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Optimization of the reflux ratio of benzene-toluene stage distillation columns by the Cuckoo algorithm

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Abstract: In this study, an enthalpy-concentration method was applied in order to model a steady state continuous benzene-toluene mixture distillation column. For a distillation tower such as the benzene-toluene splitter, there are relatively few degrees of freedom that can be manipulated in order to minimize the total annualized cost. The reflux ratio can influence the steady-state operating point and therefore influence the total annualized cost. The trade-offs between reflux ratios and total annualized cost were discussed. The Cuckoo optimization algorithm was applied to obtain a correlation for the optimum value of the reflux ratio as a power function of the economic parameters of energy price and capital cost. The results show that, at low energy price or high capital cost, the optimum reflux factor is high.

Key words: Benzene-toluene mixture, distillation column, Cuckoo optimization algorithm, optimized reflux ratio, total annualized cost

1 Introduction

As an important part of most chemical plants, distillation remains as the most important separation technique in chemical process industries (Luyben, 1990) and is a complex process for modeling and controlling (Balchen and Mumme, 1988; Luyben, 1992; Shinskey, 1984). About 95 percent of the separation processes in the chemical industries use distillation columns (Enagandula and Riggs, 2006), and close control is necessary to achieve the desired product purity at minimum cost. Achieving control of an integrated distillation column is difficult due to the nonlinearities of the process, multivariable interaction, non-stationary behavior and severe disturbances inside the column (Hurowitz et al, 2003). Moreover, continuous distillation may show more dynamic behaviors during the process. The basis of distillation is vapor-liquid equilibrium. Distillation is applicable in the separation of chemical components, where concentrations in both phases differ from each other.

Diwekar et al (1989) studied the optimization of multi-component distillation columns, and presented formulation for single-fraction and multi-fraction batch distillation columns under constant and variable reflux ratios. Ren et al (2010) established a model for a stage distillation column. In order to optimize the reflux ratio by solving the nonlinear objective function, an improved particle swarm algorithm was developed for improving the searching ability of the basic particle swarm algorithm. Optimization of propylene-propane distillation was carried out by Mauhar et al (2004) using Aspen Plus simulation engine. A suitable combination of pressure and reflux ratio was found to minimize the energy consumption in the reboiler and to obtain the required product purity.

Fazlali et al (2009) optimized operating conditions of petroleum refinery distillation columns by means of a simulator with the aim to reduce energy consumption. In the next step the optimization results from the simulator were applied in the real unit. Chen and Lin (2001) studied the optimization of distillation column reflux ratios in petroleum refining. In their work, they explored the optimum reflux ratios of two distillation columns used in petroleum refining: one was a propylene splitter, and another was a debutanizer used in a fluid catalytic cracking plant.

Economic calculations are important in industrial designs. In our previous study, a simple method was developed for optimizing a methanol-water distillation column (Abolpour et al, 2013). In that study, the operating cost of each operating conditions was calculated in a range of reflux ratio from 1 to 10 in steps of 0.001. Then the value of the reflux ratio which will result in the minimum operating cost was selected as the optimum reflux ratio for that operating condition. In this study, the Cuckoo optimization algorithm was used to model a steady state continuous benzene-toluene mixture distillation column. A correlation for the optimum value of reflux ratio was obtained.

2 Modeling

2.1 Principles

The degradation of heat can drive the chemical separation

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in the distillation process (Henley and Seader, 1981; King, 1971; Robinson and Gilliland, 1950). To perform a separation by distillation a minimum quantity of internally circulating fluid is needed. The vapor-liquid countercurrent flows can be established by a continuous reflux in distillation. A liquid flow (L) is maintained at its boiling point and vapor flow (G) is circulated between stages to purify a feed flow (F) into products.

Fig. 1 shows the purification of the feed flow. The distillate (D) and bottoms (W) are enriched with the more volatile and less volatile components respectively. Fig. 1 shows six valves available to control the column, with which the valves 2 and 3 control the reflux ratio (Abolpour et al, 2013).

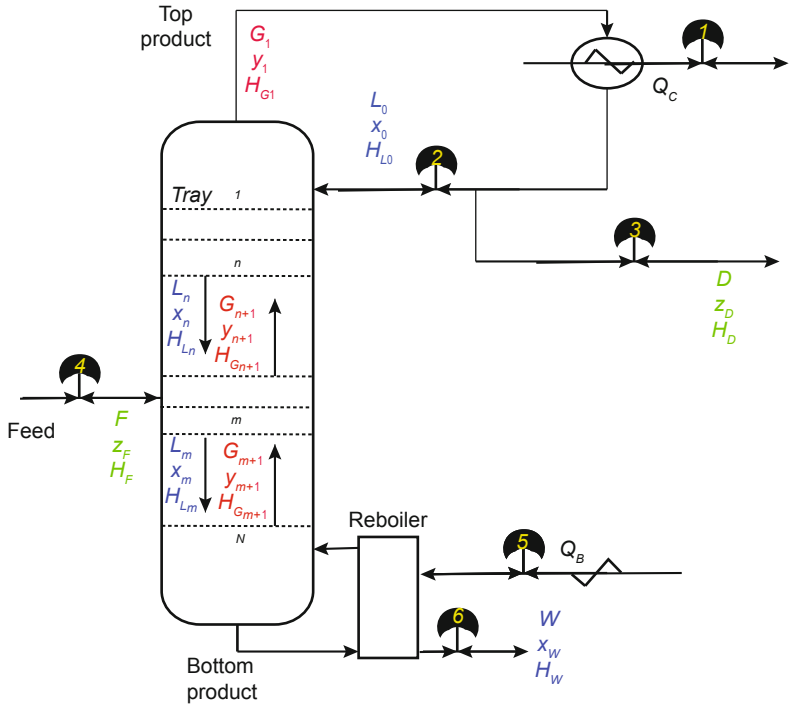

Fig. 1 Schematic of a distillation column (Abolpour et al, 2013)

2.2 Governing equations

The liquid and vapor flows do not change in a section of distillation column without heat exchangers or side-stream inputs or outputs. Assuming constant flows and considering mass balance obtains linear relations (i.e. operating lines, Eqs. (8) and (11)) for the component concentrations in the flow streams passing between adjacent stages. Equilibrium conditions limit the concentrations of flow streams leaving a stage. Therefore, the concentration differences in the flow streams at a point of column are bounded by the operating lines and the equilibrium curve. In the mentioned isolated column, heat losses are assumed to be negligible. Therefore, mole and enthalpy (H) balances can be written as the following equations:

$$F = D + W \tag{1}$$

$$Fz_F = Dz_D + Wx_W \tag{2}$$

$$Q_B = DH_D + WH_W - FH_F + Q_C \tag{3}$$

The product may be liquid, vapor, or a mixture of both, but the reflux should be liquid. The reflux ratio ($R = \frac{L_0}{D}$) is the molar ratio of reflux to withdrawn distillate. Using mole and enthalpy balances over the condenser we have:

$$G_1 = D(R+1) \tag{4}$$

$$G_1 y_1 = Dz_D + L_0 x_0 \tag{5}$$

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

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

$$G_{n+1} = L_n + D \tag{7}$$

$$G_{n+1}y_{n+1} = L_n x_n + Dz_D \tag{8}$$

$$G_{n+1}H_{G_{n+1}} = L_n H_n + DH_D + Q_C \tag{9}$$

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

$$\bar{L}_m = \bar{G}_{m+1} + W \tag{10}$$

$$\bar{L}_m x_m = \bar{G}_{m+1} y_{m+1} + Wx_W \tag{11}$$

$$\bar{L}_m H_m = \bar{G}_{m+1} H_{\bar{G}_{m+1}} + WH_W - Q_B \tag{12}$$

Eqs. (1) to (12) are fundamental equations to define the problem and their solutions give information about the distillation column.

2.3 Graphical solution method

The Ponchon-Savarit graphical method was used to investigate the relationship between tray numbers, liquid/vapor ratios, and product compositions (Treybal, 1981). The liquid enthalpy can be obtained by the following equation:

$$H_L = \left[xM_{\text{Benzene}} C_{P,\text{Benzene}} + (1-x) M_{\text{Toluene}} C_{P,\text{Toluene}} \right] (T - T_{\text{ref}}) \tag{13}$$

where C_{P} is the heat capacity of pure liquid (Perry and Green, 1999), and T_{ref} is the reference temperature (19.54 °C). It is assumed that the unmixed liquids are first heated to the bubble point of the liquid (T_D), and then vaporized at this temperature, and finally the vapors are mixed. Therefore, the gas enthalpy can be obtained by the following equation:

$$\begin{aligned} H_G = {} & yM_{\text{Benzene}} \left[C_{P,\text{Benzene}} (T_D - T_{\text{ref}}) + \lambda_{\text{Benzene}} \right] \\ & + (1-y) M_{\text{Toluene}} \left[C_{P,\text{Toluene}} (T_D - T_{\text{ref}}) + \lambda_{\text{Toluene}} \right] \end{aligned} \tag{14}$$

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

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

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

$$\frac{x_D - x_F}{x_F - x_W} = \frac{Q' - H_F}{H_F - Q''} \tag{17}$$

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

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

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

2.4 Methodology

A computer program was written using MATLAB v.7.6 software. Matrix operation facilities were used to reduce computation time. The solution procedure is described as below and more descriptions on the dimensionless mathematical model are presented in literature (Treybal, 1981).

- Equilibrium tie-line from y_1 (where $y_{1=}\, x_D$) locates x_1.
- x_1 connected to $\left[z_D, Q'\right]$ locates y_2.
- Equilibrium tie-line from y_2 locates x_2.
- x_2 connected to $\left[z_D, Q'\right]$ locates y_3.
- And so on as y_n connected to $\left[z_D, Q'\right]$ 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 (i.e. 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 lie from x_w locates y_{N+1}.
- Straight line connecting y_{N+1} to the lower operating point $\left[x_W, Q''\right]$ 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 $\left[x_W, Q''\right]$ 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.

2.5 Cuckoo optimization algorithm

Fig. 2 shows a flowchart of the proposed algorithm. This algorithm starts with an initial population (i.e. mature cuckoos and eggs). These initial cuckoos lay some eggs in some host birds' nests. Some of these eggs that are similar to the host bird's eggs grow up and become a mature cuckoo. Other eggs are killed by host birds. The grown eggs reveal the suitability of their nests. The more eggs that survive in a nest the more profit is gained in that nest. Therefore, the nest in which more eggs survive will be the term that cuckoo optimization algorithm is going to optimize.

Birds search for the most suitable nest to lay eggs to maximize their eggs survival rate. The mature cuckoos make some societies. The cuckoos immigrate toward the best habitat of all societies. Therefore, during the survival competition some of the cuckoos or their eggs die and the surviving cuckoo societies emigrate to a better environment and start laying eggs. This survival effort hopefully converges to a state that there is only one cuckoo society with the same profit values (Rajabioun, 2011).

3 Results and discussion

3.1 Evaluation of the model

The graphical model was evaluated by using the HYSYS v.3.2 simulator at the operating conditions in Table 1. The

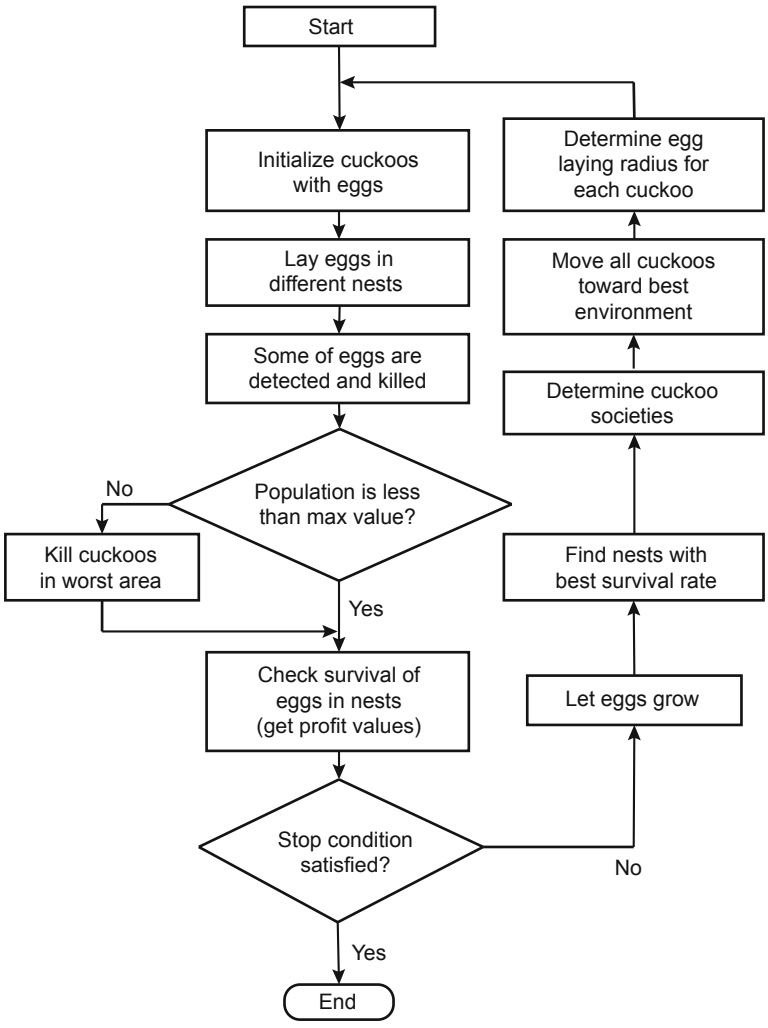

Fig. 2 Flowchart of Cuckoo optimization algorithm (Rajabioun, 2011)

results are given in Table 2. It can be seen that there is good agreement between the results of the graphical model and the values calculated with the HYSYS simulator for the assumed conditions. 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 the distillation column

Items	Value
Lighter component	benzene
Heavier component	toluene
System pressure, kPa	101.325
Temperature of feed, ºC	25
Feed flow rate, kmole/hr	100
Mole fraction of lighter component in feed	0.5
Mole fraction of lighter component in liquid phase in condenser	0.99
Mole fraction of lighter component in liquid phase in reboiler	0.01
β = reflux ratio/minimum reflux ratio	1.247

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

Items	HYSYS simulation	Graphical model
Minimum number of trays	10.666	9.1687
Actual number of trays	23.097	21
Optimal feed stage	11.545	10
Condenser temperature, ºC	80.71	80.65
Reboiler temperature, ºC	110	110.09
Condenser duty, kW	1208.1	1071.7
Reboiler duty, kW	1504.4	1405.6
Minimum reflux ratio	1.413	1.192

It should be noted that, the HYSYS simulator uses the McCabe-Thiele method (1925) to simulate a distillation column. This method is the simplest method for the analysis of binary distillation and uses the fact that the composition at each tray is determined by the mole fraction of each of components. This method is based on the assumptions of constant molar overflow, which requires the molar heats of

vaporization of the feed components be equal to each other, a mole of vapor having to be condensed for every mole of vaporized liquid, and heat effects such as heats of solution are negligible. These simplifier assumptions can decrease the model accuracy. On the other hand, applying an optimizer algorithm to the HYSYS simulator for obtaining an optimum condition for a distillation column is not possible for the users of this software. Therefore, the Ponchon-Savarit method, which is more accurate than the McCabe-Thiele method, was used to develop a computer program using MATLAB software to simulate this distillation column and then optimize the operating condition of this column.

3.2 Predictions from the graphical model

The *x-y* and *H-xy* diagrams of the graphical model for the conditions in Table 1 are shown in Figs. 3 and 4. As shown in Figs. 5 and 6, the mole fraction of benzene in both liquid and vapor phases decreases down the distillation column, and the temperature of solution increases from top to the bottom of the column.

3.3 Optimum reflux ratio

The optimum condition for a distillation column is used to achieve separation under the most profitable operating conditions. Several parameters (e.g. the diameter, reflux ratio and operating pressure of the column, and the temperature of the condenser and reboiler, etc.) can be adjusted to optimize the total annualized cost (Talifu and Luo, 2005). The optimization of the reflux ratio is of vital importance profit-wise. In the present research, first a suitable graphical model was proposed and then this model was optimized using the Cuckoo optimization algorithm.

The cost value is a function of the number of trays and also the total required duty (i.e. the sum of reboiler and condenser duties). At the minimum reflux ratio, the column requires an infinite number of trays, and consequently the capital cost becomes infinite, but the energy cost would be the least. As reflux ratio (R) increases, the number of trays rapidly decreases, until it reaches a minimum. The heating and cooling requirements increase almost proportionally with reflux ratio. For a stage distillation column, neglecting the costs of raw materials and labor, the operational costs can be defined as:

Total annualized cost = Capital cost + Energy cost

The total annualized cost curve must therefore pass though a minimum at the optimum reflux ratio. Therefore, an economic parameter (φ) is defined as below (Abolpour et al, 2013):

$$\varphi = \frac{\text{Energy cost}\,(\$\cdot \text{kw}^{-1}\cdot \text{hr}^{-1})}{\text{Energy cost}\,(\$\cdot \text{kw}^{-1}\cdot \text{hr}^{-1}) + \text{Capital cost}\,(\$\cdot \text{hr}^{-1})} \tag{18}$$

Now the reflux ratio can be optimized by minimizing the total annualized cost, which is calculated by the following equation:

$$\Phi = 365\times 24\left[Q_{tot}\varphi + N_{act}(1-\varphi)\right] \tag{19}$$

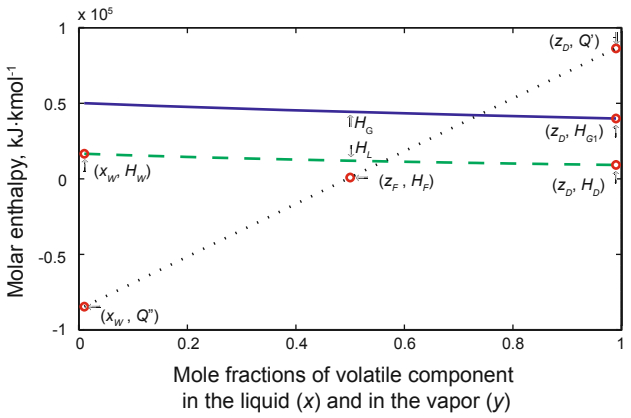

Fig. 3 Enthalpy-concentration diagram of solved graphical model for conditions in Table 2

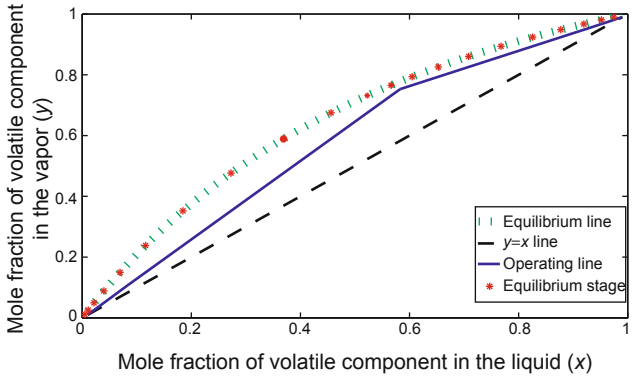

Fig. 4 Vapor-liquid equilibrium diagram of solved graphical model for conditions in Table 2

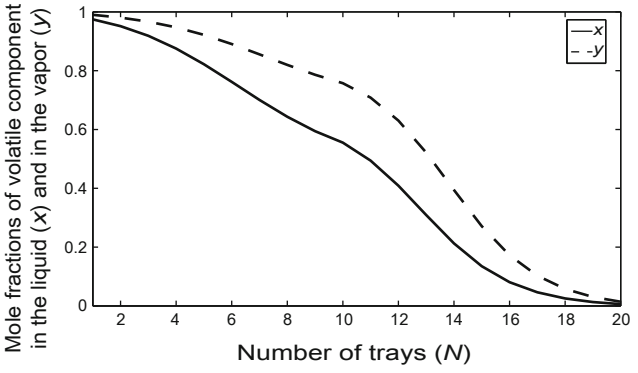

Fig. 5 Predicted mole fraction of benzene in vapor and liquid phases using the graphical model at the conditions in Table 2

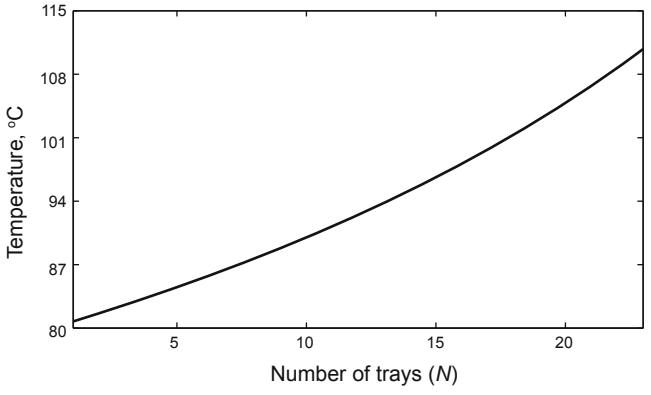

Fig. 6 Predicted solution temperature using the graphical model at the conditions in Table 2

Fig. 7 shows the results of the calculated cost value at each iteration of the Cuckoo optimization algorithm for the listed parameters in Table 2 and φ=0.02 (Abolpour et al, 2013). In this case, the minimum value of the reflux factor (β) is 1.247, which is used to compare the current model with the HYSYS simulator results. Fig. 7 also compares the current Cuckoo algorithm with two traditional algorithms (i.e. golden section search and genetic algorithm). It can be seen that the Cuckoo optimization algorithm is faster than the golden section search and the genetic algorithm for predicting the target parameter. The excellence of Cuckoo optimization algorithm is also shown in our previous study (Kaydani and Mohebbi, 2013).

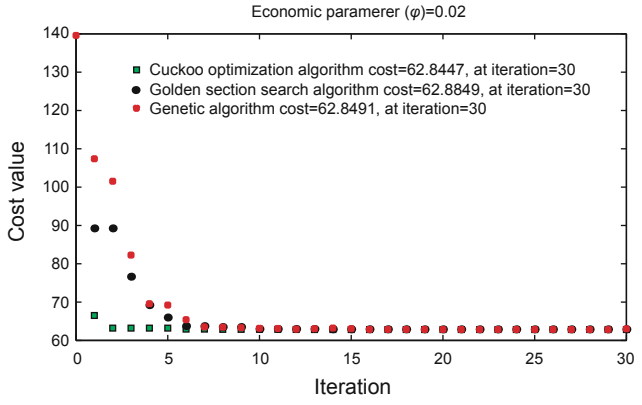

Fig. 7 The Cuckoo optimization algorithm iterations for conditions in Table 2

Fig. 8 shows the effect of economic parameter (φ) on the optimum reflux factor (β_{opt}). As one can see in Fig 8, at low energy price or high capital cost (i.e. small value of φ), the optimum reflux factor is high, and at low capital cost or high energy price (i.e. large value of φ), the optimum reflux factor is low. The fitting formulation for optimum value of reflux factor would be:

$$\beta_{opt} = 0.1068\varphi^{-0.4422} + 0.6446 \quad (20)$$

This relation can be used for all the operating conditions of a benzene-toluene distillation column with negligible error.

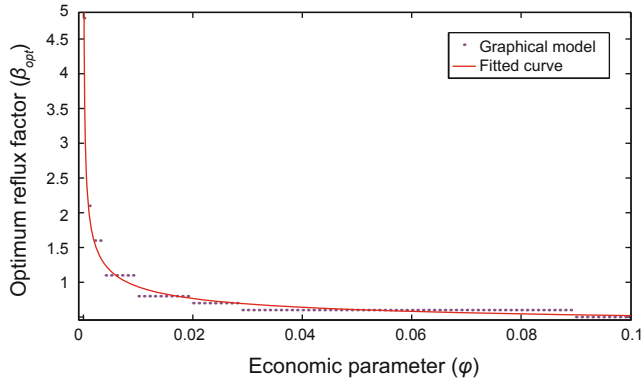

Fig. 8 Effect of economic parameter (φ) on the optimum reflux factor (β_{opt})

For instance, if feed temperature is set to be 50 °C, the error is about 1.6%, and if x_w=0.002 and z_D=0.97, this value is about 3.2%.

3.4 Effects of the operating pressure and feed temperature

Fig. 9 shows the effects of operating pressure on temperature of solution and mole fraction of benzene in liquid and vapor phases. It can be seen that with an increase of operating pressure the temperature of solution and also the mole fraction of benzene in both liquid and vapor phases on the trays increase. Higher pressure can cause an increase in the saturation temperature of the liquid. Therefore, more energy will be required for separation of these two components in the distillation column. From the other point of view, a column with a lower pressure facilitates separation and therefore less trays are required, as seen in Fig. 9 (i.e. at 100 kPa operating pressure, the number of equilibrium stages is 21 and at 300 kPa operating pressure, the number of equilibrium stages is 23). Therefore, it is clear that, high operating pressure increases the total annualized cost, which has no optimum value (i.e. lower pressure is better).

Fig. 10 shows the effects of feed temperature on the temperature of solution and the mole fraction of benzene in liquid and vapor phases. As one can see from Fig. 10, with an increase of the feed temperature the mole fractions of benzene in both liquid and vapor phases decrease, but the temperature of the solution in the column does not change

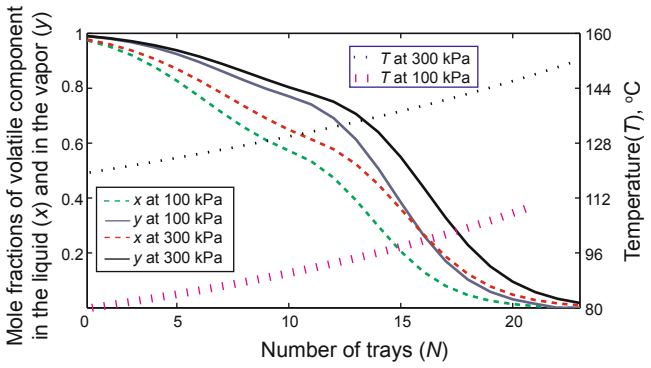

Fig. 9 Effects of operating pressure on temperature of solution and mole fraction of benzene in liquid and vapor phases

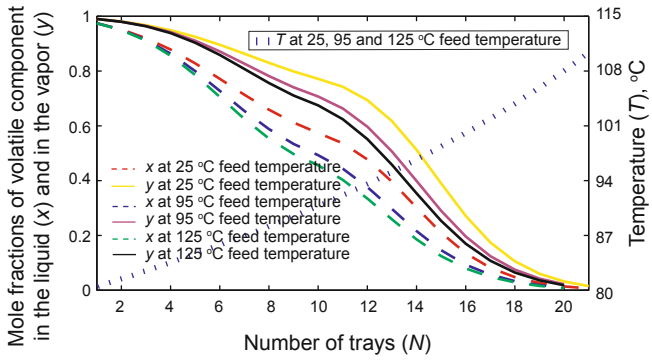

Fig. 10 Effects of feed temperature on temperature of solution and mole fraction of benzene in liquid and vapor phases

significantly. The temperature of the feed supplies some of the required energy for distillation. It should be noted that, the feed conditions (i.e. sub-cold liquid at 25 °C, two phases at 95 °C and super-heated vapor at 125 °C for the solution of benzene-toluene) affect the *x-y* and *H-xy* (Fig. 3) diagrams. This parameter (feed temperature) affects the required number of trays in the column. An increase of the feed temperature will decrease the total annualized cost. The optimum value of feed temperature is a function of the initial conditions of the available feed.

4 Conclusions

A graphical model for the operating profit of benzene-toluene stage distillation columns was developed to optimize the operating reflux ratio of the column by the Cuckoo optimization algorithm. The model was then evaluated with the HYSYS simulator and it was observed that the results from the model agree well with simulator 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 price and capital cost. It was concluded that at low energy price or high capital cost, the optimum reflux factor is high, whereas at low capital cost or high energy price, the optimum reflux factor is low.

For more accuracy, the Ponchon-Savarit graphical method was used to model this distillation column. This shows that the Cuckoo optimization algorithm is fast enough to optimize this column. This column also could be optimized to obtain optimum values of the all of operating parameters such as operating pressure and feed temperature, but other parameters except reflux ratio, have no significant effects on the total annualized cost for optimization.

List of symbols

C_P	Heat capacity at constant pressure , J·g^{-1}
D	Distillate rate, kmol·hr^{-1}
F	Feed rate, kmol·hr^{-1}
G	Vapor flow rate, kmol·hr^{-1}
G_1	The flow rate of exited vapor from top of the column, kmol·hr^{-1}
$\overline{G}_{m+1}$	The flow rate of exited vapor from the tray number m+1 of stripping section of the column, kmol·hr^{-1}
G_{n+1}	The flow rate of exited vapor from the tray number n+1 of enriching section of the column, kmol·hr^{-1}
H	Molar enthalpy, J·mol^{-1}
H_D	Molar enthalpy of distillate product at the top of column, J·mol^{-1}
H_F	Molar enthalpy of feed flow, J·mol^{-1}
H_{G1}	Molar enthalpy of G_1, J·mol^{-1}
H_{L0}	Molar enthalpy of L_0, J·mol^{-1}
H_{Lm}	Molar enthalpy of $\overline{L}_m$, J·mol^{-1}
H_{Ln}	Molar enthalpy of L_n, J·mol^{-1}
$H_{\overline{G}_{m+1}}$	Molar enthalpy of $\overline{G}_{m+1}$, J·mol^{-1}
$H_{G_{n+1}}$	Molar enthalpy of G_{n+1}, J·mol^{-1}
H_W	Molar enthalpy of residue product at the bottom of column, J·mol^{-1}
L	Liquid flow rate, kmol·hr^{-1}
$\overline{L}_m$	The flow rate of exited liquid from the tray number m of stripping section of the column, kmol·hr^{-1}
L_n	The flow rate of exited liquid from the tray number n of enriching section of the column, kmol·hr^{-1}
L_0	External reflux rate, kmol·hr^{-1}
M	Molecular weight, g·mol^{-1}
N_{act}	Actual number of trays
Q_B	Heat added in the reboiler, kW
Q_C	Heat removed in the condenser, kW
Q_{tot}	Total duty, kW
R	Reflux ratio
T	Solution temperature, °C
W	Residue rate, kmol·hr^{-1}
x	Mole fraction of volatile component in the liquid
x_0	Mole fraction of volatile component in L_0
x_m	Mole fraction of volatile component in the exited liquid flow from the tray number m of stripping section of the column
x_n	Mole fraction of volatile component in the exited liquid flow from the tray number n of enriching section of the column
x_W	Mole fraction of volatile component in the residue product at the bottom of column
y	Mole fraction of volatile component in the vapor
y_1	Mole fraction of volatile component in G_1
y_{m+1}	Mole fraction of volatile component in the exited gas flow from the tray number m+1 of stripping section of the column
y_{n+1}	Mole fraction of volatile component in the exited gas flow from the tray number n+1 of enriching section of the column
z	Average mole fraction of volatile component in the mixture of liquid and vapor phases
z_D	Average mole fraction of volatile component in the mixture of liquid and vapor of distillate product at the top of column
z_F	Average mole fraction of volatile component in the feed flow
β	Reflux factor
β_{opt}	Optimum reflux factor
λ	Latent heat of vaporization, J·g^{-1}
φ	Economic parameter
Φ	Total annualized cost parameter, \$·year^{-1}

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