
Short-Cut Methods for Multicomponent Batch Distillation

A. Narváez-García, J.C. Zavala-Loría,
A. Ruiz-Marín and Y. Canedo-López

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Abstract

This work present the batch distillation shortcut methods developed from the Fenske-Underwood-Gilliland (FUG) method of continuous distillation. In addition, a comparison between the results of shortcut method developed by Diwekar and Narváez-García et al. is done. The results of both methods are compared for validation with the results using the rigorous method presented by Domenech and Enjalbert. The results indicate no significant differences in both shortcut methods being the maximum deviation found between the two shortcut methods is less than 3%. Then, the use of any of both methods is in the ease or difficulty of the solution each of the model equations. Both methods were implemented using Fortran programming. Multidistbatch® software was used for the rigorous method.

Keywords: shortcut method, FUG, batch distillation

1. Introduction

Batch distillation is a process widely used for separation of small quantities of chemical compound of the one mixture as the recovery of small quantities of hazardous materials in waste streams, recovery of solvents, as well as, for pharmaceutical and biotechnological products with high added value, among others. Therefore, the development of mathematical models for the prediction of a process has a high interest in recent times [1-4].

Batch distillation is a flexible process because one equipment can obtain the separation of all the components of the mixture, while the continuous process [5] requires a number of columns distillation equal to the number of components minus one ($n - 1$). Another advantage

of batch distillation process is the use of the same equipment for the mixture separation with different compositions or different mixtures [6].

On the other hand, the disadvantage of the batch distillation with respect to continuous distillation is that only small amounts of products can be obtained of the mixture. Another disadvantage is the production of waste unwanted for each cuts, however, these residual cuts can be separated into the same column [7].

A batch distillation column can be operated using any of the following policies [1]:

- (1) Constant reflux.
- (2) Variable reflux.
- (3) Optimal reflux.
- (4) Reflux profile.

The process behavior can be predicted by developing mathematical models based on mass and energy balances. The mathematical models obtained can be classified as [1, 8, 9]:

- (1) Simplified (shortcut method).
- (2) Semirigorous.
- (3) Rigorous.
- (4) Order reduction.

Currently the rigorous models have an area of great interest and these require especially the use of computers with high accuracy and processing capabilities; however, simplified methods can be applied with the use of the equipment such as tablets, smart phones, and/or laptops with smaller capacity of data processing, which makes possible the search for predicting the behavior of the process [2, 10]. In addition, the use of this kind of methods is a tool for obtaining initial data for the mathematical optimization.

Unlike the rigorous methods that considered the dynamics of the complete column, the shortcut methods are mathematical models that predict the behavior of the process considering the least amount of equations, usually making an overall material balance and partial balances considering a component any "*i*." The main limiting factor of these shortcut methods is to find a functional relationship between the concentrations of the dome and the bottom.

The shortcut methods are justified because these require a minor calculus time and memory requirements, as well as, an acceptable accuracy in the results obtained with respect to the rigorous method. These are an appropriate tool to obtain initial values for the mathematical optimization of some process, when the complexity of the methods required data very close to the solution.

The shortcut method is also used for the columns design and obtaining of limit conditions as minimum reflux ratio, R_{\min} and minimum number of stage N_{\min} . On the other hand, the shortcut methods are very simple to apply and to program, therefore, are useful in the teaching-learning process.

The two most important shortcut methods reported in the literature made use of the Fenske-Underwood-Gilliland (*FUG*) method developed for continuous distillation, but considering that the feed changes at every instant; that is, the bottom product in the current time is the feed for the next time (step).

The first of the shortcut methods was developed by Diwekar [11] and reported in the literature by Diwekar and Madhavan [12]. This method was developed considering the policies of constant and variable reflux. This method used the Hengstebeck-Geddes equation. This method also performs the comparison between the values of the minimum reflux ratio of Underwood and minimum reflux ratio of Gilliland, which increases the computational time because it uses an additional iterative process.

The second method was reported by Sundaram and Evans [13] and only considered the constant reflux policy and the Fenske Equation. The model obtains a solution in two parts; an outer loop that solves material balances and internal one that solves the functional relationship between the compositions of the dome and the bottom using the *FUG* method. The mathematical model developed initially considered:

- (1) Constant relative volatilities.
- (2) Constant molar flow.
- (3) Negligible vapor and liquid accumulation in trays and the condenser.

Based on the work of Sundaram and Evans [13], Narváez-García et al. [10] developed a mathematical model for batch distillation process using a variable reflux policy.

The present studies show the most important shortcut methods used to predict the behavior of the batch distillation process.

2. Important definitions

For the use of the Underwood equations, this work considered separations Class I and Class II. In according to Shiras et al. [14] defined Class I and Class II as follows:

Class I: “Separations such that, with infinite plates, all components of the feed are present in both the top product and bottom product.”

Class II: “Separations such that, with infinite plates, some of the components are completely in the top product or completely in the bottom product.”

Similarly, an important concept in model developments is the key component light (*lk*) and heavy key component (*hk*) defined as follows:

Light key component (*lk*): Light component that is present in the residue in important amounts.

Heavy key component (*hk*): Heavy component that is present in the distillate in important amounts.

3. Reflux policies

When a fraction of the product obtained is fed back into the process and this can be done on four operations of the process: (1) constant reflux, (2) variable reflux, (3) optimum reflux, and (4) profile of reflux. In either case, the reflux ratio (R) is defined as

$$R = \frac{L}{\frac{dD}{dt}} = \frac{L}{D(t)} = \frac{L}{D} \quad (1)$$

where L is the reflux in the dome and D the product flow.

For some type of reflux used, it should be considered if there is accumulation of liquid and vapor in each of the trays as well as in the reflux tank. Another aspect that should be considered is where the initial feed is introduced because when it is performed from the reflux tank, the accumulation in each of the stages is equal to feed initial concentration, if conversely, the feed is introduced in the reboiler and column is operated without reflux, the concentration of each of the trays is equal to the concentration of the vapor phase and will be in equilibrium with the feed [15].

Constant reflux: In constant reflux policy, the product concentration varies with time because new feed input does not exist, so that the initial mole fractions of the more volatile are depleted and the molar fraction of the final distillate is an average.

Variable reflux: The batch distillation process with a variable reflux policy is used when it is desired to obtain a constant product concentration. In others words, reflux ratio is modified such that at each instant the same concentration of distillate is obtained.

Optimal reflux: For optimum reflux policy, the process used an objective function directly related to a control variable, which usually is the reflux ratio. This function is solved by applying mathematical methods such as dynamic programming, variation calculation, pontryagin maximum principle or nonlinear programming (NLP), among others. In general, the process is considered as an optimal control problem and the most common cases studied in the literature are [16]: (a) maximum distillate problem, (b) minimum time problem, (c) maximum profit problem, (d) minimum energy problem, and (e) maximum thermodynamic efficiency problem.

Reflux profile: For this case, a combination of constant reflux and variable reflux are used for obtaining a given concentration of the desired product in a time given. This operation policy is a derivation of the optimization process.

4. Materials and methods

In this work is considered a batch distillation column with the following characteristics:

- Adiabatic column.
- Theoretical trays.

- Partial reboiler.
- Total condenser.
- Constant pressure.
- Constant relative volatility.
- Negligible accumulation (holdup) of liquid and vapor.
- Constant molar flows through the column.

The mathematical model of the column is obtained by performing a total mass balance and partial mass balances to component " i ." The Fenske-Underwood-Gilliland method is used to find the functional relationship between the compositions of the bottom and the dome of the column.

Although it presents the development of the model, considering the policies of operation of constant and variable reflux, these are presented in only four cases of study for the shortcut method to reflux variable considering the contribution to the state of the art of the authors.

In each case, it is considered that the mixture is fed to the boiling temperature. The error tolerance is 10^{-4} , the integration step is $\Delta t = 10^{-1}$ h and the time of production is required to deplete the lighter component. It has been considered a feed of 200 kmol and a vapor flow of 110 kmol h⁻¹. For these cases, it is considered that the relative volatility is constant throughout the process.

The value of the vapor flow was established so that it allows to deplete the most volatile component in a small operation time. For the ternary and quaternary mixtures only first cut is considered. For validation, the results of both methods, Diwekar [11] and Narváez-García et al. [10], are compared with the results using the rigorous method presented by Domenech and Enjalbert [17]. This model is used because it is considered as a low holdup. To solve each one of the cases was made a program in Fortran language.

5. Simplified mathematical models

The complete mathematical model of a batch distillation column considering the dynamics of the process consists of a system of differential equations and algebra (DAEs) added by equations that allow the calculation of the thermodynamic properties and hydraulic conditions of the column. The solution of the system can be very complex depending on the state equations used to predict the behavior of the gas phase (Soave, Redlich-Kwong Peng-Robinson, etc.) or the solution of the models used to predict the liquid phase behavior (Wilson, NRTL, UNIQUAC, UNIFAC, etc.).

According to Diwekar [9], the number of equations in a rigorous mathematical model of a batch distillation, which considers a mixture of components nc and N trays is equal to $(N + 2)(2nc + 1)$, where $N + 2$ considers the reboiler and condenser-tank reflux. Further, the number

of equations consider the total restrictions in each of the stages ($\sum x = \sum y = 1$), the expression of reflux ratio ($R = L / D$), and liquid (L) and vapor (V) flows calculations along the column. The number of equations increases if the calculation of other variables of interest such as the column hydraulic or thermodynamic efficiency is considered.

The solution of this equation system is complex and requires intensive use of computers with adequate processing capacity, which affects costs in the area of process simulation. Therefore, it is needed to consider some simplifications to the mathematical model to reduce the data processing time.

Reductions to the batch distillation mathematical model are possible if it is considered that the process is continuous, with a feed that changes in every moment as shown in **Figure 1** [1, 10], which allows to use equations Fenske [18], Underwood [19], and Gilliland [20] of continuous distillation (*FUG* method).

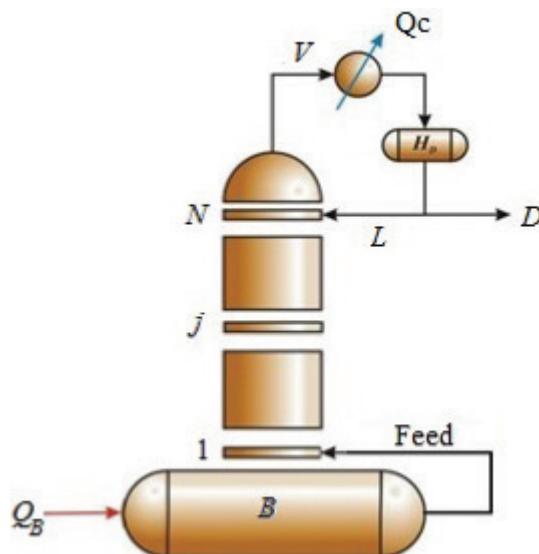


Figure 1. Scheme of a batch distillation column for the shortcut method.

Gilliland correlation can be replaced by the correlation Eduljee [21] because the mathematical expression is simpler for numerical works. The shortcut method considers:

- (1) Constant molar flow along the column.
- (2) Constant relative volatilities throughout the process.
- (3) Negligible fluid and vapor accumulation within the column.

Constant molar flow is based on the assumption that the enthalpy of vaporization is the same for all components, which is correct if the mixture consists of very similar compounds.

The simplification is more restrictive from shortcut method to consider constant relative volatilities throughout the process. This consideration significantly reduces the number of calculations in the model, especially because the iterative processes of liquid-vapor equilibrium does not apply. When the relative volatility cannot be considered as a constant amount along the time or the column, polynomial expressions or Winn [22] equation can be used to estimate the changes; therefore, Diwekar [11] suggested that the relative volatilities can be used to calculate in every moment of the process using an average between the values of the bottom and the dome.

Finally, the vapor accumulation in a distillation column can be neglected because it is much less than the cumulative amount of liquid, and the accumulation of fluid in the column can be neglected, considering that this accumulation is less than the liquid accumulated in the reboiler. Under these circumstances, the two most important shortcut methods for batch distillation in the literature were reported by Diwekar [11], Sundaram and Evans [13], and Narvaez-García et al. [17].

5.1. Shortcut methods derived from FUG method

5.1.1. Shortcut method developed by Diwekar [11]

The first shortcut method for batch distillation presented here was developed by Diwekar [11]. This method considers a global balance in the column and their respective partial balances (component “*i*”); each of the equations used in the method are presented below:

Global balance:

$$\frac{dB}{dt} = -D; \quad B_0 = F \quad (2)$$

where *D* is the distillate obtained by a mass balance in the dome of the column:

$$D = \frac{V}{R+1} \quad (3)$$

where *R* is the reflux ratio:

$$R = \frac{L}{D} \quad (4)$$

Partial balance with respect to a component (*i*):

$$\frac{d[Bx_B^{(i)}]}{dt} = -Dx_D^{(i)} \quad (5)$$

$$B \frac{dx_B^{(i)}}{dt} + x_B^{(i)} \frac{dB}{dt} = -Dx_D^{(i)} \quad (6)$$

$$B \frac{dx_B^{(i)}}{dt} + x_B^{(i)} \frac{dB}{dt} = -Dx_D^{(i)} = \left(\frac{dB}{dt}\right)x_D^{(i)} \quad (7)$$

and substituting in Eq. (2) is obtained:

$$B \frac{dx_B^{(i)}}{dt} - D x_B^{(i)} = -D x_D^{(i)} \quad (8)$$

substituting in Eq. (3) is obtained:

$$\frac{d x_B^{(i)}}{dt} = \frac{D}{B} [x_B^{(i)} - x_D^{(i)}]; \quad x_{B_0}^{(i)} = x_{F_0}^{(i)} \quad (9)$$

$$\frac{d x_B^{(i)}}{dt} = \frac{V}{B(R+1)} [x_B^{(i)} - x_D^{(i)}]; \quad x_{B_0}^{(i)} = x_{F_0}^{(i)} \quad (10)$$

A material balance is also performed for the reference component (k) and the ratio between the component (i) and the component (k).

$$\frac{d x_B^{(k)}}{dt} = \frac{D}{B} [x_B^{(k)} - x_D^{(k)}] = \frac{V}{B(R+1)} [x_B^{(k)} - x_D^{(k)}]; \quad x_{B_0}^{(k)} = x_{F_0}^{(k)} \quad (11)$$

$$\frac{d x_B^{(i)}}{d x_B^{(k)}} = \frac{\frac{D}{B} [x_B^{(i)} - x_D^{(i)}]}{\frac{D}{B} [x_B^{(k)} - x_D^{(k)}]}; \quad x_{B_0}^{(i)} = x_{F_0}^{(i)}; \quad i = 1, 2, \dots, n; i \neq k \quad (12)$$

$$\frac{d x_B^{(i)}}{d x_B^{(k)}} = \frac{[x_B^{(i)} - x_D^{(i)}]}{[x_B^{(k)} - x_D^{(k)}]}; \quad x_{B_0}^{(i)} = x_{F_0}^{(i)}; \quad i = 1, 2, \dots, n; i \neq k \quad (13)$$

$$d x_B^{(i)} = \frac{[x_B^{(i)} - x_D^{(i)}]}{[x_B^{(k)} - x_D^{(k)}]} d x_B^{(k)}; \quad x_{B_0}^{(i)} = x_{F_0}^{(i)}; \quad i = 1, 2, \dots, n; i \neq k \quad (14)$$

Eqs. (2) and (14) can be discretized if considered very small changes, then considering Eq. (2), is obtained:

$$\frac{\Delta B}{\Delta t} = -D \quad (15)$$

$$\Delta B = -D \Delta t \quad (16)$$

$$B_{new} = B_{old} - D \Delta t \quad (17)$$

Using Eq. (3) is obtained:

$$B_{new} = B_{old} - \left(\frac{V}{R+1} \right) \Delta t \quad (18)$$

Considering Eq. (14) is obtained:

$$\Delta x_B^{(i)} = \frac{[x_B^{(i)} - x_D^{(i)}]_{new}}{[x_B^{(k)} - x_D^{(k)}]_{old}} \Delta x_B^{(k)}; \quad x_{B_0}^{(i)} = x_{F_0}^{(i)}; \quad i = 1, 2, \dots, n; i \neq k \quad (19)$$

$$x_{B,new}^{(i)} = x_{B,old}^{(i)} + \frac{[x_B^{(i)} - x_D^{(i)}]_{old}}{[x_B^{(k)} - x_D^{(k)}]_{old}} \Delta x_B^{(k)}; \quad x_{B_0}^{(i)} = x_{F_0}^{(i)}; \quad i = 1, 2, \dots, n; i \neq k \quad (20)$$

The functional relationship between the concentrations of the dome and the bottom for this method is obtained using the equation Hengestebbeck-Geddes:

$$x_D^{(i)} = \left(\frac{\alpha_i}{\alpha_k} \right)^{C_1} \left[\frac{x_D^{(k)}}{x_B^{(k)}} x_B^{(i)} \right]; \quad i = 1, 2, \dots, n; i \neq k \quad (21)$$

being α the relative volatility and C_1 a constant equal to the minimum number of trays of Fenske equation. It is also necessary to use the equations of Underwood and Gilliland or Eduljee:

$$\sum_{i=1}^{nc} \frac{\alpha_i x_B^{(i)}}{\alpha_i - \theta} = 0 \quad (22)$$

$$R_{min} = -1 + \sum_{i=1}^{nc} \frac{\alpha_i x_D^{(i)}}{\alpha_i - \theta} \quad (23)$$

$$Y = 1 - \exp \left[\frac{(1+54.4X)(X-1)}{(11+117.2X)\sqrt{X}} \right] \quad (24)$$

The Eduljee correlation is

$$Y = 0.75(1 - X^{0.5668}) \quad (25)$$

being, in both cases:

$$X = \frac{R - R_{\min}}{R + 1} \quad (26)$$

$$Y = \frac{N - N_{\min}}{N + 1} \quad (27)$$

In the case of a constant reflux policy, Diwekar [11] uses a function that relates the minimum reflux ratio obtained with Underwood equation ($R_{\min U}$) and the minimum reflux ratio obtained with Gilliland Equation ($R_{\min G}$) can be expressed as

$$f_c = \frac{R_{\min U}}{R} - \frac{R_{\min G}}{R} = 0 \quad (28)$$

In the variable reflux case, Diwekar [11] uses a function obtained from the equation Hengstebeck-Geddes (Eq. (21)), considering the sum of all components, and applying the sum in both members of this equation is obtained:

$$\sum_{i=1}^{nc} x_D^{(i)} = \sum_{i=1}^{nc} \left(\frac{\alpha_i}{\alpha_k} \right)^{C_1} \left[\frac{x_B^{(k)}}{x_B^{(k)}} x_B^{(i)} \right] = 1 \quad (29)$$

$$\frac{x_B^{(k)}}{x_D^{(k)}} = \sum_{i=1}^{nc} \left(\frac{\alpha_i}{\alpha_k} \right)^{C_1} x_B^{(i)} \quad (30)$$

Therefore, the function is

$$f_v = \left\{ \sum_{i=1}^{nc} \left[\left(\frac{\alpha_i}{\alpha_k} \right)^{C_1} x_B^{(i)} \right] \right\} - \frac{x_B^{(k)}}{x_D^{(k)}} \quad (31)$$

In this method, it is necessary to consider a reference component, hence, using the equation Hengstebeck-Geddes (Eq. (21)) and separating the concentration of the reference component (k):

$$x_D^{(k)} = \frac{x_B^{(k)}}{\sum_{i=1}^{nc} \left[\left(\frac{\alpha_i}{\alpha_k} \right)^{C_1} x_B^{(i)} \right]} \quad (32)$$

With the developed mathematical models, it is necessary to consider finding the solution; therefore, the solution algorithm is shown below.

5.1.1.1. Diwekar solution algorithm

The shortcut method developed by Diwekar [11] is setup by the system of Eqs. (1)–(32). To solve this system of equations, it is necessary to follow the next steps:

Constant reflux policy.

- (1) Steady-state concentrations are calculated considering that $C_1 = N$.
 - (a) The concentration of component reference (k) in the dome (Eq. (32)) is calculated.
 - (b) Other concentrations are calculated using the Hengstebeck-Geddes equation (Eq. (22)).
 - (c) Increase the time (Δt).
 - (d) New concentrations (Eq. (20)) and the remaining amount in the reboiler (Eq. (18)) are calculated.

- (2) To propose an initial value of C_1 , which will be adjusted by an iterative process.
- (3) To calculate the reference component concentration in the dome (Eq. (32)).
- (4) Other concentrations are calculated using Equation Hengestebeck-Geddes (Eq. (21)).
- (5) To solve Underwood equations (22) and (23).
- (6) To solve Gilliland equation.
 - (a) First Eq. (24).
 - (b) Second Eq. (26).
 - (c) Finally, Eq. (27).
- (7) Verify that the obtained value by Underwood equations is the same to that obtained by Equation Gilliland.
 - (a) To use Eq. (31).
 - (b) If this is not true it is necessary to change the value of C_1 with some iterative process as the Newton-Raphson method.
 - (c) The process is repeated from step 2 to achieve convergence.
 - (d) If this is true go to step 8.
- (8) Increase the time (Δt).
- (9) Calculate new concentrations (Eq. (20)) and the remaining amount in the reboiler (Eq. (18)).
- (10) The process is repeated until the desired time production.

Variable reflux policy.

- (1) Steady-state concentrations are calculated considering that $C_1 = N$.
 - (a) Consider constant the concentration of reference component (k) in the dome.
 - (b) Other concentrations are calculated using the equation Hengestebeck-Geddes equations (Eq. (21)).
 - (c) Increase the time (Δt).
 - (d) New concentrations (Eq. (20)) and the remaining amount in the reboiler (Eq. (18)) are calculated.
- (2) To propose an initial value of C_1 , which will be adjusted by an iterative process.
- (3) Verify that Eq. (31) is zero.
 - (a) If this is not true it is necessary to change the value of C_1 with some iterative process as the Newton-Raphson method until converge.

- (4) Other concentrations are calculated using Equation Hengestebeck-Geddes (Eq. (21)).
- (5) To solve Underwood equations (22) and (23).
- (6) To solve Gilliland equation.
 - (a) First Eq. (27).
 - (b) Second Eq. (24).
- (7) Calculate the value of the reflux ratio R with Eq. (26).
- (8) Increase the time (Δt).
- (9) Calculate new concentrations (Eq. (20)) and the remaining amount in the reboiler (Eq. (18)).
- (10) The process is repeated until the desired time production.

5.1.2. Shortcut method developed by Sundaram and Evans [13] using a constant reflux policy

In the method of Sundaram and Evans [13], the total material balance (Eq. (2)) and partial (Eq. (4)) are similar to the method of Diwekar [11], and Eqs. (18) and (20) are the same; however, Eq. (20) may be a function of the remaining liquid in the bottom; therefore, Eq. (6) calculates the change in the mole fractions in the bottom, then:

$$d x_B^{(i)} = [x_D^{(i)} - x_B^{(i)}] \frac{dB}{B} \quad (33)$$

Considering very small changes in the above equation; therefore, it is obtained:

$$\Delta x_B^{(i)} = [x_D^{(i)} - x_B^{(i)}]_{\text{old}} \frac{\Delta B}{B_{\text{old}}} \quad (34)$$

$$x_{B,\text{new}}^{(i)} = x_{B,\text{old}}^{(i)} + [x_D^{(i)} - x_B^{(i)}]_{\text{old}} \frac{(B_{\text{new}} - B_{\text{old}})}{B_{\text{old}}}, \quad x_{B_0}^{(i)} = x_{F_0}^{(i)}; i = 1, 2, \dots, n \quad (35)$$

Using the reference component (k) in the partial balance, instead of component (i), it is obtained:

$$d x_B^{(k)} = [x_D^{(k)} - x_B^{(k)}] \frac{dB}{B} \quad (36)$$

and considering very small changes in Eq. (24) can be obtained:

$$\frac{(B_{\text{new}} - B_{\text{old}})}{B_{\text{old}}} = \frac{\Delta x_B^{(k)}}{[x_D^{(k)} - x_B^{(k)}]_{\text{old}}} \quad (37)$$

Substituting Eq. (37) into Eq. (35), Eq. (20) is obtained. Eq. (28) is easily solved; however, Eq. (30) and Eq. (35) are much more complex because they require the functional relationship between the concentrations of the bottom and the dome.

The functional relationship between the concentrations of the dome and the bottom is calculated using the Fenske equation considering the minimum number of separation stages (N_{\min}) with the mole fractions of the dome (x_D) and bottom (x_B):

$$N_{\min} = \frac{\ln \left[\frac{x_D^{(i)} x_B^{(k)}}{x_D^{(k)} x_B^{(i)}} \right]}{\ln(\alpha_i)} \quad (38)$$

The Underwood equation for Class I mixtures and the Gilliland or Eduljee equations are used. In the original work of Sundaram and Evans [13] the equations for mixtures Class II were not considered.

When the mixture is classified as a multicomponent system Class I, the Underwood equation that relates the R_{\min} it can be expressed as [22]:

$$R_{\min} = \frac{\left[\frac{x_D^{(lk)}}{x_B^{(lk)}} \right] - \alpha_{lk,lk} \left[\frac{x_D^{(lk)}}{x_B^{(lk)}} \right]}{\alpha_{lk,lk} - 1} \quad (39)$$

In this method, it is also necessary to consider the composition of a component (k) of reference; then, using the Fenske equation, the composition of the reference component is isolated. Therefore, it is necessary to considerer the sum of all components. From Eq. (35), the following is obtained:

$$x_D^{(i)} = x_B^{(i)} \left[\frac{x_D^{(k)}}{x_B^{(k)}} \right] \alpha_i^{N_{\min}}; \quad i = 1, 2, \dots, n; i \neq k \quad (40)$$

$$\sum_{i=1}^n x_D^{(i)} = \sum_{i=1}^n x_B^{(i)} \left[\frac{x_D^{(k)}}{x_B^{(k)}} \right] \alpha_i^{N_{\min}} = 1 \quad (41)$$

$$x_D^{(k)} = \frac{x_B^{(k)}}{\sum_{i=1}^n (\alpha_i^{N_{\min}} x_B^{(i)})} \quad (42)$$

With all the mathematical equations of the shortcut method, the next step is to provide an appropriate methodology for the solution.

5.1.2.1. Sundaram and Evans [13] solution algorithm

The mathematical model of Sundaram and Evans is formed by the system of Eqs. (35), (37)–(42). To solve this system, follow the next steps:

- (1) Steady-state concentrations are calculated considering that $N_{\min} = N$.
 - (a) The concentration of reference component (k) in the dome (Eq. (42)) is calculated.
 - (b) Other concentrations are calculated using Fenske Eq. (40).
 - (c) Increase the time (Δt).
 - (d) New concentrations (Eq. (35)) and the remaining amount in the reboiler (Eq. (37)) are calculated.
- (2) The R_{\min} and N_{\min} are calculated.
 - (a) For R_{\min} Eq. (39) is used.
 - (b) For N_{\min} Eq. (38) is used.
 - (c) Eqs. (38) and (39) are solved using an iterative process.
- (3) Calculate the reference component concentration in the dome (Eq. (42)).
- (4) The other concentrations are calculated using the Fenske Eq. (40).
- (5) Back to step 2 until achieve the desired production time.

5.1.3. Short method developed by Narváez-García et al. [10] using a variable reflux policy

This proposal is based on the concepts of Sundaram and Evans [13]. It is initiated by calculating the reflux ratio required to obtain the desired product; therefore, using Eq. (26) and solving it, the following is obtained:

$$R = \frac{X + R_{\min}}{1 - X} \quad (43)$$

Eq. (43) requires the calculation of R_{\min} , which you can get from one of the equations of Underwood (Eq. (23)) as shown below:

$$R_{\min} = -1 + \sum_{i=1}^{nc} \frac{\alpha_i x_B^{(i)}}{\alpha_i - \theta} \quad (44)$$

Eq. (23) requires the calculation of θ , so Eq. (22) is used:

$$\sum_{i=1}^{nc} \frac{\alpha_i x_B^{(i)}}{\alpha_i - \theta} = 0 \quad (45)$$

Also, it is necessary to obtain the concentrations in the dome, therefore using the Fenske Equation (38) for the component (i):

$$x_D^{(i)} = x_B^{(i)} \left[\frac{x_D^{(k)}}{x_B^{(k)}} \right] \alpha_i^{N_{\min}}; \quad i = 1, 2, \dots, n; i \neq k \quad (46)$$

Applying a sum process considering all the components of the mixture and calculating the composition of the reference component (k) and is obtained:

$$x_D^{(k)} = \frac{x_B^{(k)}}{\sum_{i=1}^{nc} (\alpha_i^{N_{\min}} x_B^{(i)})} \quad (47)$$

Eqs. (40) and (42) require the calculation of the N_{\min} . Eq. (23) also requires the calculation of X ; therefore, using Eqs. (25) and (27), the following is obtained;

$$X = \left[1 - \left(\frac{4}{3} \right) \left(\frac{N - N_{\min}}{N + 1} \right) \right]^{1.7643} \quad (48)$$

Eq. (48) requires the N_{\min} value, therefore, it is necessary to obtain N_{\min} for the shortcut method. In this sense the Fenske equation allows to calculate the minimum number of trays when the light key component (lk) and the heavy key component ($hk = k$) are considered, then:

$$N_{\min} = \frac{\log \left\{ \left[\frac{x_D^{(lk)}}{x_D^{(k)}} \right] \left[\frac{x_B^{(k)}}{x_B^{(lk)}} \right] \right\}}{\log(\alpha_{lk,k})} \quad (49)$$

where:

$$x_D^{(lk)} = \left[\frac{x_D^{(k)}}{x_B^{(k)}} \right] x_B^{(lk)} \alpha_{lk,k}^{N_{\min}} \quad (50)$$

To change Eq. (49) in function of known values, $x_D^{(k)}$ should be replaced by an $x_D^{(lk)}$ expression, therefore, knowing that $\sum_{i=1}^{nc} x_D^{(i)} = 1$, then:

$$\sum_{i=1}^{nc} x_D^{(i)} - x_D^{(lk)} = 1 - x_D^{(lk)} \quad (51)$$

Substituting Eq. (40) into Eq. (51), the following is obtained:

$$\sum_{i=1}^{n_c} \left\{ \left[\frac{x_D^{(lk)}}{x_B^{(lk)}} \right] (\alpha_{i,k})^{N_{\min}} x_B^{(i)} \right\} - x_D^{(lk)} = 1 - x_D^{(lk)} \quad (52)$$

Substituting Eq. (50) in Eq. (52), the following is obtained:

$$\sum_{i=1}^{n_c} \left\{ \left[\frac{x_D^{(lk)}}{x_B^{(lk)}} \right] (\alpha_{i,k})^{N_{\min}} x_B^{(i)} \right\} - \left[\frac{x_D^{(lk)}}{x_B^{(lk)}} \right] x_B^{(lk)} \alpha_{lk,k}^{N_{\min}} = 1 - x_D^{(lk)} \quad (53)$$

$$x_D^{(k)} = \frac{[1 - x_D^{(lk)}] x_B^{(k)}}{\sum_{i=1}^{n_c} \alpha_{i,k}^{N_{\min}} x_B^{(i)} - x_B^{(lk)} \alpha_{lk,k}^{N_{\min}}} = \frac{[1 - x_D^{(lk)}] x_B^{(k)}}{\sum_{i=2}^{n_c} \alpha_{i,k}^{N_{\min}} x_B^{(i)}} \quad (54)$$

and, Eq. (49) becomes:

$$N_{\min} = \frac{\log \left\{ \left[\frac{x_D^{(lk)} \sum_{i=2}^{n_c} \alpha_{i,k}^{N_{\min}} x_B^{(i)}}{[1 - x_D^{(lk)}] x_B^{(lk)}} \right] \right\}}{\log(\alpha_{lk,k})} \quad (55)$$

Eq. (55) requires an iterative process for the solution of N_{\min} ; therefore, using the Newton-Raphson method, the following is obtained:

$$1 - x_D^{(lk)} = \left[\frac{x_D^{(lk)}}{x_B^{(lk)}} \right] \sum_{i=2}^{n_c} \left(\frac{\alpha_{i,k}}{\alpha_{lk,k}} \right)^{N_{\min}} x_B^{(i)} \quad (56)$$

$$f(N_{\min}) = \left\{ \left[\frac{x_D^{(lk)}}{x_B^{(lk)}} \right] \sum_{i=2}^{n_c} \left[x_B^{(i)} \left(\frac{\alpha_{i,k}}{\alpha_{lk,k}} \right)^{N_{\min}} \right] \right\} - [1 - x_D^{(lk)}] = 0 \quad (57)$$

$$f'(N_{\min}) = \left[\frac{x_D^{(lk)}}{x_B^{(lk)}} \right] \left\{ \left[\sum_{i=2}^{n_c} x_B^{(i)} \left(\frac{\alpha_{i,k}}{\alpha_{lk,k}} \right)^{N_{\min}} \right] \times \ln \left(\frac{\alpha_{i,k}}{\alpha_{lk,k}} \right) \right\} \quad (58)$$

$$(N_{\min})_{\text{actual}} = (N_{\min})_{\text{anterior}} - \frac{f(N_{\min})_{\text{anterior}}}{f'(N_{\min})_{\text{anterior}}} \quad (59)$$

With the N_{\min} value, the reflux ratio and other values relating to the variable N_{\min} can be calculated. The proposed solution to the developed method is addressed in the following section.

It is notable that both the model of Diwekar [11] and this model started from the same material balances (global and partial), and in other words, both works are developed following the same method; however, the functional relationship between the concentrations of the dome and bottom is different equations. **Table 1** presents a comparison between the equations of the two models.

In fact the equations of Underwood and Gilliland are the same in each model, and the difference is the way of how the values of the N_{\min} are obtained. Narváez-García et al. [10] used the Fenske equation, while Diwekar [11] used the equation of Hengstebeck-Geddes.

While calculation times are similar in both models, the Narváez-García et al. model has an advantage over the Diwekar model when the separation of mixtures Class I is performed due to the use of a simplified Underwood equation (Eq. (39)). This does not happen with the model of Diwekar because the original equations of Underwood are always considered.

Diwekar [11]	Narváez-García et al. [10]
$f_v = \left\{ \sum_{i=1}^{nc} \left[x_B^{(i)} \left(\frac{\alpha_i}{\alpha_k} \right)^{C_i} \right] \right\} - \frac{x_D^{(k)}}{x_D^{(k)}} = 0$	$f(N_{\min}) = \left\{ \left[\frac{x_D^{(k)}}{x_B^{(k)}} \right] \sum_{i=2}^{nc} \left[x_B^{(i)} \left(\frac{\alpha_{i,k}}{\alpha_{i,k}} \right)^{N_{\min}} \right] \right\} - [1 - x_D^{(k)}] = 0$
$x_D^{(i)} = x_B^{(i)} \left[\frac{x_D^{(k)}}{x_B^{(k)}} \right] \left(\frac{\alpha_i}{\alpha_k} \right)^{C_i};$ $i = 1, 2, \dots, n; i \neq k$	$x_D^{(i)} = x_B^{(i)} \left[\frac{x_D^{(k)}}{x_B^{(k)}} \right] \alpha_i^{N_{\min}};$ $i = 1, 2, \dots, n; i \neq k$
$x_D^{(k)} = \frac{x_B^{(k)}}{\sum_{i=1}^{nc} (\alpha_i^{N_{\min}} x_B^{(i)})}$	$x_D^{(k)} = \frac{[1 - x_D^{(k)}] x_B^{(k)}}{\sum_{i=2}^{nc} \alpha_{i,k}^{N_{\min}} x_B^{(i)}}$
$B_{\text{actual}} = B_{\text{anterior}} - \left(\frac{V}{R+1} \right) \Delta t$	$B_{\text{actual}} = B_{\text{anterior}} + \frac{\Delta x_B^{(k)}}{[x_D^{(k)} - x_B^{(k)}]_{\text{anterior}}} B_{\text{anterior}}$
$x_{B_{\text{actual}}}^{(i)} = x_{B_{\text{anterior}}}^{(i)} + \frac{[x_B^{(i)} - x_D^{(k)}]_{\text{anterior}}}{[x_B^{(i)} - x_D^{(k)}]_{\text{anterior}}} \Delta x_B^{(k)};$	$x_{B_{\text{actual}}}^{(i)} = x_{B_{\text{anterior}}}^{(i)} + [x_D^{(i)} - x_B^{(i)}]_{\text{anterior}} \frac{(B_{\text{actual}} - B_{\text{anterior}})}{B_{\text{anterior}}};$
$x_{B_0}^{(i)} = x_{F_0}^{(i)}; i = 1, 2, \dots, n; i \neq k$	$x_{B_0}^{(i)} = x_{F_0}^{(i)}; i = 1, 2, \dots, n$
$\sum_{i=1}^n \frac{\alpha_i x_B^{(i)}}{\alpha_i - \theta} = 0; R_{\min} = -1 + \sum_{i=1}^n \frac{\alpha_i x_D^{(i)}}{\alpha_i - \theta}; \text{ CLASS II}$	
Not considered	$R_{\min} = \frac{\left[\frac{x_D^{(k)}}{x_B^{(k)}} \right] - \alpha_{ik,k} \left[\frac{x_D^{(k)}}{x_B^{(k)}} \right]}{\alpha_{ik,k} - 1}; \text{ CLASS I}$
$Y = 1 - \exp \left[\frac{(1+54.4X)(X-1)}{(11+117.2X)\sqrt{X}} \right]; X = \frac{R - R_{\min}}{R+1}; Y = \frac{N - N_{\min}}{N+1}$	

Table 1. Comparing the Diwekar [11] and Narváez-García et al. [10] shortcut method using variable reflux policy.

5.1.3.1. Solution algorithm (Narváez-García et al. [1])

The mathematical model by Narváez-García et al. [10] is conformed for the system of Eqs. (22) and (23) or (39), (35), (37), (43), (48), (49), (54), (55), (57), (58), and (59). The main objective of this system of equations is to calculate the value of the reflux ratio and for this Eq. (40) is used.

Eq. (43) requires the value of X and R_{\min} . The value of X is related to the minimum number of trays (N_{\min}) through Eqs. (48) and (49); therefore, first N_{\min} is calculated, starting with an assumed value and is iterated until it converges to the correct value of N_{\min} .

The Newton-Raphson iterative method used Eqs. (57)–(59). These equations are only function of the dome and bottom concentrations of as well as of the relative volatilities.

The value obtained of X allows to find the value of $R_{\min'}$ which is solve using the Underwood equation (39). However, to get the value of R_{\min} before it is necessary to calculate the mole fractions of the dome (x_D) using Eqs. (40) and (54). With the values of X and R_{\min} will be calculated the reflux ratio R (Eq. (43)) and now it is possible to calculate the amount remaining in the reboiler using Eq. (37) and the bottom concentration using Eq. (35).

6. Cases of study

The mathematical models of the shortcut method presented in this work have been solved considering various mixtures: binary, ternary, and quaternary. Being the variable reflux policy more complicated than the constant reflux policy, only are presented cases considering the variable reflux policy. The input conditions to the process are shown in **Table 2**.

Case	Feed molar fraction				Relatives volatilities (α)				N^*	k	$x_D^{q\omega}$
	1	2	3	4	1	2	3	4			
1	0.40	0.20	0.30	0.10	1.67	1.25	1.00	0.83	5	3	0.70
2	0.33	0.33	0.34	–	1.33	1.00	0.67	–	10	2	0.80
3	0.50	0.50	–	–	2.40	1.00	–	–	9	2	0.95

N^* = Number of trays, k = Reference, Component = 1, 2, 3, 4.

Table 2. Input conditions for cases of study.

7. Results and discussion

The results of the cases of the study are shown below. Considering that, the mole fraction of the desired component is a constant amount, the profiles of the reflux ratios, the remaining amounts in the bottom and its concentrations are obtained. To validate the results of the reflux rate obtained by the shortcut methods, a comparison between the profile of the reflux ratio obtained and the profile obtained with a rigorous method was performed.

7.1. Case 1

Figures 2, 4, and 5 show the results obtained with the short methods of Diwekar [11] and Narváez-García et al. [10]. **Figure 3** shows the result comparison between the shortcut method and the rigorous method.

The comparison of the results between the two shortcut methods (**Figures 2, 4, and 5**) allows to establish that there are no significant differences. The maximum deviation for reflux was 1.5%, the amount remaining in the reboiler was 0.55 %, and concentrations in the bottom was 2%.

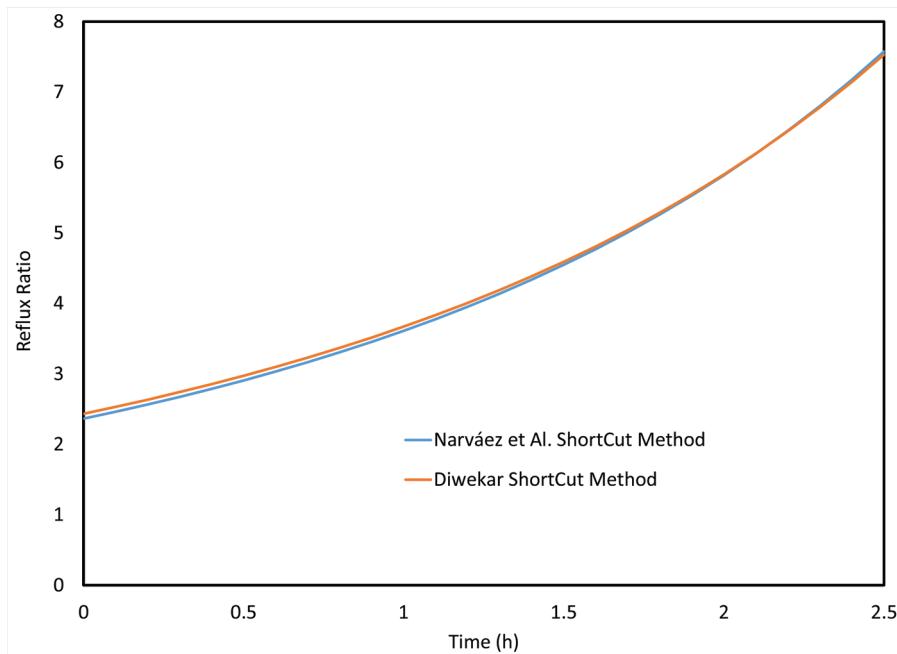


Figure 2. Reflux ratio profiles obtained with the shortcut methods.

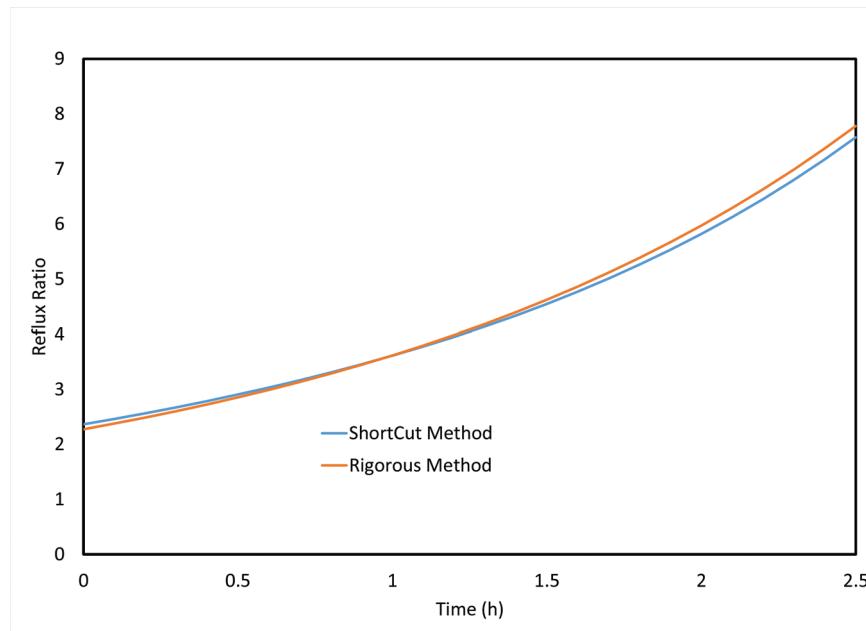


Figure 3. Comparison of profiles of reflux ratio using the shortcut method and a rigorous method.

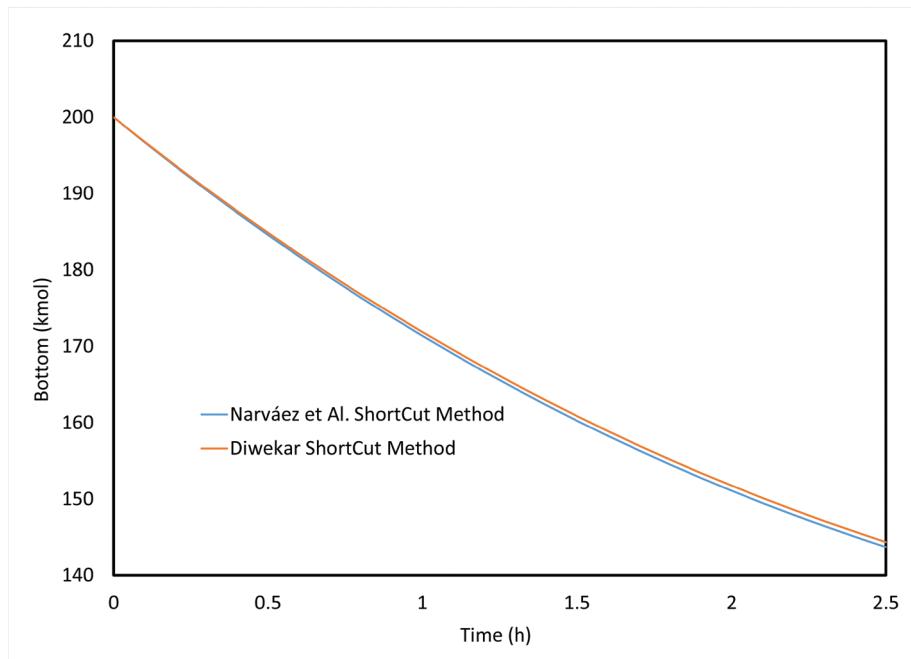


Figure 4. Remaining amount in the reboiler obtained by shortcut methods.

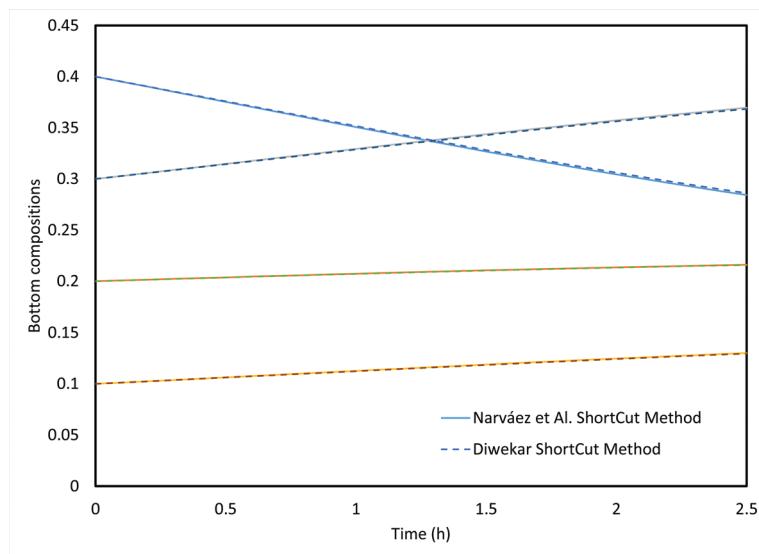


Figure 5. Concentration profiles in the reboiler obtained by shortcut methods.

As for the comparison between the shortcut method and the rigorous method (**Figure 3**), the deviations are within an acceptable range of 9.7% maximum considering the reflux ratio is calculated.

7.2. Case 2

Figures 6, 8, and 9 show the results obtained with the short methods of Diwekar [11] and Narváez-García et al. [10]. **Figure 3** shows the results comparison between the shortcut method and the rigorous method.

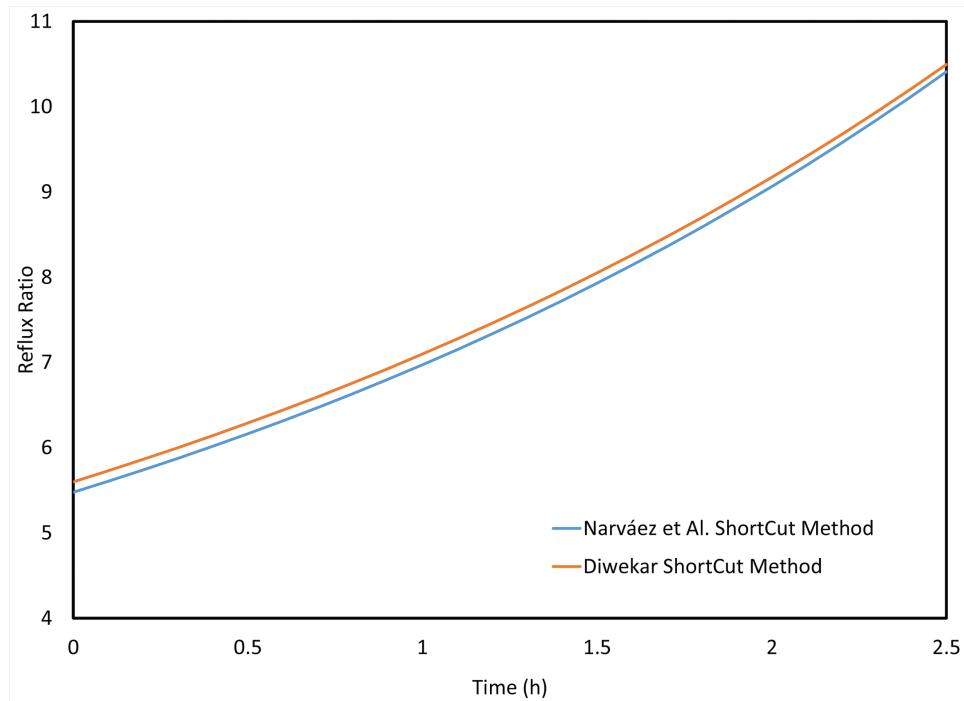


Figure 6. Reflux ratio profiles obtained by shortcut methods.

The results between both short methods (**Figures 6, 8, and 9**) allow to establish that there are no significant differences. The maximum deviation for calculated reflux ratio was 2.2%, for the amount remaining in the reboiler was 0.29%, and the deviation in the bottom concentrations was 0.67%. As for the comparison between the shortcut method and the rigorous method (**Figure 7**), the deviations are within an acceptable range of 9.7% maximum considering the reflux ratio is calculated.

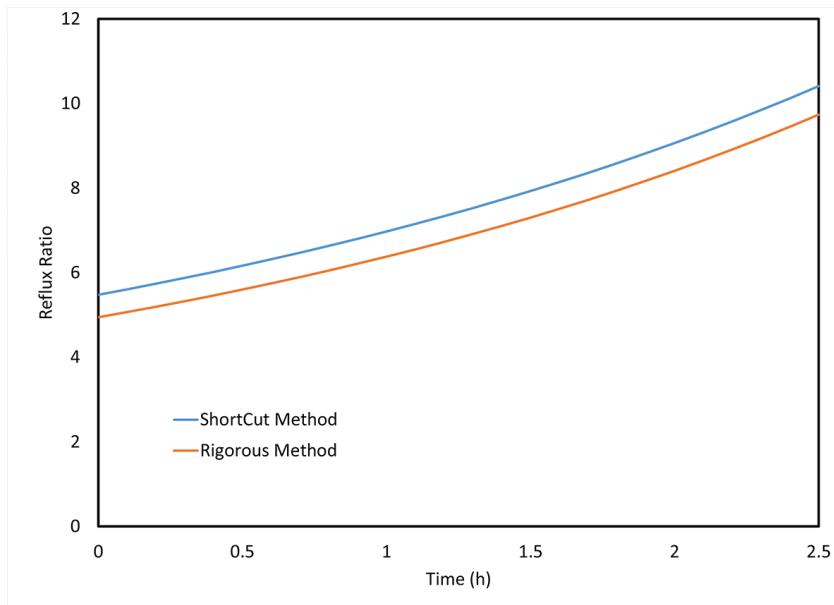


Figure 7. Comparison of profiles of reflux ratio obtained using the shortcut method and a rigorous method.

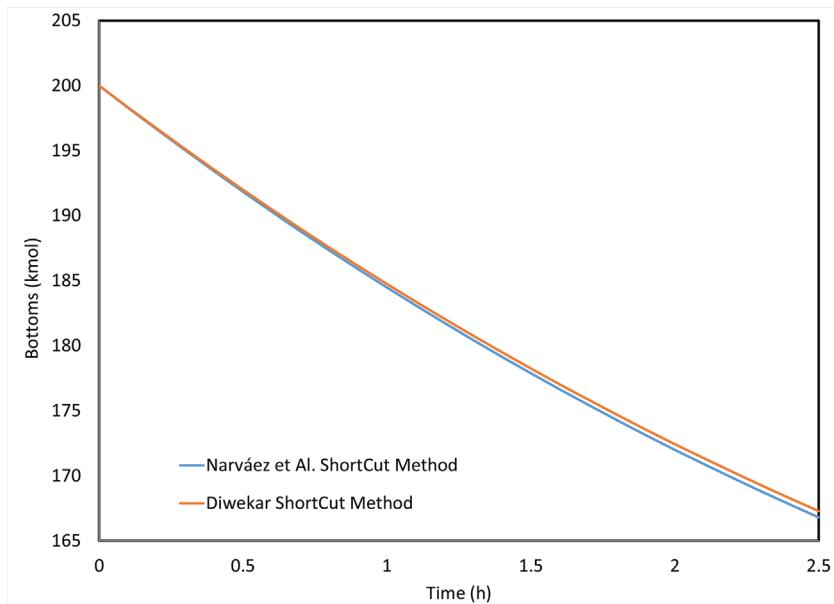


Figure 8. Remaining amount in the reboiler obtained by shortcut methods.

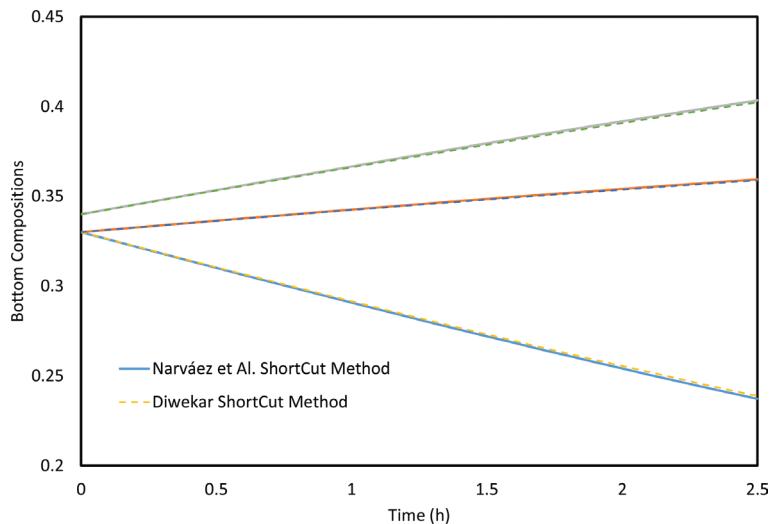


Figure 9. Concentration profiles in the reboiler obtained by shortcut methods.

7.3. Case 3

Figures 10, 12, and 13 show the results obtained with the short methods of Diwekar [11] and Narváez-García et al. [10]. Figure 11 shows the results comparison between the shortcut method and the rigorous method.

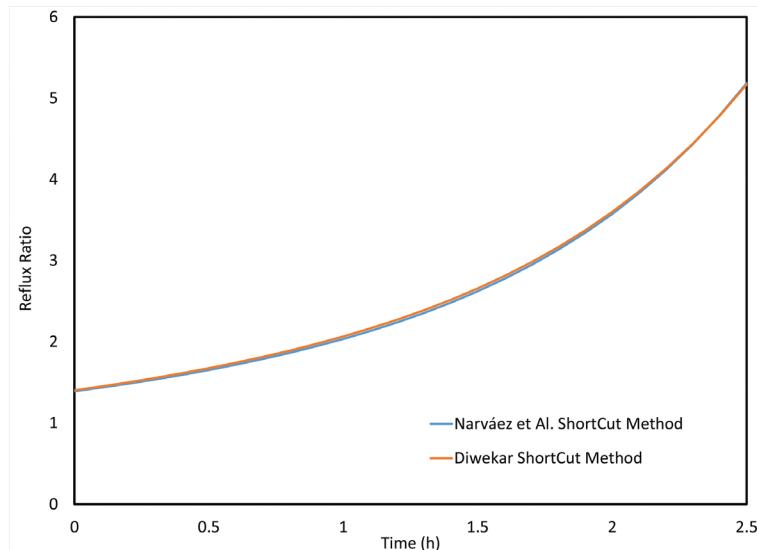


Figure 10. Reflux ratio profiles obtained by shortcut methods.

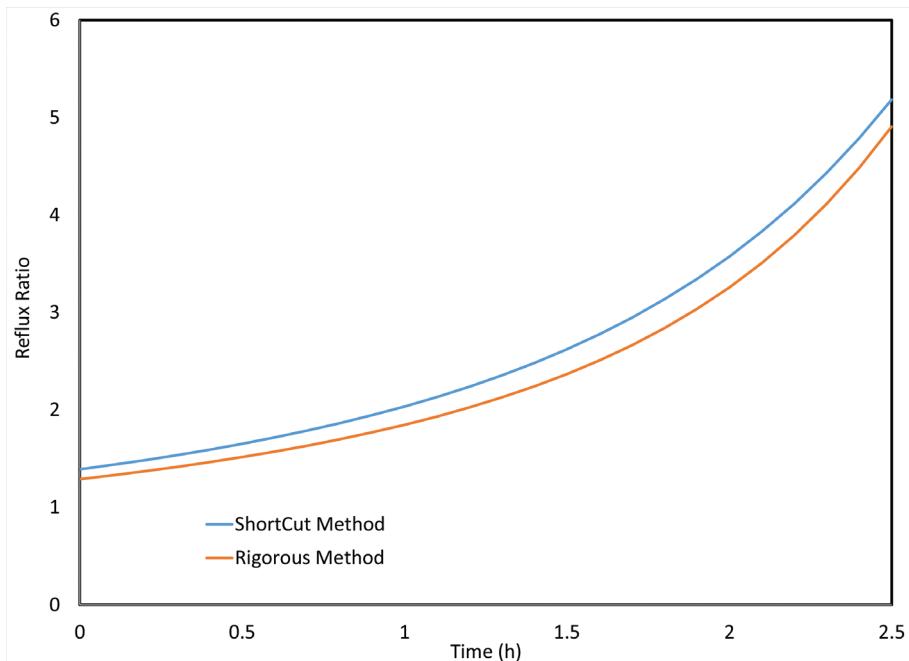


Figure 11. Comparison of profiles of reflux ratio obtained using the shortcut method and a rigorous method.

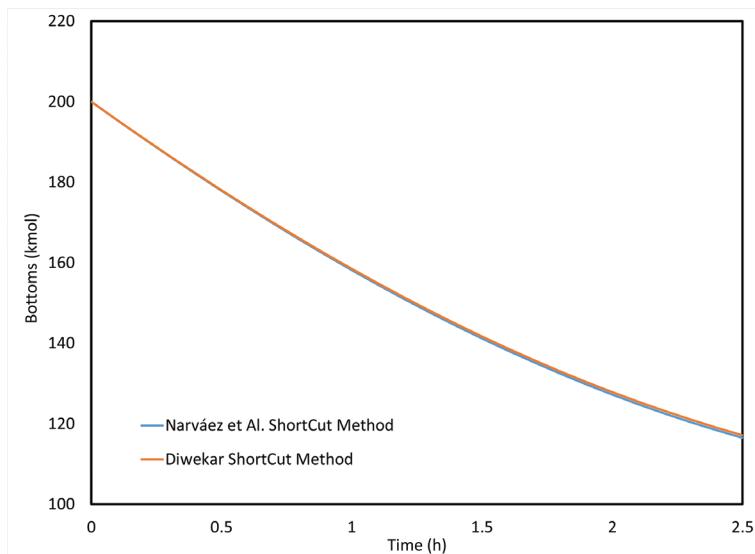


Figure 12. Remaining amount in the reboiler obtained by shortcut methods.

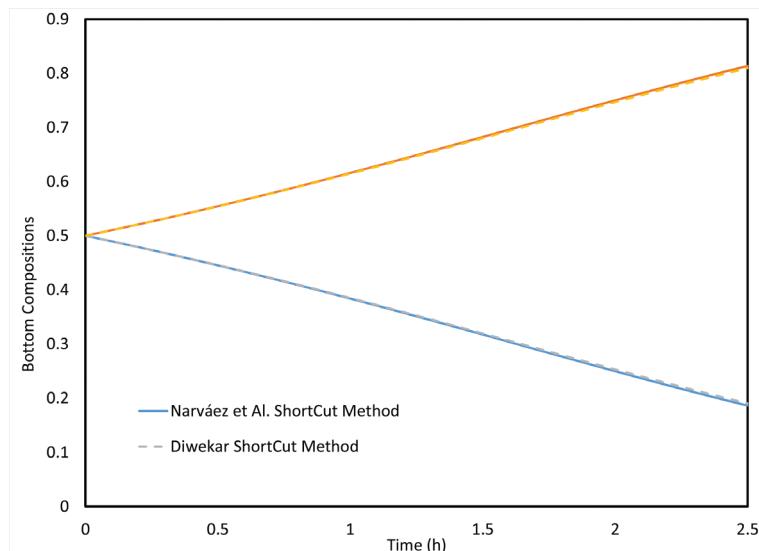


Figure 13. Concentration profiles in the reboiler obtained by shortcut methods.

The results between both short methods (**Figures 10, 12, and 13**) allow to establish that there are no significant differences. The maximum deviation for calculated reflux ratio was 2.7%, the amount remaining in the reboiler was 0.45%, and the deviation in the bottom concentrations was 0.63%. As for the comparison between the shortcut method and the rigorous method (**Figure 11**), the deviations are within an acceptable range of 3.8% maximum considering the reflux ratio is calculated.

In general, as shown in each of the figures, the maximum deviation found between the two shortcut methods considering a policy of variable reflux is less than 3% and, in this sense, the use of either of the two depends on the ease of application of the method.

In this case, the method developed by Narváez-García et al. [10] is better because it is adjusted to the original equations of the FUG method.

Similarly, to validate the shortcut methods considering a variable reflux policy, we had presented a comparison between the profiles of the reflux ratio which shows that you can have up to 9.7% difference between the results of the shortcut method and the rigorous method, of course, this difference is due to the simplifications of the short method, however, the difference falls within an acceptable range and this validated the shortcut methods presented. The maximum difference found between the concentrations of the bottom was less than 2%.

In all cases, the behavior of the profiles is adequate for the batch distillation process; in other words, greater process time is necessary for a greater reflux and the more volatile component is depleted.

8. Conclusions

In this chapter, we have presented the shortcut methods developed by Diwekar [11], Sundaram and Evans [13], and Narváez-García et al. [10]. Considering the complexity of the solution only, the shortcut method with a variable reflux policy is solved. The results were validated using a rigorous method. It is considered that the results of the shortcut methods are very close with respect to the rigorous method results.

Author details

A. Narváez-García¹, J.C. Zavala-Loría^{2*}, A. Ruiz-Marín¹ and Y. Canedo-López¹

*Address all correspondence to: jose.zavala@unini.edu.mx

1 Faculty of Chemical Sciences and Petroleum, Autonomous University of Carmen, Carmen City, Campeche, Mexico

2 Iberoamerican International University, San Francisco de Campeche, Campeche, Mexico

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