

Economic Optimization of the Reflux Ratio of Two Components Stage Distillation Columns

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Abstract

Distillation columns are complex processes for modeling and controlling. These columns are significant parts of most chemical industries for separation of components. Control of this process is essential for achieving certain purity for products with a minimum cost. However, nonlinearities, multivariable interaction, non-stationary behavior and severity of disturbances inside the column made this process too complex for controlling. In this study a graphical method is applied to model steady state continuous two components distillation column. First, a MATLAB code was developed to solve the mathematical model of the column. Then, the column was simulated using HYSYS software. Finally, the reflux ratio of this column was optimized to minimize the operating cost. A formula is presented to calculate the optimum value of this reflux ratio as an exponential function of a certain economic parameter of energy prices and depreciation costs. It is resulted that at low energy prices or high equipment depreciation costs, the optimum reflux factor is high.

Keyword: Two Components Mixture; Distillation Column; Optimized Reflux Ratio; Operating Costs

Introduction

Distillation columns are complex processes for modeling and controlling that are significant parts of most chemical industries for separation of components (Luyben, 1990; Balchen and Mumme, 1998; Luyben, 1992; Shinskey, 1984; Enagandula and Riggs, 2006). Control of this process is essential for achieving certain purity for products with a minimum cost. But, nonlinearities, multivariable interaction, non stationary behavior and severity of disturbances inside the column made this process too complex for controlling (Hurowitz, 2003). The basis of this process is thermodynamic vapor-liquid equilibrium (VLE). Distillation causes the separation of chemical components and provides different concentrations in both phases.

Diwekar et al. (1985) optimized the multicomponent batch distillation columns and formulated the optimization problem for the single-fraction and multi-fraction batch distillation columns

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operating under variable and constant reflux conditions. Ren et al. (2010) presented a mathematical model for operation profits with reflux ratio of a stage distillation column. They solved the nonlinear objective function with an improved particle swarm algorithm to optimize the reflux ratio. Mauhar et al. optimized the distillation process of Propylene-Propane using Aspen Plus simulation engine, based on the real operating data taken from the factory (Mauhar et al. 2004). They optimized the right combination of pressure and reflux rate to minimize the energy consumption in the reboiler and to obtain the required product purity. Fazlali et al. (2009) optimized operating conditions of an atmospheric distillation unit of a petroleum refinery using a simulator for earning more overhead products. They presented a net economical balance between the increments of the overhead products and the energy consumption for an energy saving in the refinery. Chen and Lin (2001) obtained the optimum reflux ratio of distillation towers in petroleum refining processes (propylene splitter and debutanizer plants) using an optimization software. In the present study, the enthalpy-concentration method (Treybal, 1981) is used to simulate steady state continuous two components distillation columns. This study accommodates the experience of the authors in both fields as they modeled binary distillation columns via general coding language, MATLAB as well as industrial dynamic simulation package, HYSYS.

Method and material

Distillation uses the degradation of heat to drive a chemical separation (Henley and Seader, 1981; King, 1971; Robinson and Gilliland, 1950). To achieve separation by distillation or other equilibrium countercurrent exchange processes a minimum quantity of internally circulating fluid is required. In distillation the vapor-liquid countercurrent flows are typically established by a continuous reflux. A flow of liquid (L) maintained at its boiling point and of vapor (G) are circulated between stages in order to purify a quantity of feed per unit time (F) into products. Figure 1 depicts the purification of the feed flow where the distillate (D) is being enriched with the more volatile component and bottoms (W) with the less volatile. In this Figure, the trays are numbered top to down, and subscripts indicate the tray from which a stream originates. The bar sign over a variable indicates that it applies to the section of the column below the point of introduction of the feed. x , y and z are mole fractions of the more volatile component in liquid, vapor and a mixture of the two phases, respectively. Also, Q_C and Q_B are the heats of condenser and reboiler, respectively. In distillation heat is added below the feed point, that is, to the stripping section of the column, to drive off volatile materials into the descending liquid stream. Similarly, heat is removed above the feed point, that is, to the rectifying section of the column, to condense less volatile materials out of the ascending vapor stream. This Figure introduces the variables used and points out the six valves available to control the column. No matter which valve is used for composition control or how it is used, fundamentally there are three factors that could be manipulated: The feed split, the fractionation, and the reflux ratio. An overall material balance for the column indicates that the distillate plus the bottoms should equal the feed flow. The feed split is simply the ratio of the distillate to bottoms. The other fundamental variable is the fractionation which is the amount of separation that occurs per stage. The overall fractionation in a column depends on the number of stages, the energy input, and the difficulty of the separation. Valves number 2 and 3 controls the reflux ratio in the distillation operation. In a distillation column the liquid and vapor flows are almost unchanged in a subsection containing no heat exchangers or side-stream inputs or outputs. By assuming constant flows and considering mass balance, one can obtain linear relations, known as operating lines, for the components concentrations in the flow streams passing between adjacent stages. Equilibrium curves limit the

concentrations of flow streams leaving a stage. Thus, concentration differences in the flow streams at any point in the column are bounded by the operating lines and the equilibrium curve.

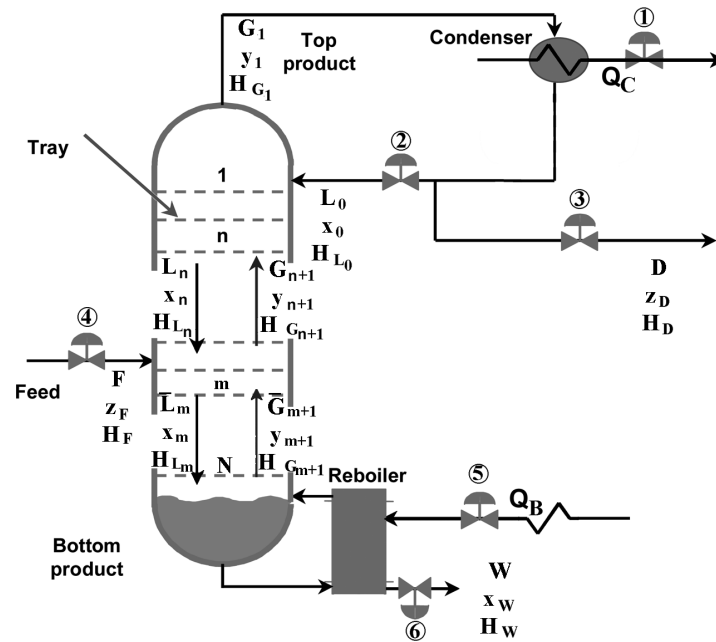


Figure 1. Schematic of distillation column.

In the aforementioned isolated column, heat losses are assumed to be negligible. Therefore, using overall mole and enthalpy (H) balances we have:

$$F = D + W \quad (1)$$

$$Fz_F = Dz_D + Wx_W \quad (2)$$

$$Q_B = DH_D + Wx_W - FH_F + Q_C \quad (3)$$

The distillate product may be liquid, vapor, or a mixture of both. The reflux, however, should be liquid. The molar ratio of reflux to withdrawn distillate is taken as the reflux ratio ($R = \frac{L_0}{D}$).

Therefore, using mole and enthalpy balances over the condenser we have:

$$G_1 = D(R + 1) \quad (4)$$

$$G_1 y_1 = Dz_D + L_0 x_0 \quad (5)$$

$$Q_C = D[(R + 1)H_{G_1} - RH_{L_0} - H_D] \quad (6)$$

Mole and enthalpy balances for the enriching section (section of the column above the feed point) would be as follows:

$$G_{n+1} = L_n + D \quad (7)$$

$$G_{n+1} y_{n+1} = L_n x_n + Dz_D \quad (8)$$

$$G_{n+1} H_{G_{n+1}} = L_n H_n + DH_D + Q_C \quad (9)$$

Also, mole and enthalpy balances for stripping section (section of the column below the feed point) are:

$$\bar{L}_m = \bar{G}_{m+1} + W \quad (10)$$

$$\bar{L}_m x_m = \bar{G}_{m+1} y_{m+1} + W x_W \quad (11)$$

$$\bar{L}_m H_m = \bar{G}_{m+1} H_{\bar{G}_{m+1}} + W H_W - Q_B \quad (12)$$

Equations 1 to 12 are basic equations for complete definition of the problem and their solutions gives out information about the behavior of the distillation column under different conditions.

In this section Ponchon-Savarit graphical method was used to develop the relation between tray numbers, liquid/vapor ratios, and product compositions (Treybal, 1981). Although this method can handle many situations, it requires detailed enthalpy data as well. Assuming ideal liquid solution, liquid enthalpy is obtained by the following equation:

$$H_L = \left[x M_{Methanol} C_{P,Methanol} + (1-x) M_{Water} C_{P,Water} \right] (T - T_{ref}) \quad (13)$$

Where C_P is heat capacity of pure liquid (Perry and Green, 1999), and T_{ref} is the reference temperature (which is 292.69 K in this work). For the present purpose, saturated vapor enthalpies can be calculated by assuming that the unmixed liquids are first heated to the dew point of the liquid T_D , and then vaporized at this temperature, where the vapors are mixed. Therefore, gas enthalpies are obtained by the following equation:

$$H_G = y M_{Methanol} \left[C_{P,Methanol} (T_D - T_{ref}) + \lambda_{Methanol} \right] + (1-y) M_{Water} \left[C_{P,Water} (T_D - T_{ref}) + \lambda_{Water} \right] \quad (14)$$

Where λ is the latent heat of evaporation of pure substance at T_D (Perry and Green, 1999). Combining equations 1 to 12 yields to the following equations:

$$\frac{z_D - y_{n+1}}{y_{n+1} - x_n} = \frac{Q' - H_{G_{n+1}}}{H_{G_{n+1}} - H_{L_n}} \quad (15)$$

$$\frac{y_{m+1} - x_W}{y_{m+1} - x_m} = \frac{H_{\bar{G}_{m+1}} - Q''}{H_{\bar{G}_{m+1}} - H_{\bar{L}_m}} \quad (16)$$

$$\frac{x_D - x_F}{x_F - x_W} = \frac{Q' - H_F}{H_F - Q''} \quad (17)$$

Where, $Q' = (H_D + \frac{Q_C}{D})$ is the heat removed per mole of distillate in the condenser. Also $Q'' = (H_W - \frac{Q_B}{W})$ is the net flow of heat per mole of residue. Equations 15 to 17 represent seven points as listed below:

$$[z_D, Q'], [y_{n+1}, H_{G_{n+1}}], [x_n, H_{L_n}], [x_W, Q''], [y_{m+1}, H_{\bar{G}_{m+1}}], [x_m, H_{\bar{L}_m}], [z_F, H_F]$$

$[z_D, Q']$ and $[x_W, Q'']$ are fixed. These equations represent a set of straight lines on the H_{x_i}, y_i diagram which pass $[z_D, Q']$, $[x_W, Q'']$, and $[z_F, H_F]$ known as upper operating point, lower operating point, and feed point, respectively.

The minimum reflux ratio (R_m) is the maximum ratio which requires an infinite number of trays for the desired separation, and it is associated with the minimum reboiler heat load and condenser cooling load for the separation. Also the minimum number of trays (N_m) is obtained when the reflux ratio equals infinity.

Modelling

A code was developed using MATLAB. In order to reduce computation time, matrix operation facilities were used. These operators can minimize the number of loops applied in the program. The solution procedure is described as below and more descriptions on the dimensionless mathematical model are presented in references (Treybal, 1981).

Equilibrium tie-line from y_1 (where $y_1 = x_D$) locates x_1 . x_1 connected to $[z_D, Q']$ locates y_2 . Equilibrium tie-line from y_2 locates x_2 . x_2 connected to $[z_D, Q']$ locates y_3 . And so on as y_n connected to $[z_D, Q']$ locates x_n . This trend continues up to a point where the tie-line passes z_F , namely the feed composition. In this way the equilibrium stages are determined (each tie line represent an equilibrium stage). Locate x_W at intersection of $x=x_W$ and the bubble point curve. The reboiler is taken as an equilibrium stage; hence x_W and y_{N+1} are in equilibrium with each other. The tie line from x_W locates y_{N+1} . Straight line connecting y_{N+1} to the lower operating point $[x_W, Q'']$ locates x_N on the saturated liquid bubble point curve. x_N locates y_N with the equilibrium tie line equation. Straight line connecting y_N to the operating point $[x_W, Q'']$ locates x_{N+1} . And so on, using tie line and operating point relations for number of equilibrium stages until x_F is reached or crossed by a tie line.

Results and discussions

The graphical model was evaluated by HYSYS simulation for operating conditions of Table 1 and the results are presented in Table 2. It can be seen that results from the graphical model agree well with the HYSYS simulation results for the assumed condition. Given the complexity of distillation and the influence of many parameters involved, the prediction from the model has proved to be very accurate.

Table 1. Operating conditions of distillation column.

Lighter component	Benzene	Methanol	mXylene
Heavier component	Toluene	Water	oXylene
System pressure (kpa)	101.325	101.325	101.325
Temperature of food (K)	298.15	298.15	298.15
feed flow rate (kmole/hr)	100	100	100
mole fraction of lighter component in food	0.5	0.5	0.5
mole fraction of lighter component in liquid phase in condenser	0.99	0.99	0.99
mole fraction of lighter component in liquid phase in reboiler	0.01	0.01	0.01
β =reflux ratio/minimum reflux ratio	1.2342	1.247	1.1

The x-y and H-xy diagrams of the graphical model for the conditions of Table 1 are given in Figures 2 and 3. As shown in Figures 4 and 5, mole fraction of lighter component in both liquid and vapor phases and also the temperature of solution decrease down the distillation column.

Table 2. Comparison the results of graphical model (programmed by MATLAB) and HYSYS simulation.

	Benzene-Toluene		Methanol-Water		mXylene-oZylene	
	HYSYS simulation	Graphical model	HYSYS simulation	Graphical model	HYSYS simulation	Graphical model
Minimum number of trays	10.666	9.1687	6.41	5.859	80.207	65.61
Actual number of trays	23.097	21	16.216	14	187.011	154
Optimal feed stage	11.545	10	8.108	7	93.505	77
Condenser temperature (K)	353.86	353.797	340.37	338.415	412.19	412.328
Reboiler temperature (K)	383.15	383.242	370.34	372.477	416.85	717.404
Condenser duty ($kJ \cdot hr^{-1}$)	4.349×10^6	3.858×10^6	3.319×10^6	3.228×10^6	3.456×10^7	2.701×10^7
Reboiler duty ($kJ \cdot hr^{-1}$)	5.416×10^6	5.06×10^6	3.838×10^6	3.692×10^6	3.694×10^7	2.969×10^7
Minimum reflux ratio	1.413	1.1921	0.594	0.666	16.124	12.657

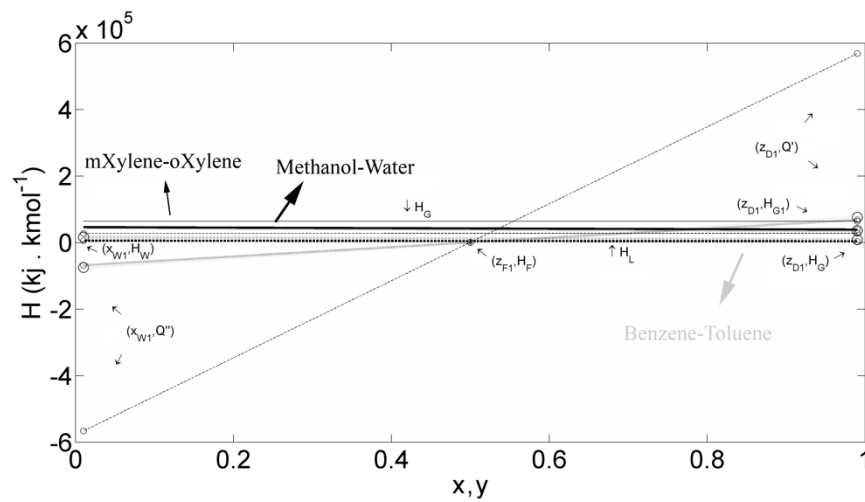


Figure 2. Enthalpy-Concentration diagram of solved graphical model for conditions of Table 2.

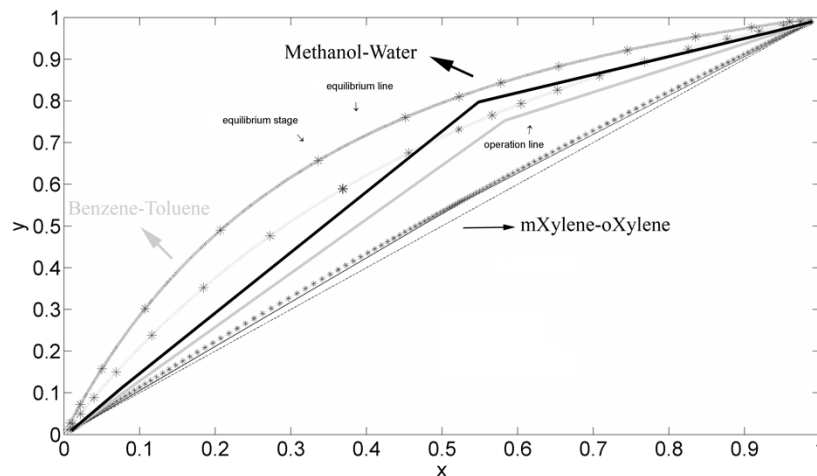


Figure 3. Vapor-Liquid equilibrium diagram of solved graphical model for conditions of Table 2.

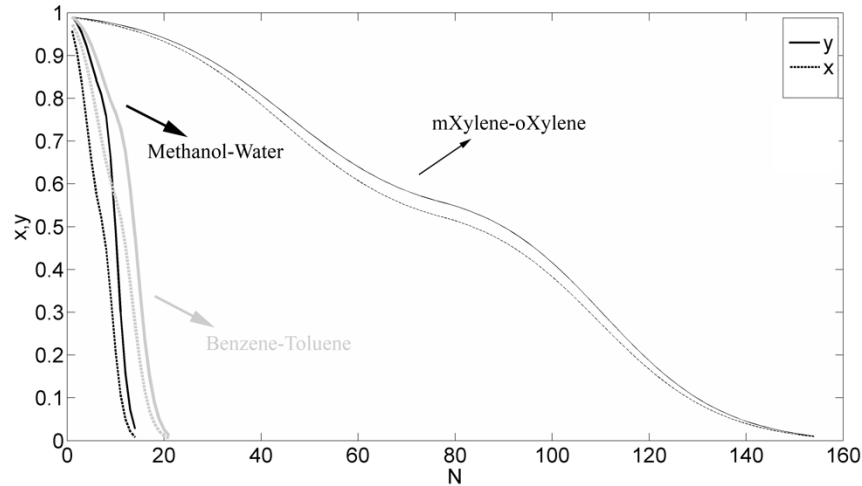


Figure 4. Predicted mole fraction of light component in vapor and liquid phases by graphical model for conditions of Table 2.

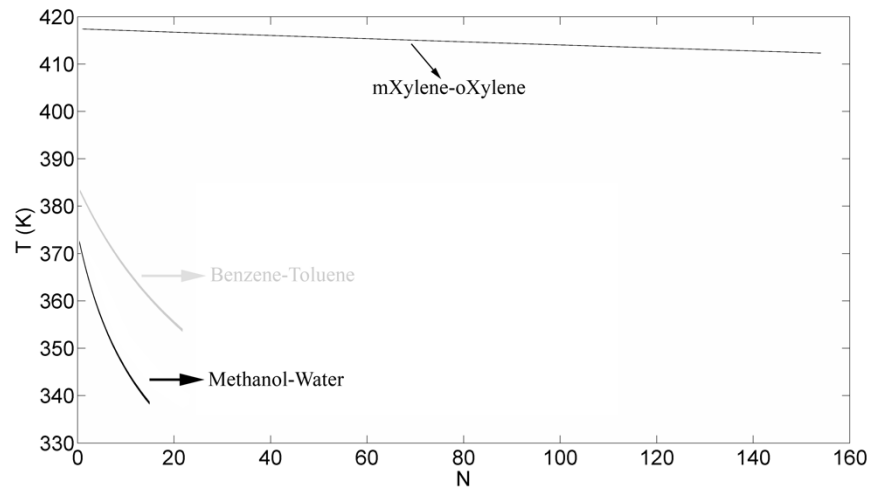


Figure 5. Predicted solution temperature by graphical model for conditions in Table 2.

As with all the industrial processes, the optimum situation for a distillation process is to achieve separation under the most profitable operating conditions. For an operating distillation column, several parameters can be adjusted to optimize the operating costs, e.g. the diameter of the column, reflux ratio, operating pressure, temperature of the condenser and reboiler, etc. (Talifu and Luo, 2005). The optimization of the reflux ratio is of vital importance profit-wise. Any reflux ratio between minimum and infinity provides the desired separation, with the corresponding number of theoretical trays required, varying from infinity to the minimum. Determination of the number of trays for several values of R , together with the limiting values of N_m and R_m , usually allows plotting a curve with sufficient accuracy for most purposes.

Figure 6 shows the effect of β on the actual number of trays and also the total required duty (sum of reboiler and condenser duties). As shown in the Figure, with an increase in β , total required duty undergoes a liner increase, but the actual number of trays decreases nonlinearly. At the minimum reflux ratio, the column requires an infinite number of trays, and consequently the equipment depreciation costs become infinite, but the energy costs would be the least. As R increases, the number of trays rapidly decreases, until it reaches a minimum. The heating and

cooling requirements increase almost proportionally with reflux ratio, as shown. For a stage distillation column, dispensing the costs of raw materials and labor, the operational costs can be defined as:

$$\text{Operational costs} = \text{Equipment depreciation costs} + \text{Energy costs}$$

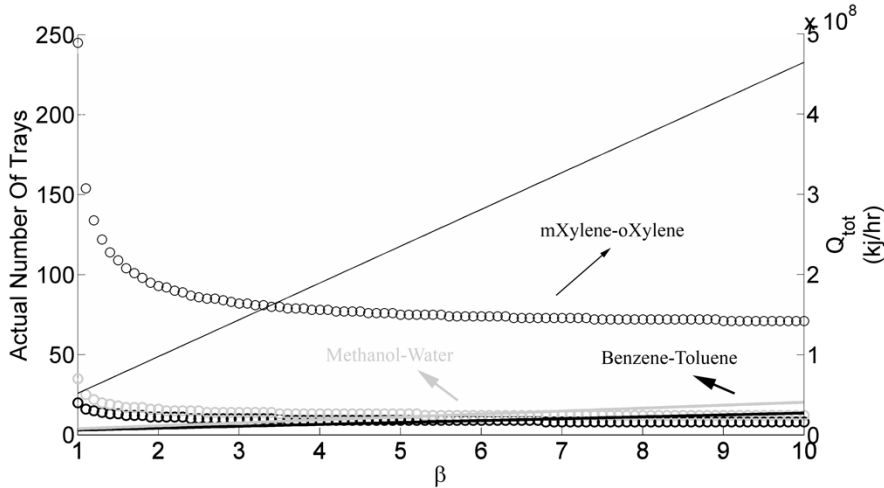


Figure 6. Effect of β on the actual number of trays and total required duty for conditions of Table 2.

The operating cost curve must therefore pass through a minimum at the optimum reflux ratio. Therefore, we define an economic parameter (ϕ) as blow:

$$\phi = \frac{\text{Energy Cost } (\$.kw^{-1}.hr^{-1})}{\text{Energy Cost } (\$.kw^{-1}.hr^{-1}) + \text{One Tray Depreciation Cost } (\$.hr^{-1})} \quad (18)$$

Now we can optimize the reflux ratio through minimizing the operating cost parameter which is calculated by the following equation, as shown in Figure 7 (for listed parameters of Table 2 and $\phi=0.02$). In this case, the minimum value for β is 1.247, which was used to compare current model with HYSYS simulation results.

$$\Phi = \frac{Q_{tot}}{3600} \phi + N_{act} (1 - \phi) \quad (19)$$

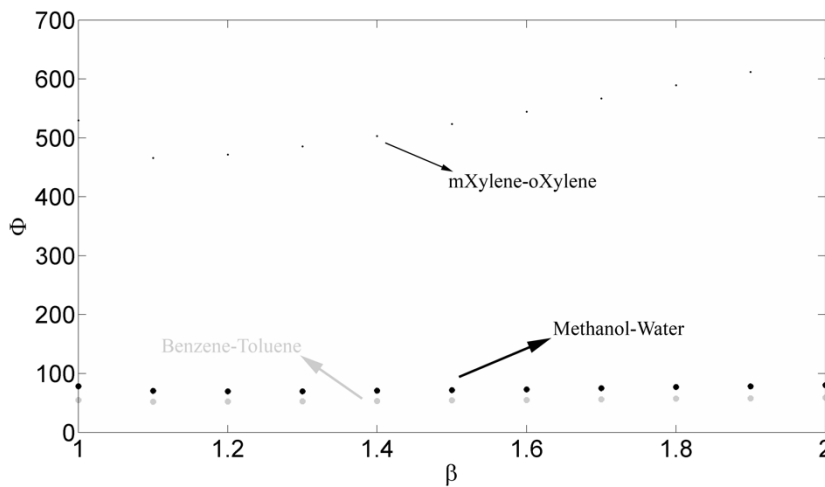


Figure 7. Most economical (optimum) reflux ratio for conditions of Table 2.

Figure 8 shows the effect of economic parameter on the optimum reflux factor (β_{opt}). As shown in this Figure, at low energy prices or high equipment depreciation costs (smaller value of ϕ), the optimum reflux factor is high, and at low equipment depreciation costs or high energy prices (larger value of ϕ), the optimum reflux factor is low. The fitting formulations for optimum values of reflux factor would be:

$$\text{Methanol-Water: } \beta_{opt} = 0.1068\phi^{-0.4422} + 0.6446 \quad (20)$$

$$\text{Benzene-Toluene: } \beta_{opt} = 0.09864\phi^{-0.4166} + 0.7628 \quad (21)$$

$$\text{mXylene-oXylene: } \beta_{opt} = 0.03108\phi^{-0.5456} + 0.8959 \quad (22)$$

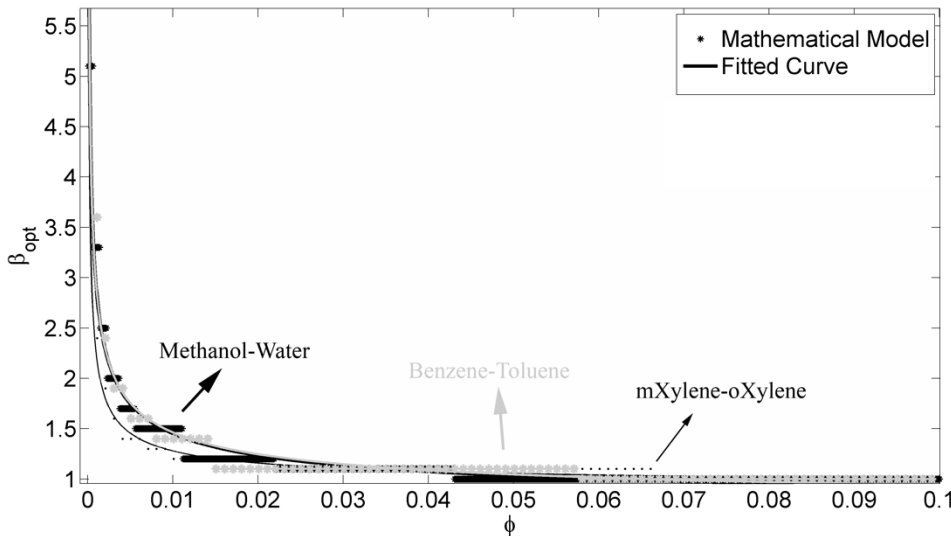


Figure 8. Effect of economic parameter (ϕ) on the optimum reflux factor (β_{opt}).

The presented method can be used for all operating conditions of two components distillation columns with negligible error.

Conclusion

Distillation columns are important parts of separation procedure in the chemical industries. Modeling of this column is necessary for controlling the process and also achieving certain purity for products with a minimum cost. But, nonlinearities, multivariable interaction, non-stationary behavior and severity of disturbances inside the column made this process too complex for modelling. The Ponchon-Savarit graphical method was used to develop the relation between tray numbers, liquid/vapor ratios, and product compositions. This model was established to optimize the operating reflux ratio of the column for the operating profit of two components (*i.e.* Methanol-Water, Benzene-Toluene, and mXylene-oXylene) stage distillation column. This graphical model was evaluated by HYSYS simulation. It was observed that the results from the model agree well with simulation results. Finally, a fitting relation was introduced to calculate the optimum reflux ratio of the distillation column. The optimum reflux factor was defined as a function of energy prices and equipment depreciation costs. It was concluded that at low energy prices or high equipment depreciation costs, the optimum reflux factor is high, whereas at low equipment depreciation costs or high energy prices, the optimum reflux factor is low.

List of Symbols

C_p	Heat capacity at constant pressure (j.gr-1)
D	Distillate rate (kmol.hr-1)
F	Feed rate (kmol.hr-1)
G	Vapor rate in enriching section (kmol.hr-1)
\bar{G}	Vapor rate in stripping section (kmol.hr-1)
H	Molar enthalpy (j.mol-1)
L	Liquid rate in enriching section (kmol.hr-1)
\bar{L}	Liquid rate in stripping section (kmol.hr-1)
L_0	External reflux rate (kmol.hr-1)
M	Molecular weight (gr.mol-1)
N_{act}	Actual number of trays
N_{min}	Minimum number of trays
Q_B	Heat added in the reboiler (kj.hr-1)
Q_C	Heat removed in the condenser (kj.hr-1)
Q_{tot}	Total duty (kj.hr-1)
R	Reflux ratio
R_m	Minimum reflux ratio
T	Solution temperature (K)
W	Residue rate (kmol.hr-1)
x	Mole fraction of more volatile component in the liquid
y	Mole fraction of more volatile component in the vapor
Z	Average mole fraction of more volatile component in the mixture of liquid and vapor phases
B	Reflux factor
β_{opt}	Optimum reflux factor
λ	Latent heat of vaporization (j.gr-1)
Φ	Economic parameter

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