equation:

$$K^{(i)} = \frac{y^{(i)}}{x^{(i)}} = \frac{P_i^{sat}}{P} \; ; i = 1, 2,\ldots,n \tag{6}$$

For non-ideal mixtures, we can use the following equation:

$$K^{(i)} = \frac{y^{(i)}}{x^{(i)}} = \frac{\gamma_i P_i^{sat}}{\widehat{\phi}_i P} \; ; i = 1, 2,\ldots,n \tag{7}$$

Where $K^{(i)}$ is the constant of the VLE, and $y^{(i)}$ is the mole fraction of the vapor phase, $x^{(i)}$ is the mole fraction of the liquid phase, γ_i represents the activity coefficient, P^{sat} is the saturation pressure and $\widehat{\phi}_i$ denotes the partial fugacity coefficient, all referring to component i, and P represents the system pressure. Activity coefficients can be obtained with a solution model (Wilson, NRTL, etc.) or the Chao-Seader correlation. The fugacity coefficients can be obtained with an equation of state (Redlich-Kwong, Soave, Peng-Robinson, etc.)

At standard or low pressures P_i^{sat} can be obtained with Antoine's equation.

$$\ln\left[P_i^{sat} \right] = A_i - \frac{B_i}{T + C_i} \; ; i = 1, 2,\ldots,n \tag{8}$$

Coefficients A_i, B_i and C_i appear in literature related to this area of study.

3. Thermodynamic efficiency

By definition, the thermodynamic efficiency (η_t) of a process based on availability or exergy is defined as:

$$\eta_t = \left(\frac{W_{min}}{W_{total}} \right)_{sep} = \left(\frac{W_{min}}{W_{min} + LW} \right)_{sep} \tag{9}$$

where W is the work and LW is the total loss of work.

Since the minimum work is determined by changes in exergy, they can be determined using the First and Second Law of Thermodynamics. Figure 2 shows the control volume used to obtain the equations that represent thermodynamic efficiency in batch distillation.

Figure 2 shows that the process can exchange energy with the environment but does not perform any mechanical work. The energy balance (enthalpy) given by the First Law of Thermodynamics, considering the reboiler, the column of trays and the condenser-reflux drum, is:

$$\frac{d(mI)_{sist}}{dt} = \frac{d(BI_B)}{dt} + \sum_{i=1}^{n} \frac{d(H_t I_t)_i}{dt} + \frac{d(H_D I_{rt})}{dt} \tag{10}$$

where:

$$\frac{d(mI)_{sist}}{dt} = Q_0 + Q_B - Q_C - DI_D \tag{11}$$

According to the Second Law of Thermodynamics, the entropy balance is:

$$\frac{d(mS)_{sist}}{dt} = \frac{d(BS_B)}{dt} + \sum_{i=1}^{n} \frac{d(H_t S_t)_i}{dt} + \frac{d(H_D S_{rt})}{dt} \tag{12}$$

where:

$$\frac{d(mS)_{sist}}{dt} = \frac{Q_0}{T_0} + \frac{Q_B}{T_B} - \frac{Q_C}{T_C} - DS_D + d(S_{irr}) \tag{13}$$
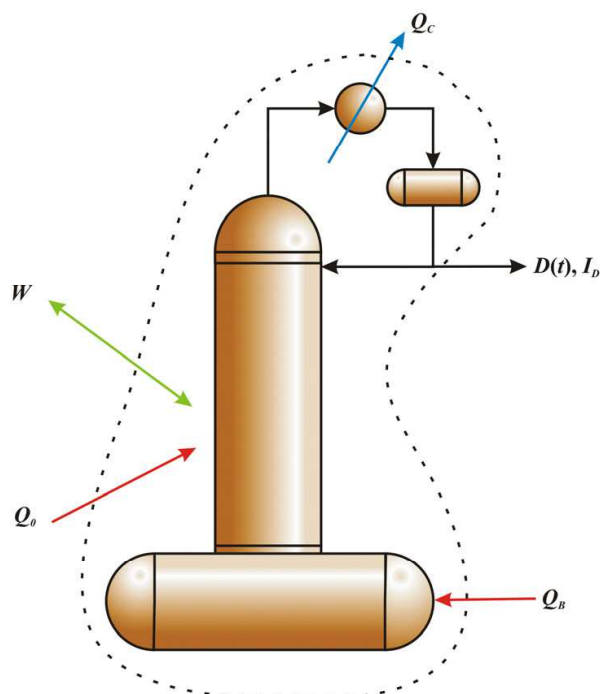

Fig. 2. Control volume for batch process.

I represents enthalpy, S is entropy, Q is the amount of heat, C represents the condenser, D represents the distillate, B represents the bottoms, m is the system mass, 0 is the reference state, t is the stage or tray and T is the temperature. The available work can be obtained if we combine equations (11) and (13). To do so, equation (13) must be multiplied by the temperature of the reference state T_0 (it is considered that the reference state is liquid at 25 °C and 1.0 atm):

$$\frac{d(mT_0 S)_{sist}}{dt} = Q_0 + \frac{T_0}{T_B} Q_B - \frac{T_0}{T_C} Q_C - DT_0 S_D + T_0 d(S_{irr})$$

$$\frac{d(mI)_{sist}}{dt} - \frac{d(mT_0 S)_{sist}}{dt} = Q_0 + Q_B - Q_C - DI_D - Q_0 - \frac{T_0}{T_B} Q_B + \frac{T_0}{T_C} Q_C + DT_0 S_D - T_0 d(S_{irr})$$

$$\frac{d\left[m\left(I - T_0 S\right)\right]}{dt} = \left(1 - \frac{T_0}{T_B}\right)Q_B - \left(1 - \frac{T_0}{T_C}\right)Q_C - D\left(I_D - T_0 S_D\right) - T_0 d\left(S_{irr}\right) \tag{14}$$

the availability is represented as $\mathcal{A} = I - T_0 S$, then:

$$\frac{d\left(m\mathcal{A}\right)_{sist}}{dt} = \left(1 - \frac{T_0}{T_B}\right)Q_B - \left(1 - \frac{T_0}{T_C}\right)Q_C - D\mathcal{A}_D - T_0 d\left(S_{irr}\right) \tag{15}$$

$$\frac{d\left(m\mathcal{A}\right)_{sist}}{dt} = \left(1 - \frac{T_0}{T_B}\right)Q_B - \left(1 - \frac{T_0}{T_C}\right)Q_C - D\mathcal{A}_D - LW \tag{16}$$

Where the loss of work is defined as $LW = T_0 dS_{irr}$. The terms of the right hand side of Equation (16) represent the difference between the exergy or the availability of flows entering and leaving the system. The term on the left hand side is the change of exergy in the system. Finding the values in Equation (16), the work loss is:

$$LW = \left(1 - \frac{T_0}{T_B}\right)Q_B - \left(1 - \frac{T_0}{T_C}\right)Q_C - D\mathcal{A}_D - \frac{d\left(m\mathcal{A}\right)_{sist}}{dt} \tag{17}$$

$\dfrac{d\left(m\mathcal{A}\right)_{sist}}{dt}$ can be calculated, if discretised, by multiplying Equation (12) by T_0 minus Equation (10):

$$\frac{\Delta\left(m\mathcal{A}\right)_{sist}}{\Delta t} = \frac{\Delta\left(B\mathcal{A}_B\right) + \sum_{i=1}^{n}\Delta\left(H_t\mathcal{A}_t\right)_i + \Delta\left(H_D\mathcal{A}_{rt}\right)}{\Delta t} \tag{18}$$

Another way to estimate the value of $\dfrac{d\left(m\mathcal{A}\right)_{sist}}{dt}$ is by applying an exergy balance at the bottom of the column. Applying an exergy balance in the reboiler, we have:

$$\frac{d\left(m\mathcal{A}\right)_{sist}}{dt} = \frac{d\left(B\mathcal{A}_B\right)}{dt} = B\frac{d\left(\mathcal{A}_B\right)}{dt} + \mathcal{A}_B\frac{d\left(B\right)}{dt} \tag{19}$$

Introducing Equation (1) from Table (1) in Equation (19), we obtain:

$$\frac{d\left(B\mathcal{A}_B\right)}{dt} = B\frac{d\left(\mathcal{A}_B\right)}{dt} - D\mathcal{A}_B \tag{20}$$

According to Kim and Diwekar (2000) and Zavala-Loría and Coronado-Velasco (2008), the total exergy can be calculated from its physical component ($\mathcal{A}_{phis}$) and its chemical component ($\mathcal{A}_{chem}$), i.e.:

$$\mathcal{A} = \mathcal{A}_{phis} + \mathcal{A}_{chem} \tag{21}$$

where $\mathcal{A}_{phis}$ considers the physical processes that involve thermal interactions with the surroundings and $\mathcal{A}_{chem}$ considers the mass and heat transfer with the surroundings. The main contribution to this energy is due to mixing effects and can be estimated from the chemical potential at low pressures (Kim and Diwekar, 2000). $\mathcal{A}_{phis}$ is relatively lower than $\mathcal{A}_{chem}$. Thus, the physical component can be regarded as constant for all chemical species and the derivative of this term is eliminated. The chemical component of exergy for an ideal mixture can be expressed as:

$$\mathcal{A}_{chem} = RT_0 \sum_i x^{(i)} \ln\left[x^{(i)}\right] \tag{22}$$

whereas a non-ideal mixture can be calculated as:

$$\mathcal{A}_{chem} = RT_0 \sum_i x^{(i)} \ln\left[\gamma_i x^{(i)}\right] \tag{23}$$

and the exergy exchange in the reboiler for an ideal mixture can be calculated as:

$$\mathcal{A}_B = \mathcal{A}_{B_{phis}} + \mathcal{A}_{B_{chem}} = \mathcal{A}_{B_{phis}} + RT_0 \sum_i x_B^{(i)} \ln\left[x_B^{(i)}\right] \tag{24}$$

for a non-ideal mixture:

$$\mathcal{A}_B = \mathcal{A}_{B_{phis}} + \mathcal{A}_{B_{chem}} = \mathcal{A}_{B_{phis}} + RT_0 \sum_i x_B^{(i)} \ln\left[\gamma_{B,i} x_B^{(i)}\right] \tag{25}$$

Taking the derivative of Equations (24) and (25) yields:

$$\frac{d\left(\mathcal{A}_B\right)}{dt} = \frac{d\left(\mathcal{A}_{B_{chem}}\right)}{dt} = RT_0 \frac{d\left\{\sum_i x_B^{(i)} \ln\left[x_B^{(i)}\right]\right\}}{dt} \tag{26}$$

$$\frac{d\left(\mathcal{A}_B\right)}{dt} = \frac{d\left(\mathcal{A}_{B_{chem}}\right)}{dt} = RT_0 \frac{d\left\{\sum_i x_B^{(i)} \ln\left[\gamma_{B,i} x_B^{(i)}\right]\right\}}{dt} \tag{27}$$

The derivative of the term on the right hand side of Equations (26) and (27) can be represented in terms of the mathematical model of the column; thus, substituting Equation (2) of Table 1 yields:

$$\frac{d\left\{\sum_i x_B^{(i)} \ln\left[x_B^{(i)}\right]\right\}}{dt} = \sum_i\left\{\left[1 + \ln x_B^{(i)}\right]\frac{dx_B^{(i)}}{dt}\right\}$$
$$= \left(\frac{V}{B}\right)\sum_i\left\{x_B^{(i)} - y_B^{(i)} + \left(\frac{L}{V}\right)\left[x_1^{(i)} - x_B^{(i)}\right]\right\} \tag{28}$$

$$\frac{d\left\{\sum_i x_B^{(i)} \ln\left[\gamma_{i,B} x_B^{(i)}\right]\right\}}{dt} = \sum_i \left\{\left[1 + \ln\gamma_{i,B} x_B^{(i)}\right]\frac{dx_B^{(i)}}{dt} + \frac{x_B^{(i)}}{\gamma_{i,B}}\frac{d\gamma_{i,B}}{dt}\right\}$$

$$= \left(\frac{V}{B}\right)\sum_i\left\{x_B^{(i)} - y_B^{(i)} + \left(\frac{L}{V}\right)\left[x_1^{(i)} - x_B^{(i)}\right]\right\}\left[1 + \ln\gamma_{i,B} x_B^{(i)}\right] \qquad (29)$$

$$+ \sum_i\left[\frac{x_B^{(i)}}{\gamma_{i,B}}\frac{d\gamma_{i,B}}{dt}\right]$$

Substituting Equation (28) on the right hand side of Equation (20) for an ideal mixture, and Equation (29) on the right hand side of Equation (20) for a non-ideal mixture yields:

Ideal Mixture:

$$\frac{d\left(B\mathcal{A}_B\right)}{dt} = VRT_0\sum_i\left\{x_B^{(i)} - y_B^{(i)} + \left(\frac{L}{V}\right)\left[x_1^{(i)} - x_B^{(i)}\right]\right\}\left\{1 + \ln\left[x_B^{(i)}\right]\right\}$$

$$- D\left\{\mathcal{A}_{B,phis} + RT_0\sum_i x_B^{(i)} \ln\left[x_B^{(i)}\right]\right\} \qquad (30)$$

Non-ideal Mixture:

$$\frac{d\left(B\mathcal{A}_B\right)}{dt} = VRT_0\sum_i\left\{x_B^{(i)} - y_B^{(i)} + \left(\frac{L}{V}\right)\left[x_1^{(i)} - x_B^{(i)}\right]\right\}\left[1 + \ln\gamma_{i,B} x_B^{(i)}\right]$$

$$+ BRT_0\sum_i\left[\frac{x_B^{(i)}}{\gamma_{i,B}}\frac{d\gamma_{i,B}}{dt}\right] \qquad (31)$$

$$- D_t\left[\mathcal{A}_{B,phis} + RT_0\sum_i x_B^{(i)} \ln\gamma_{i,B} x_B^{(i)}\right]$$

The exergy of the current production (dome) that will be used in Equation (6) for an ideal mixture can be calculated as:

$$\mathcal{A}_D = \mathcal{A}_{D,phis} + RT_0\sum_i x_D^{(i)} \ln\left[x_D^{(i)}\right] \qquad (32)$$

for a non-ideal mixture:

$$\mathcal{A}_D = \mathcal{A}_{D,phis} + RT_0\sum_i x_D^{(i)} \ln\left[\gamma_{i,D} x_D^{(i)}\right] \qquad (33)$$

The exergy transfer associated with the transmission of energy as heat in the process can be calculated by the energy balances in the reboiler and condenser. Considering that ΔH^{vap} is the same for each component and is not related to the temperature of the process, the Clausius-Clapeyron equation can be used to calculate ΔH^{vap}, and the first two terms on the right hand side of Equation (16) can be calculated by the following equation;

Ideal Mixture:

$$\left(1 - \frac{T_0}{T_B}\right)Q_B - \left(1 - \frac{T_0}{T_D}\right)Q_D = V\Delta H^{vap}T_0\left(\frac{1}{T_C} - \frac{1}{T_B}\right) \tag{34}$$

and considering constant relative volatility:

$$\left(1 - \frac{T_0}{T_B}\right)Q_B - \left(1 - \frac{T_0}{T_D}\right)Q_D = VRT_0\ln\left[\frac{x_D^{(1)}(\alpha_1 - 1) + 1}{x_B^{(1)}(\alpha_1 - 1) + 1}\right] \tag{35}$$

Non-ideal Mixture:

$$\left(1 - \frac{T_0}{T_B}\right)Q_B - \left(1 - \frac{T_0}{T_D}\right)Q_D = VRT_0\ln\left(\frac{\gamma_{1,D}\Phi_{1,B}K_{1,B}}{\gamma_{1,B}\Phi_{1,D}K_{1,D}}\right) \tag{36}$$

where, K is the liquid-vapor equilibrium constant and Φ is defined as:

$$\Phi_k \equiv \frac{\widehat{\phi_k}}{\phi_k^{sat}}\exp\left[-\frac{V_k\left(P - P_k^{sat}\right)}{RT}\right]; k = 1, 2, \ldots,n \tag{37}$$

Therefore, the term for exergy loss or work loss, LW in Equation (17) for an ideal mixture, can be calculated with Equation (35) and for a non-ideal mixture with Equation (36):

Ideal Mixture:

$$LW = VRT_0\ln\left[\frac{x_D^{(1)}(\alpha_1 - 1) + 1}{x_B^{(1)}(\alpha_1 - 1) + 1}\right] + DRT_0\left\{\sum_i x_B^{(i)}\ln\left[x_B^{(i)}\right] - \sum_i x_D^{(i)}\left[\ln x_D^{(i)}\right]\right\}$$

$$+ D\left(\mathcal{A}_{B,phis} - \mathcal{A}_{D,phis}\right) \tag{38}$$

$$- VRT_0\sum_i\left\{x_B^{(i)} - y_B^{(i)} + \left(\frac{L}{V}\right)\left[x_1^{(i)} - x_B^{(i)}\right]\right\}\left[1 + \ln x_B^{(i)}\right]$$

Non-ideal Mixture:

$$LW = VRT_0\ln\left(\frac{\gamma_{1,D}\Phi_{1,B}K_{1,B}}{\gamma_{1,B}\Phi_{1,D}K_{1,D}}\right) + D_tRT_0\left\{\sum_i x_B^{(i)}\ln\left[\gamma_{i,B}x_B^{(i)}\right] - \sum_i x_D^{(i)}\ln\left[\gamma_{i,D}x_D^{(i)}\right]\right\}$$

$$+ D_t\left(\mathcal{A}_{B,phis} - \mathcal{A}_{D,phis}\right)$$

$$- VRT_0\sum_i\left\{x_B^{(i)} - y_B^{(i)} + \left(\frac{L}{V}\right)\left[x_1^{(i)} - x_B^{(i)}\right]\right\}\left\{1 + \ln\left[\gamma_{i,B}x_B^{(i)}\right]\right\} \tag{39}$$

$$- BRT_0\sum_i\left[\frac{x_B^{(i)}}{\gamma_{i,B}}\frac{d\gamma_{i,B}}{dt}\right]$$

Considering that $\mathcal{A}_{B,phis} - \mathcal{A}_{D,phis} \approx 0$, then:

Ideal Mixture:

$$LW = VRT_0 \ln\left[\frac{x_D^{(1)}(\alpha_1 - 1) + 1}{x_B^{(1)}(\alpha_1 - 1) + 1}\right]$$

$$+ DRT_0 \left\{\sum_i x_B^{(i)} \ln\left[x_B^{(i)}\right] - \sum_i x_D^{(i)} \left[\ln x_D^{(i)}\right]\right\} \tag{40}$$

$$- VRT_0 \sum_i \left\{x_B^{(i)} - y_B^{(i)} + \left(\frac{L}{V}\right)\left[x_1^{(i)} - x_B^{(i)}\right]\right\}\left[1 + \ln x_B^{(i)}\right]$$

Non-ideal Mixture:

$$LW = VRT_0 \ln\left(\frac{\gamma_{1,D}\Phi_{1,B}K_{1,B}}{\gamma_{1,B}\Phi_{1,D}K_{1,D}}\right) + DRT_0\left\{\sum_i x_B^{(i)} \ln\left[\gamma_{i,B}x_B^{(i)}\right] - \sum_i x_D^{(i)} \ln\left[\gamma_{i,D}x_D^{(i)}\right]\right\}$$

$$- VRT_0 \sum_i \left\{x_B^{(i)} - y_B^{(i)} + \left(\frac{L}{V}\right)\left[x_1^{(i)} - x_B^{(i)}\right]\right\}\left\{1 + \ln\left[\gamma_{i,B}x_B^{(i)}\right]\right\} - BRT_0 \sum_i \left[\frac{x_B^{(i)}}{\gamma_{i,B}}\frac{d\gamma_{i,B}}{dt}\right] \tag{41}$$

the minimum work can be calculated as:

Ideal Mixture:

$$W_{\min} = DRT_0 \left\{\sum_i x_D^{(i)} \ln\left[x_D^{(i)}\right] - \sum_i x_B^{(i)} \ln\left[x_B^{(i)}\right]\right\}$$

$$+ VRT_0 \sum_i \left\{x_B^{(i)} - y_B^{(i)} + \left(\frac{L}{V}\right)\left[x_1^{(i)} - x_B^{(i)}\right]\right\}\left\{1 + \ln\left[x_B^{(i)}\right]\right\} \tag{42}$$

Non-ideal Mixture:

$$W_{\min} = DRT_0 \left\{\sum_i x_D^{(i)} \ln\left[\gamma_{i,D}x_D^{(i)}\right] - \sum_i x_B^{(i)} \ln\left[\gamma_{i,B}x_B^{(i)}\right]\right\}$$

$$+ VRT_0 \sum_i \left\{x_B^{(i)} - y_B^{(i)} + \left(\frac{L}{V}\right)\left[x_1^{(i)} - x_B^{(i)}\right]\right\}\left\{1 + \ln\left[\gamma_{i,B}x_B^{(i)}\right]\right\}$$

$$+ BRT_0 \sum_i \left[\frac{x_B^{(i)}}{\gamma_{i,B}}\frac{d\gamma_{i,B}}{dt}\right] \tag{43}$$

and the thermodynamic efficiency [Equation (9)] results in:

Ideal Mixture:

$$\eta_t = \frac{\sum_i \left\{x_D^{(i)} \ln\left[x_D^{(i)}\right] - x_B^{(i)} \ln\left[x_B^{(i)}\right]\right\} + \left\{R\left[x_1^{(i)} - y_B^{(i)}\right] + x_B^{(i)} - y_B^{(i)}\right\}\left\{1 + \ln\left[x_B^{(i)}\right]\right\}}{(R+1)\ln\left[\dfrac{x_D^{(1)}(\alpha_1 - 1) + 1}{x_B^{(1)}(\alpha_1 - 1) + 1}\right]} \tag{44}$$

Non-ideal Mixture:

$$\eta_t = \frac{\sum_i \left\{ x_D^{(i)} \ln \gamma_{i,D} x_D^{(i)} - x_B^{(i)} \ln \gamma_{i,B} x_B^{(i)} + \left(R \left[x_1^{(i)} - y_B^{(i)} \right] + x_B^{(i)} - y_B^{(i)} \right) \left[1 + \ln \gamma_{i,B} x_B^{(i)} \right] + \left(\frac{B}{V} \right) \left[\frac{x_B^{(i)}}{\gamma_{i,B}} \frac{d\gamma_{i,B}}{dt} \right] \right\}}{(R+1) \ln \left(\frac{K_{1,B}}{K_{1,D}} \frac{\Phi_{1,B}}{\Phi_{1,D}} \frac{\gamma_{1,D}}{\gamma_{1,B}} \right)} \tag{45}$$

Equation (45) can be reduced if one considers that the changes of activity coefficients in the reboiler are so small that they can be neglected. Then:

$$\eta_t = \frac{\sum_i \left\{ x_B^{(i)} + x_D^{(i)} \ln \gamma_{i,D} x_D^{(i)} + \left[R \left(x_1^{(i)} - y_B^{(i)} \right) - y_B^{(i)} \right] \left[1 + \ln \gamma_{i,B} x_B^{(i)} \right] \right\}}{(R+1) \ln \left(\frac{K_{1,B}}{K_{1,D}} \frac{\Phi_{1,B}}{\Phi_{1,D}} \frac{\gamma_{1,D}}{\gamma_{1,B}} \right)} \tag{46}$$

If the gas phase is ideal or close to ideality, then Equation (46) can be reduced even more:

$$\eta_t = \frac{\sum_i \left\{ x_B^{(i)} + x_D^{(i)} \ln \gamma_{i,D} x_D^{(i)} + \left[R \left(x_1^{(i)} - y_B^{(i)} \right) - y_B^{(i)} \right] \left[1 + \ln \gamma_{i,B} x_B^{(i)} \right] \right\}}{(R+1) \ln \left(\frac{K_{1,B}}{K_{1,D}} \frac{\gamma_{1,D}}{\gamma_{1,B}} \right)} \tag{47}$$

The solution of Equation (45) or its simplifications [Equation (46) and (47)] require the calculation of activity coefficients of the mixtures, which can be obtained with an appropriate solution model (Wilson, NRTL, UNIQUAC, UNIFAC, etc.). According to Equations (44), (45), (46) and (47), the thermodynamic efficiency not only depends on the reflux ratio but on the concentration of components in both phases and the kind of mixture. A convenient way to express thermodynamic efficiency is the average thermodynamic equation used by Zavala Loría (2004), Zavala et al. (2007), Zavala and Coronado (2008). and Zavala et al. (2011) to solve the maximum thermodynamic efficiency problem:

$$\eta_{average} = \frac{\int_0^t \eta_t dt}{t} \tag{48}$$

4. Results and discussion

Using the First and Second Law of Thermodynamics, this work has developed an expression for calculating the thermodynamic efficiency of a batch distillation process [Equations (44) and (45)]. To solve the mathematical model, the feeding was introduced at the top of the column at boiling temperature, neglecting the accumulation of vapor in each stage. The process was performed with total condenser, atmospheric pressure and adiabatic column.

To solve the model, two mixtures were considered. The first one is an ideal mixture of Hexane/Benzene/Chlorobenzene (HBC); the second one is a non-ideal mixture of Ethanol-Water (EW).

Case of study 1: Hexane/Benzene/Chlorobenzene mixture

The conditions and data used to solve the mathematical model of thermodynamic efficiency are given in Table 2. Relative volatilities were calculated with the Soave-Redlich-Kwong equation of state.

Variable/Parameter	Amount	Units
Feed (F)	200.00	kmol
Vapor flow (V)	240.00	kmol/h
Condenser liquid holdup (H_D)	5.00	kmol
Tray liquid holdup (H_T)	1.00	kmol
Batch time	1.00	h
Z_{Hexane}	0.20	
$Z_{Benzene}$	0.30	
$Z_{Chlorobenzene}$	0.50	
a_{Hexane}	8.54	
$a_{Benzene}$	4.71	
Number of trays	15	
Reflux ratio (Constant)	5	

Table 2. Data used to solve the mathematical model of thermodynamic efficiency

The first step for the resolution of the mathematical model was to reach the steady state to extract the product during one hour. Figure 3, shows the concentrations at the top of the column (including the steady state).
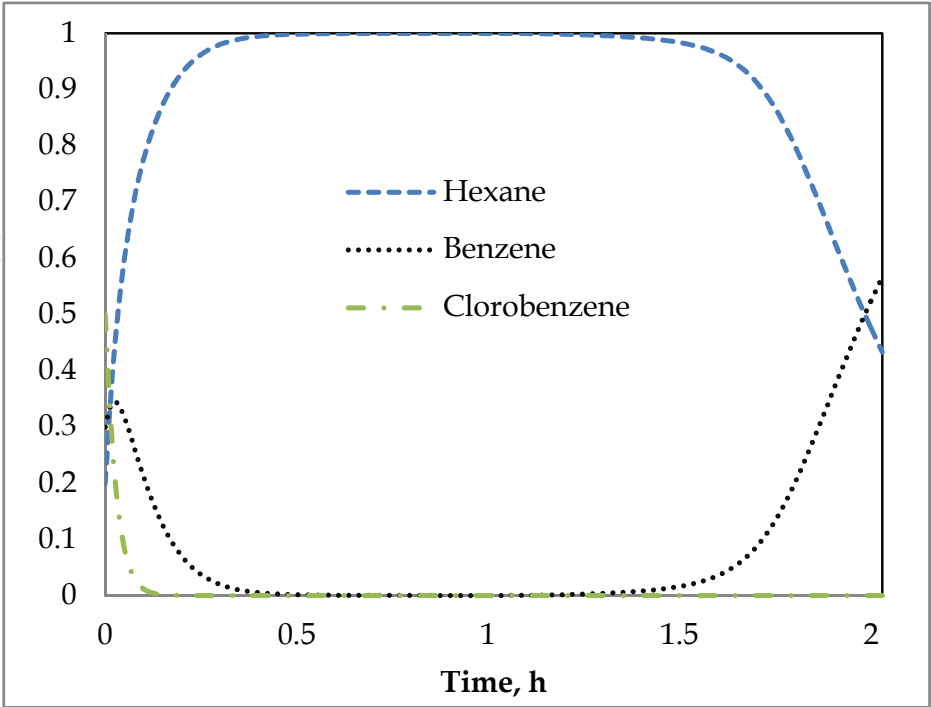
Fig. 3. Concentrations at the top of the column.

The average thermodynamic efficiency is 17.58% for this production time while the average concentration of the most volatile component at the top of the column is 88.55% mol. Table 3, shows the variations observed when the reflux ratio is changed.

Reflux ratio	$\eta_{average}$ (%)	$x^{(1)}_{D,average}$ (%)
2	55.60	49.50
3	28.61	64.34
4	20.60	77.66
5	17.58	88.55
6	16.16	95.55
7	15.08	98.51
8	14.02	99.40

Table 3. Thermodynamic efficiency behavior based on variations in the reflux ratio.

Figure 4 shows the thermodynamic efficiency behavior in the product obtaining.
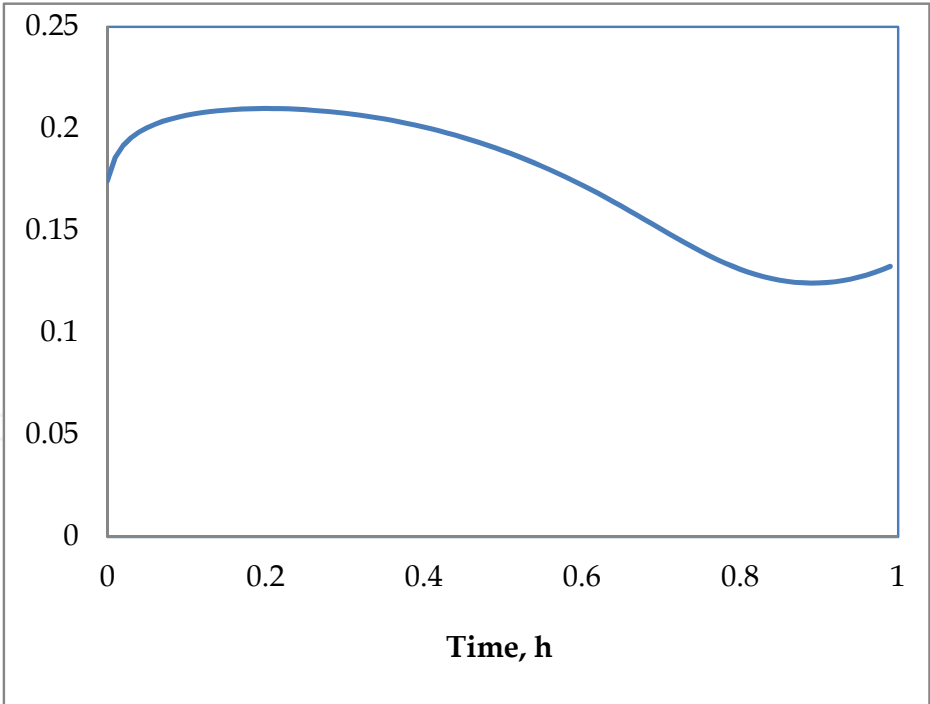
Fig. 4. Thermodynamic efficiency behavior in the product obtaining.

Such variations make evident the influence of the reflux ratio over the thermodynamic efficiency; in other words, the thermodynamic efficiency of the process is smaller when the reflux ratio is higher. We also could observe that the reflux ratio affects the product concentration. If the reflux ratio increases the product concentration increases as well.

Case of study 2: Ethanol/Water mixture

The conditions used for solving the mathematical model of thermodynamic efficiency for a non ideal mixture (Ethanol/Water) are given in Table 4. Wilson's equation was used to obtain the activity coefficients; the vapor phase is considered to have an ideal behavior. The steady state was reached when Ethanol presented a purity level of 89.61% mol obtained using Wilson's equation.

3.045 hours was the period of time needed to reach the steady state, we obtained an average thermodynamic efficiency of 36.96% and the product presented an average concentration of 86.74% mol of the most volatile component.

Variable/Parameter	Amount	Units
Feed (F)	100.00	
Vapor flow (V)	120.00	
Condenser liquid holdup (H_D)	5.00	
Tray liquid holdup (H_T)	1.00	kmol
Batch time	2.00	kmol/h
$Z_{Ethanol}$	0.50	kmol
Z_{Water}	0.50	kmol
$a_{Ethanol}$	8.54	h
a_{Water}	4.71	
Number of trays	15	
Reflux ratio (Constant)	2	

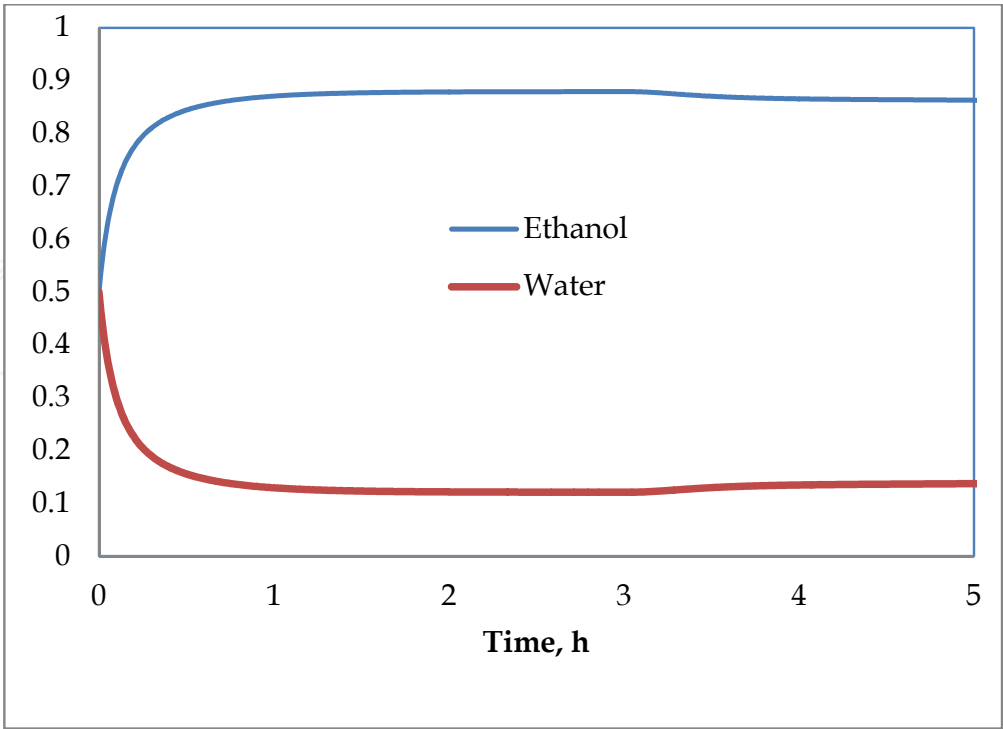Table 4. Data used to solve the mathematical model of thermodynamic efficiency.

Fig. 5. Concentration profiles at the top of the column.

Figure 5 shows the behavior of the concentrations at the top of the column, while the behavior of punctual thermodynamic efficiency is shown in Figure 6. Table 5 shows the variations observed when different reflux ratios are used.
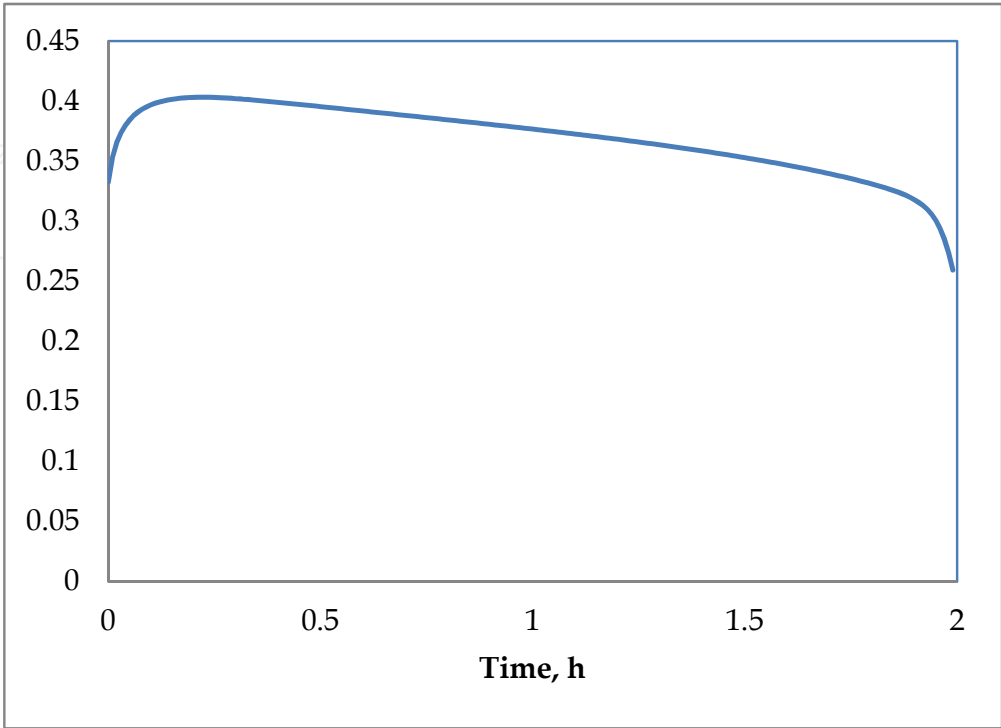

Fig. 6. Thermodynamic efficiency profile (obtaining product).

Reflux ratio	$\eta_{average}$ (%)	$x_{D,average}^{(1)}$ (%)
5	36.96	86.74
6	32.75	86.96
7	29.24	87.12
8	26.38	87.24
9	24.00	87.32
10	22.02	87.39

Table 5. Thermodynamic efficiency behavior with regards to the reflux ratio variation.

As in the last case, we observe that when the reflux ratio increases, the efficiency decreases; however, the concentration of the most volatile component presents also an increment. We can formulate the following heuristic rule: If the variables of the process are maintained, the reflux ratio will have an inverse effect on the thermodynamic efficiency of the process.

5. Concluding remarks

Using the First and Second Law of Thermodynamics (exergy concept), this work has developed an expression for calculating the thermodynamic efficiency of a batch distillation

process. The resulting equation was used to find the batch distillation thermodynamic efficiency for an ideal mixture and a non-ideal mixture. The equation obtained is a generalization of the equation developed by Zavala-Loría et al. (2007), Zavala and Coronado (2008) and Zavala et al. (2011).

The results obtained by solving the Equations, allowed us to observe the relationship between reflux and thermodynamic efficiency of the process. Furthermore, variables such as the product purity are affected by the reflux ratio, in other words, the purity of the product requires a greater amount of reflux to obtain a higher concentration.

6. Nomenclature

|	
H_j	molar hold-up on tray j
H_D	molar hold-up on the condenser
I	enthalpy (J/mol)
S	entropy (J/mol K)
V	vapor flow rate (mol/h)
L	liquid flow rate (mol/h)
D	distillate flow rate (mol/h)
B	amount of moles in the reboiler, mol
n	number of components
N	number of trays in the column
R_t	reflux ratio
t	time (h)
W	work (J)
LW	work loss (J)
z	mole fraction in the feed
$x_j^{(i)}$	mole fraction in the liquid of component i at plate j
$y_j^{(i)}$	mole fraction in the vapor of component i at plate j
$x_B^{(i)}$	mole fraction in the liquid of component i in the reboiler
$x_D^{(i)}$	mole fraction in the vapor of component i in the distillate
$K_j^{(i)}$	equilibrium constant
T	temperature
A	availability
η_t	punctual thermodynamic efficiency
ΔH^{vap}	vaporization heat

Subindex

0	reference
c	condenser
f	end
D	distillate
B	boiler or reboiler
t	time

7. References

Luyben, William L. (1990); Process modeling, Simulation and Control for Chemical Engineers; McGraw-Hill. Second edition, 725 pp.

Kim, K.J., Diwekar, U.M. (2000); Comparing Batch Column Configurations: Parametric Study Involving Multiple Objetives; Aiche Journal, 46(12), pp. 2475-2488.

Zavala-Loría, J.C. (2004); Optimización del Proceso de Destilación Discontinua; Tesis Doctoral, Departamento de Ingeniería Química, Instituto Tecnológico de Celaya, Celaya, Guanajuato, México.

Zavala, José C., Córdova, Atl., Cerón, Rosa M. and Palí, Ramón J. (2007); Thermodynamic efficiencies of a conventional batch column; Int. J. Exergy, 4(4), pp. 371-383.

Zavala, J. C. and Coronado, Cristina (2008); Optimal Control Problem in Batch Distillation Using Thermodynamic Efficiency; Ind. Eng. Chem. Res., 47, pp. 2788-2793.

Zavala-Loría, J. C., Ruiz-Marín, A. and Coronado-Velásco, Cristina (2011); Maximum Thermodynamic Efficiency Problem in Batch Distillation; Brazilian Journal of Chemical Engineering, 28(2), pp. 333-342.
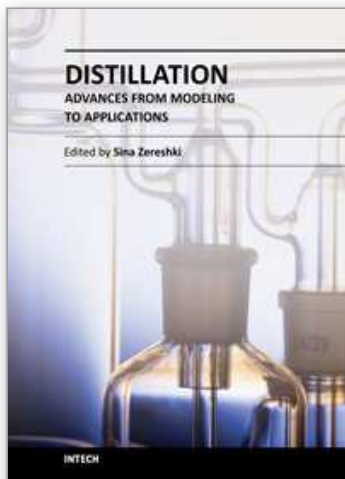
Distillation - Advances from Modeling to Applications

Edited by Dr. Sina Zereshki

Distillation modeling and several applications mostly in food processing field are discussed under three sections in the present book. The provided modeling chapters aimed both the thermodynamic mathematical fundamentals and the simulation of distillation process. The practical experiences and case studies involve mainly the food and beverage industry and odor and aroma extraction. This book could certainly give the interested researchers in distillation field a useful insight.

How to reference

In order to correctly reference this scholarly work, feel free to copy and paste the following:

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