

MAXIMUM THERMODYNAMIC EFFICIENCY PROBLEM IN BATCH DISTILLATION

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Abstract - A dynamic batch distillation study of the non-ideal mixture Ethanol-Water is presented. The objective of the study was to calculate an average thermodynamic efficiency of the process under an optimal constant reflux policy and the objective function includes a given production time in order to obtain the desired product quality (measured as the average mole fraction of the accumulated product). An expression for computing the thermodynamic efficiency is presented. The simulation of the column uses a mathematical model considering the complete dynamics of the operation and the problem of optimal control resulting in a non-linear programming problem. A dynamic optimization technique based on a SQP method was used to solve the problem. The average thermodynamic efficiency for the separation process under the conditions presented was 37.95%.

Keywords: Batch distillation; Thermodynamic Efficiency; Optimal Control Problem.

INTRODUCTION

Optimizing the operation of a batch distillation process is known as an optimal control problem, which has received considerable attention in the literature. The control variable frequently used in the optimization process of batch distillation is the reflux ratio and it is convenient to use an objective function directly related to the control variable. The objective functions are solved by applying mathematical methods such as dynamic programming, calculus of variations, Pontryagin's maximum principle, genetic algorithms, neural networks and nonlinear programming (NLP), among others.

In general, the most common problems for optimal control of the batch distillation process discussed in the literature are:

- **Maximum distillate problem:** To maximize the amount of distillate for a fixed concentration of the most volatile key component for a known operating time (Converse. and Gross, 1963; Diwekar et al.,

1987; Farhat et al. 1990; Diwekar, 1992; Logsdon and Biegler, 1993; Zavala-Loría et al., 2006; Zavala-Loría and Coronado-Velásco, 2008);

- **Minimum time problem:** To minimize the operating time necessary to produce a certain amount of distillate that meets a specified concentration of the most volatile key component (Coward, 1967; Robinson, 1970; Mayur and Jackson, 1971; Hansen and Jorgensen, 1986; Mujtaba and Macchietto, 1988; Diwekar, 1992);

- **Problem of maximum profit:** To maximize a profit function for a specified concentration of product (Kerkhof and Vissers, 1978; Logsdon et al., 1990; Diwekar, 1992);

- **Problem of minimum energy:** Energy requirements are minimized to produce a certain amount of distillate to meet a specified concentration of the most volatile key component (Furlonge et al., 1999; Mukherjee et al., 2001);

- **Maximum thermodynamic efficiency problem:** To maximize the thermodynamic efficiency of the

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process in a fixed time to produce a quantity of distillate complying with a specified concentration of the most volatile key component (Zavala-Loría, 2004; Zavala-Loría and Coronado-Velásco, 2008).

Due to high energy costs, the study of energy consumption is of great interest for industry. In particular, distillation columns use a lot of energy in the form of heat for their operation. Finding how efficient the heat is used in a column operation is an important task. This idea guides the effort of the work presented here. The target is to determine how efficient the heat is used under different operational conditions; in order to do this, the thermodynamic efficiency is calculated and used for solving a problem of optimal control for a batch distillation process using a constant reflux policy. The analysis of thermodynamic efficiency in a batch distillation column has been presented by Zavala-Loría (2004), Kim and Diwekar (2000), and Zavala et al. (2007).

Recently, Zavala-Loría and Coronado-Velasco (2008) used the thermodynamic efficiency to present a new approach to the optimal control problem in a batch distillation column whose mathematical model is presented in Table 1. They considered two binary ideal mixtures: Toluene-Benzene and Cyclohexane-Toluene. The aim of this paper is to present a generalized scheme for the optimal control problem considering non-ideal mixtures.

Table 1: Mathematical model of a batch distillation column (n is the number of components and N the number of equilibrium stages).

$\frac{dB}{dt} = -D_t = -\frac{V}{R_t + 1} \quad (1)$
$\frac{dx_B^{(i)}}{dt} = \left(\frac{V}{B}\right) \left\{ x_B^{(i)} - y_B^{(i)} + \left(\frac{L}{V}\right) [x_1^{(i)} - x_B^{(i)}] \right\}; \quad (2)$ $i = 1, \dots, n$
$\frac{dx_j^{(i)}}{dt} = \left(\frac{V}{H_j}\right) \left\{ y_{j-1}^{(i)} - y_j^{(i)} + \left(\frac{L}{V}\right) [x_{j+1}^{(i)} - x_j^{(i)}] \right\}; \quad (3)$ $i = 1, \dots, n ; j = 1, \dots, N$
$\frac{dx_D^{(i)}}{dt} = \left(\frac{V}{H_D}\right) [y_n^{(i)} - x_D^{(i)}] ; \quad i = 1, \dots, n \quad (4)$
$\sum_{i=1}^n y_j^{(i)} = \sum_{i=1}^n K_j^{(i)} x_j^{(i)} = 1 ; \quad i = 1, \dots, n ; j = 1, \dots, N \quad (5)$

In the same way as in the cited work of Zavala-Loría and Coronado-Velasco (2008), in this paper

the optimal control problem arises from a mathematical model involving the thermodynamic efficiency, defined as:

$$\eta_t = \frac{W_{\min, \text{sep}}}{W_{\text{total}}} = \frac{W_{\min, \text{sep}}}{W_{\min, \text{sep}} + LW} \quad (6)$$

where $W_{\min, \text{sep}}$ is the minimum work required to obtain the specified product purity and LW is the total loss of work, total loss of availability or total loss of exergy obtained from the exergy analysis of the process shown in Figure 1.

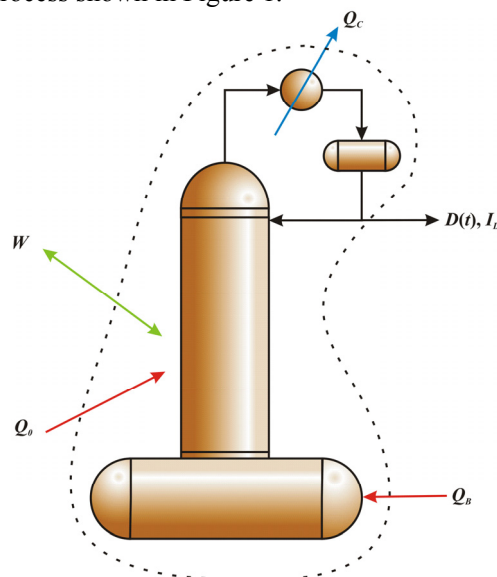


Figure 1: Control volume for discontinuous process.

The vapor-liquid equilibrium (VLE) can be represented by the following equation:

$$K^{(i)} = \frac{y^{(i)}}{x^{(i)}} = \frac{\gamma_i P_i^{\text{sat}}}{\hat{\phi}_i P} ; \quad i = 1, 2, \dots, n \quad (7)$$

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 represents the activity coefficient, P^{sat} is the saturation pressure and $\hat{\phi}$ denotes the partial fugacity coefficient, all referring to component i , and P represents the system pressure.

THERMODYNAMIC EFFICIENCY

Considering a non-isolated control volume (Figure 1), where the process can exchange energy with the environment but does not perform any mechanical work, the exergy balance of the system is:

$$\frac{d(B\mathcal{B}_B)}{dt} = \left(1 - \frac{T_0}{T_B}\right) Q_B - \left(1 - \frac{T_0}{T_D}\right) Q_D - D_t \mathcal{B}_D - LW \quad (8)$$

The terms of the right hand side of Equation (8) represent the difference between the exergy of the streams entering and leaving the system. The term on the left hand side is the change of availability in the reboiler. The function of availability or exergy is defined as:

$$\mathcal{B} = h - T_0 s \quad (9)$$

where h is the enthalpy, s is the entropy, T is the temperature. The reference state is the liquid at a temperature of 25°C and pressure of one atmosphere. By applying an exergy balance at the bottom of the column, the change of availability is given by:

$$\frac{d(B\mathcal{B}_B)}{dt} = B \frac{d(\mathcal{B}_B)}{dt} + \mathcal{B}_B \frac{d(B)}{dt} \quad (10)$$

And, since the overall material balance in the process is given by Equation (1) of Table 1, Equation (10) can be expressed as:

$$\frac{d(B\mathcal{B}_B)}{dt} = B \frac{d(\mathcal{B}_B)}{dt} - D_t \mathcal{B}_B \quad (11)$$

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

$$\mathcal{B} = \mathcal{B}_{\text{phis}} + \mathcal{B}_{\text{chem}} \quad (12)$$

$$\begin{aligned} \frac{d \left[\sum_i x_B^{(i)} \ln \gamma_{i,B} x_B^{(i)} \right]}{dt} &= \sum_i \left\{ \frac{dx_B^{(i)}}{dt} \ln \left[\gamma_{i,B} x_B^{(i)} \right] + x_B^{(i)} \frac{d(\ln \gamma_{i,B})}{dt} \right\} \\ &= \left(\frac{V}{B} \right) \sum_i \left\{ x_B^{(i)} - y_B^{(i)} + \left(\frac{L}{V} \right) \left[x_1^{(i)} - x_B^{(i)} \right] \right\} \ln \left[\gamma_{i,B} x_B^{(i)} \right] + \sum_i \left[x_B^{(i)} \frac{d(\ln \gamma_{i,B})}{dt} \right] \end{aligned} \quad (16)$$

Substituting the above equations on the right hand side of Equation (15) results in:

where $\mathcal{B}_{\text{phis}}$ considers the physical processes that involve thermal interactions with the surroundings and also 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). In addition, the physical component of availability is relatively lower than the chemical component of availability. 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 availability can be expressed as:

$$\mathcal{B}_{\text{chem}} = RT_0 \sum_i x^{(i)} \ln \left[\gamma_i x^{(i)} \right] \quad (13)$$

and the exergy exchange in the reboiler can be calculated as:

$$\begin{aligned} \mathcal{B}_B &= \mathcal{B}_{\text{phis}} + \mathcal{B}_{\text{chem}} = \\ &\mathcal{B}_{\text{phis}} + RT_0 \sum_i x_B^{(i)} \ln \left[\gamma_{B,i} x_B^{(i)} \right] \end{aligned} \quad (14)$$

Taking the derivative of Equation (14) yields:

$$\begin{aligned} \frac{d(\mathcal{B}_B)}{dt} &= \frac{d(\mathcal{B}_{\text{chem}})}{dt} = \\ &RT_0 \frac{d \left\{ \sum_i x_B^{(i)} \ln \left[\gamma_{B,i} x_B^{(i)} \right] \right\}}{dt} \end{aligned} \quad (15)$$

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

$$\frac{d(\mathcal{B}_{\mathcal{B}})}{dt} = \text{VRT}_0 \sum_i \left\{ x_{\mathcal{B}}^{(i)} - y_{\mathcal{B}}^{(i)} + \left(\frac{L}{V} \right) [x_1^{(i)} - x_{\mathcal{B}}^{(i)}] \right\} \ln \gamma_{i,\mathcal{B}} x_{\mathcal{B}}^{(i)} \quad (17)$$

$$+ \text{BRT}_0 \sum_i \left[x_{\mathcal{B}}^{(i)} \frac{d(\ln \gamma_{i,\mathcal{B}})}{dt} \right] - D_t \left[\mathcal{B}_{\mathcal{B},\text{phis}} + \text{RT}_0 \sum_i x_{\mathcal{B}}^{(i)} \ln \gamma_{i,\mathcal{B}} x_{\mathcal{B}}^{(i)} \right]$$

Similarly, the availability of current production that will be used in Equation (8) is calculated using:

$$\mathcal{B}_{\mathcal{D}} = \mathcal{B}_{\mathcal{D},\text{phis}} + \text{RT}_0 \sum_i x_{\mathcal{D}}^{(i)} \ln \gamma_{i,\mathcal{D}} x_{\mathcal{D}}^{(i)} \quad (18)$$

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 constant volume and that ΔH^{vap} is the same for each component and is not related to the temperature, then the Clausius-Clapeyron equation can be used and the first two terms on the right hand side of Equation (8) can be calculated by the following equation:

$$\left(1 - \frac{T_0}{T_{\mathcal{B}}} \right) Q_{\mathcal{B}} - \left(1 - \frac{T_0}{T_{\mathcal{D}}} \right) Q_{\mathcal{D}} = \text{VRT}_0 \ln \left(\frac{\gamma_{1,\mathcal{D}} \Phi_{1,\mathcal{B}} K_{1,\mathcal{B}}}{\gamma_{1,\mathcal{B}} \Phi_{1,\mathcal{D}} K_{1,\mathcal{D}}} \right) \quad (19)$$

where $Q = V\Delta H^{\text{vap}}$, K is the liquid-vapor equilibrium constant and Φ is defined as:

$$\Phi_k \equiv \frac{\widehat{\phi}_k}{\phi_k^{\text{sat}}} \exp \left[- \frac{V_k (P - P_k^{\text{sat}})}{RT} \right]; \quad (20)$$

$k = 1, 2, \dots, n$

Therefore, the term for exergy lost or missed work, LW , can be obtained from Equation (8);

$$LW = \text{VRT}_0 \ln \left(\frac{\gamma_{1,\mathcal{D}} \Phi_{1,\mathcal{B}} K_{1,\mathcal{B}}}{\gamma_{1,\mathcal{B}} \Phi_{1,\mathcal{D}} K_{1,\mathcal{D}}} \right) + D_t \text{RT}_0 \left[\sum_i x_{\mathcal{B}}^{(i)} \ln \gamma_{i,\mathcal{B}} x_{\mathcal{B}}^{(i)} - \sum_i x_{\mathcal{D}}^{(i)} \ln \gamma_{i,\mathcal{D}} x_{\mathcal{D}}^{(i)} \right] + D_t (\mathcal{B}_{\mathcal{B},\text{phis}} - \mathcal{B}_{\mathcal{D},\text{phis}}) \quad (21)$$

$$- \text{VRT}_0 \sum_i \left\{ x_{\mathcal{B}}^{(i)} - y_{\mathcal{B}}^{(i)} + \left(\frac{L}{V} \right) [x_1^{(i)} - x_{\mathcal{B}}^{(i)}] \right\} \ln \left[\gamma_{i,\mathcal{B}} x_{\mathcal{B}}^{(i)} \right] - \text{BRT}_0 \sum_i \left[x_{\mathcal{B}}^{(i)} \frac{d(\ln \gamma_{i,\mathcal{B}})}{dt} \right]$$

If the term $\mathcal{B}_{\mathcal{B},\text{phis}} - \mathcal{B}_{\mathcal{D},\text{phis}}$ in Equation (21) is considered to be equal to zero, then the minimum work required can be calculated as:

$$W_{\min} = D_t \text{RT}_0 \left[\sum_i x_{\mathcal{D}}^{(i)} \ln \gamma_{i,\mathcal{D}} x_{\mathcal{D}}^{(i)} - \sum_i x_{\mathcal{B}}^{(i)} \ln \gamma_{i,\mathcal{B}} x_{\mathcal{B}}^{(i)} \right] \quad (22)$$

$$+ \text{VRT}_0 \sum_i \left\{ x_{\mathcal{B}}^{(i)} - y_{\mathcal{B}}^{(i)} + \left(\frac{L}{V} \right) [x_1^{(i)} - x_{\mathcal{B}}^{(i)}] \right\} \ln \left[\gamma_{i,\mathcal{B}} x_{\mathcal{B}}^{(i)} \right] + \text{BRT}_0 \sum_i \left[x_{\mathcal{B}}^{(i)} \frac{d(\ln \gamma_{i,\mathcal{B}})}{dt} \right]$$

and the thermodynamic efficiency in Equation (6) results in:

$$\eta_t = \frac{\sum_i \left\{ x_{\mathcal{D}}^{(i)} \ln \gamma_{i,\mathcal{D}} x_{\mathcal{D}}^{(i)} - x_{\mathcal{B}}^{(i)} \ln \gamma_{i,\mathcal{B}} x_{\mathcal{B}}^{(i)} + \left(R \left[x_1^{(i)} - y_{\mathcal{B}}^{(i)} \right] + x_{\mathcal{B}}^{(i)} - y_{\mathcal{B}}^{(i)} \right) \ln \left[\gamma_{i,\mathcal{B}} x_{\mathcal{B}}^{(i)} \right] + \left(\frac{B}{V} \right) \left[x_{\mathcal{B}}^{(i)} \frac{d(\ln \gamma_{i,\mathcal{B}})}{dt} \right] \right\}}{(R+1) \ln \left(\frac{K_{1,\mathcal{B}} \Phi_{1,\mathcal{B}} \gamma_{1,\mathcal{D}}}{K_{1,\mathcal{D}} \Phi_{1,\mathcal{D}} \gamma_{1,\mathcal{B}}} \right)} \quad (23)$$

Equation (23) can be reduced if one considers that the changes of activity coefficients in the reboiler are so small that they can be neglected. Then:

$$\eta_t = \frac{\sum_i \left\{ x_B^{(i)} + x_D^{(i)} \ln \gamma_{i,D} x_D^{(i)} + \left[R \left(x_B^{(i)} - y_B^{(i)} \right) - y_B^{(i)} \right] \ln \left[\gamma_{i,B} x_B^{(i)} \right] - y_B^{(i)} \ln \gamma_{i,B} x_B^{(i)} \right\}}{(R+1) \ln \left(\frac{K_{1,B} \Phi_{1,B} \gamma_{1,D}}{K_{1,D} \Phi_{1,D} \gamma_{1,B}} \right)} \quad (24)$$

Equation (24) is consistent with the equation proposed by Zavala-Loría and Coronado-Velasco (2008) for ideal mixtures:

$$\eta_t = \frac{\sum_i \left\{ x_B^{(i)} + x_D^{(i)} \ln x_D^{(i)} + \left[R \left(x_B^{(i)} - y_B^{(i)} \right) - y_B^{(i)} \right] \ln x_B^{(i)} - y_B^{(i)} \ln x_B^{(i)} \right\}}{(R+1) \ln \left[\frac{x_D^{(1)} (\alpha_{1,2} - 1) + 1}{x_B^{(1)} (\alpha_{1,2} - 1) + 1} \right]} \quad (25)$$

The solution of Equation (23) or its simplification [Equation (24)] requires the calculation of activity coefficients of the mixtures at the top and bottom of the column, which can be obtained with an appropriate solution model.

THE OPTIMAL CONTROL PROBLEM

To solve the problem of optimal control, this paper uses Wilson's equation and activity coefficients obtained with the following equation:

$$\ln(\gamma_k) = 1 - \ln \left(\sum_j x^{(j)} \Lambda_{kj} \right) - \sum_i \left(\frac{x^{(i)} \Lambda_{ik}}{\sum_j x^{(j)} \Lambda_{ij}} \right); \quad (26)$$

$$k = 1, 2, \dots, n$$

with:

$$\Lambda_{ij} \equiv \frac{v_j}{v_i} \exp \left(- \frac{\lambda_{ij} - \lambda_{ji}}{RT} \right) \quad (27)$$

In a dynamic behavior of batch distillation, the thermodynamic efficiency is a set of values that depends not only on the energy needs of the process, but also indirectly on time since the amounts and compositions of the product streams change constantly. Then, the process optimization (optimal control problem) gives a set of values for the thermodynamic efficiency and an average (η_{av}) can be calculated for the total distillation time (t_f):

$$\eta_{av} = \frac{\int_0^{t_f} \eta_t dt}{t_f} \quad (28)$$

The problem of maximum thermodynamic efficiency arises considering that, within the production time ($0.0 \leq t \leq t_f$), an average concentration of product previously established within the valid range ($0.0 \leq x_{D,av}^{(i)} \leq 1.0$) is obtained.

The smallest possible value of the reflux ratio is zero ($R_t \geq 0.0$); therefore, the problem of optimal control can be posed as follows:

$$\text{Max}_{R_t, N, t} \eta_{av} = \frac{\int_0^{t_f} \eta_t dt}{t_f} \quad (29)$$

s.t.:

$$x_{D,av}^{(i)} = \frac{\int_0^{t_f} D_t x_D^{(i)} dt}{\int_0^{t_f} D_t dt} = x_D^*$$

The restrictions also include the equations of the mathematical model of a batch distillation process shown in Table 1 [Equations (1) to (5)]. To solve the optimal control problem, a NLP method is used for which it is necessary to discretize the state variables, done by using the technique of direct orthogonal collocation. Therefore, the system of Equations (29) plus Equations (1) to (5) can be represented as:

Maximize $_{R_t, N, t_k, x_k}$

$$\eta_{av} = \frac{1}{t_f} \sum_k w_k \eta_k \quad (k = 1, \dots, ncol + 2)$$

s.t.:

$$x_{D,av}^{(i)} = \frac{\sum_{k=1}^{ncol+2} w_k D(t)_k x_{D,k}^{(i)}}{\sum_{k=1}^{ncol+2} w_k D(t)_k} = x_{D,opt}^{(i)}$$

$$\sum_{k=1}^{ncol+2} p_k(t) B = -D(t) = -\frac{V}{R_t + 1}$$

$$\sum_{k=1}^{ncol+2} p_k(t) x_B^{(i)} = \frac{V}{B} \left\{ x_B^{(i)} - y_B^{(i)} + \frac{L}{V} [x_1^{(i)} - x_B^{(i)}] \right\}$$

$$\sum_{k=1}^{ncol+2} p_k(t) x_j^{(i)} = \frac{V}{H_j} \left\{ y_{j-1}^{(i)} - y_j^{(i)} + \frac{L}{V} [x_{j+1}^{(i)} - x_j^{(i)}] \right\} \quad (30)$$

$$\sum_{k=1}^{ncol+2} p_k(t) x_D^{(i)} = \frac{V}{H_D} \left\{ y_N^{(i)} - x_D^{(i)} \right\}$$

$$K_j^{(i)} = \frac{\hat{\phi}_j^L}{\hat{\phi}_j^V}$$

$$y_j^{(i)} = K_j^{(i)} x_j^{(i)}$$

$$\sum_{i=1}^{nc} y_j^{(i)} = 1$$

$$i = 1, \dots, nc \quad ; \quad j = 1, \dots, N$$

$$y_{j=0}^{(i)} = y_B^{(i)} \quad ; \quad x_{j=N+1}^{(i)} = x_D^{(i)}$$

$$0 \leq x \leq 1$$

$$0 \leq R_{MIN} \leq R_t$$

$$0 \leq t \leq t_f$$

where ncol is the number of collocation points, $p(t)$ are the collocation polynomial coefficients and w are the weights of the Gaussian quadrature.

RESULTS AND DISCUSSION

In this work, the batch distillation process was performed by introducing the feeding to the top of the column at its temperature of saturation, neglecting the accumulation of vapor in each stage of equilibrium, constant vapor flow along of the column, constant pressure, total condenser and adiabatic column. The operating time for the resolution of the optimal control problem is considered in the steady state (obtaining product). In this paper, the solution of the problem of maximum thermodynamic efficiency uses Sequential Quadratic Programming (SQP); the state variables are discretized and solved using the technique of direct orthogonal collocation. Also, the control variable is parameterized using optimal constant reflux.

According to the solution of Equation (23) or Equation (24), the R_t reflux ratio has an inverse effect on the thermodynamic efficiency of the process since the thermodynamic efficiency decreases when R_t increases due to increased energy needs. The binary mixture Ethanol (E)-Water (W) was used as an example to solve the optimal control problem shown in the system of Equations (30).

Case-Study: Ethanol - Water Mixture

The conditions used for solving the optimal control problem by maximizing the thermodynamic efficiency are given in Table 2. The predicted azeotropic point for the mixture of Ethanol - Water using Wilson's equation was 0.8961.

The optimum average thermodynamic efficiency obtained was 37.95%. The other results for the solution of the control problem are shown in Figures 2, 3, 4, 5, 6 and 7 and are discussed below.

Table 2: Input data for the Thermodynamic Efficiency Optimal Control Problem.

Variable/Parameter	Amount	Unit
Feed (F)	100.00	kmol
Vapor rate (V)	33.00	kmol/h
Condenser liquid holdup (H_D)	10.00	kmol
Tray liquid holdup (H_j)	1.00	kmol
Batch time (t_f)	2.00	h
$Z_{Ethanol}$	0.48	
Z_{Water}	0.52	
Theoretical stages (N)	13	
Purity constraint ($X_{D,Average}$)	0.88	

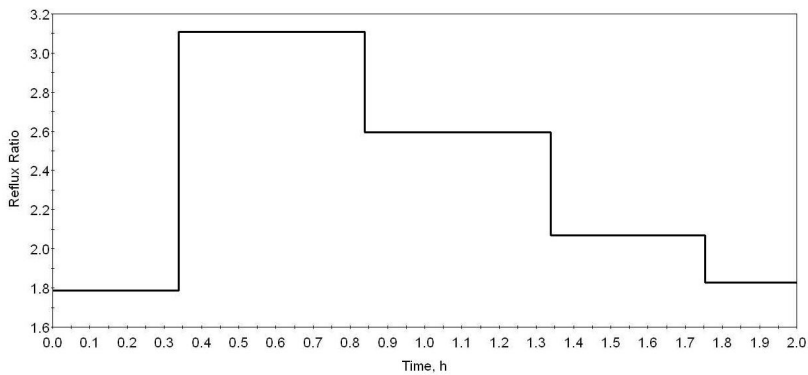


Figure 2: Reflux ratio optimal profile.

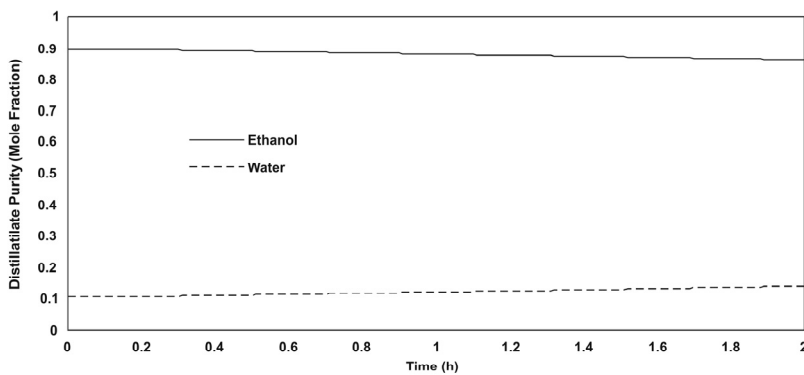


Figure 3: Profiles of product mole fraction.

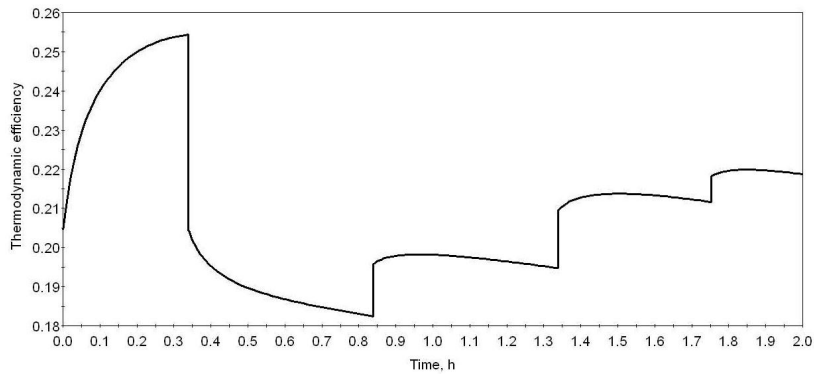


Figure 4: Thermodynamic efficiency profile.

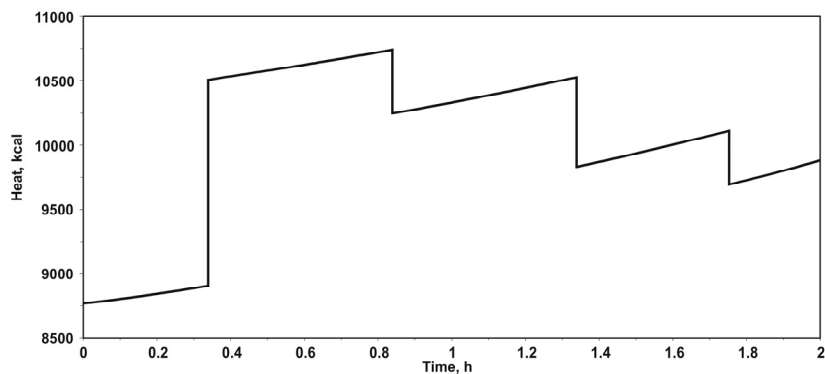


Figure 5: Heat supplied to the reboiler.

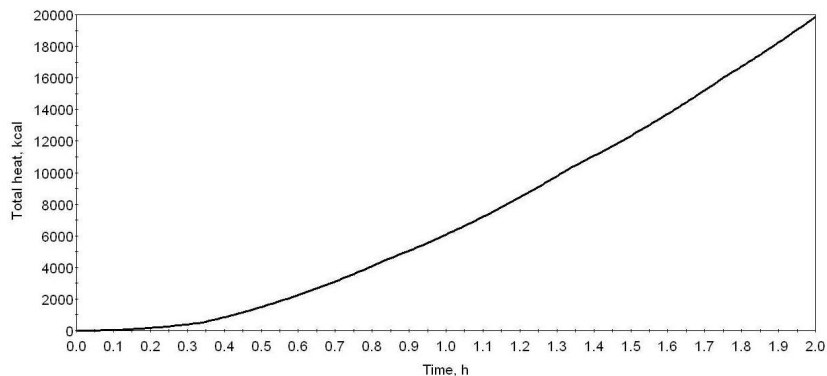


Figure 6: Heat supplied (accumulated) to the reboiler.

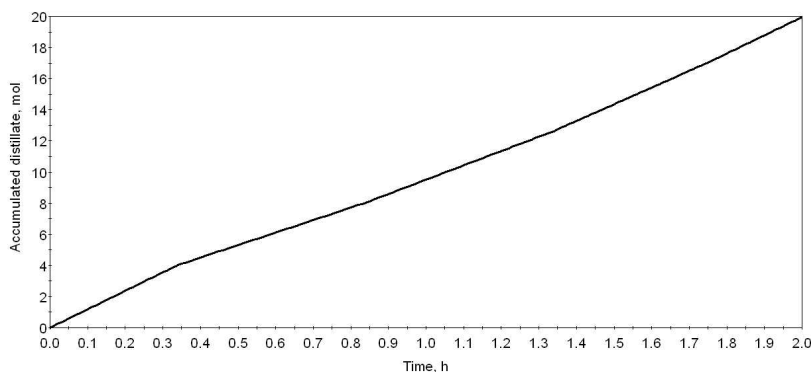


Figure 7: Profile of accumulated distillate.

In Figures 2 and 4, it is possible to observe the inverse relationship between the optimal reflux ratio and the thermodynamic efficiency. Figure 3 shows the profile of the mole fraction of the product under the desired average concentration. The effect of reflux ratio on the energy needs is also notable in Figure 5 because a smaller reflux ratio requires supply of a smaller quantity of heat. The profile of accumulated heat supplied to the process is shown in Figure 6. Figure 7 shows the accumulated distillate profile, which is 20% of the amount fed. These figures (2 to 7) are the result of the optimal control problem solution, using a NLP solver with the following conditions: 2 hours for the total time, piecewise-constant for the control type (reflux ratio) and continuous allowable values.

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 propose and solve an optimal control problem called the

maximum thermodynamic efficiency. The equation obtained is a generalization of the equation developed by Zavala-Loría and Coronado-Velasco (2008) and can be used to simulate the separation of ideal and non-ideal mixtures.

The results obtained by solving the optimal control problem allowed us to observe the relationship between reflux and thermodynamic efficiency of the process. Furthermore, variables such as the desired product purity and production time also affect the thermodynamic efficiency of the process. The increase in purity of the product requires a greater amount of reflux to obtain a concentration close to the steady state concentration obtained at total reflux. A longer production time requires a greater amount of reflux in order to achieve the desired purity due to the depletion of the components.

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NOMENCLATURE

H_j	molar hold-up on tray j	
H_D	molar hold-up on the condenser	
h	enthalpy	J/mol
s	entropy	J/mol K
V	vapor flow rate	mol/h
L	liquid flow rate	mol/h
D_t	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
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	
β	availability	
η	thermodynamic efficiency	
ΔH^{vap}	heat of vaporization	

Subscripts

0	reference
c	condenser
f	end
D	distillate
B	reboiler

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