Batch Distillation Column Design using Shortcut Method - A Review

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Abstract - *This paper introduces the batch distillation methods developed from the Fenske Underwood-Gilliland (FUG) continuous distillation method. Besides this, the results of the shortcut method developed by Diwekar and Narváez-García et al are compared. The results of both methods are compared to confirm the results using the rigorous method presented by Domenech and Enjalbert. The results show no significant difference for both shortcuts since the maximum deviation obtained between the shortcuts is less than 3%. Subsequently, the use of either of these two methods is easily found or the difficulty of each solution of the model calculations. The direct batch distillation model is effective for batch distillation and batch process design. The shortcut model is constructed using Fenske-Underwood-Gilland (FUG) calculations for continuous distillation design. The model consists of advances in time using the explicit integration scheme of the first step and solving FUG equations at any time step. The number used for model problems is used for model testing and validation. The agreement between the shortcut model is, therefore, a more complex simulation. The model can be a powerful and fast tool to be used in the design of the batch process and in the integration of batch distillation systems.*

*Key Words***: Batch Distillation, FUG method, Design of Batch Distillation Column, Shortcut Distillation Method**

1.INTRODUCTION

Batch distillation is a widely used process for separating chemical compounds in small quantities of a mixture, for the recovery of small quantities of hazardous substances in waste streams, for the recovery of solvents, as well as for the high added value of cement and biotechnology products, among others. Therefore, the development of mathematical models for the estimation of a process has been of great interest in recent times [1–4]. It is a simple process as a device can separate all parts of the mixture, while a continuous process [5] requires several columns of distillation equal to the number of minus one (n - 1) parts. Another advantage of the batch distillation process is the use of single devices for mixing with different compositions or different mixes [6]. On the other hand, the disadvantage of batch distillation in the case of continuous distillation is that only a small number of products can be obtained from the mixture. Another disadvantage is that each cutter

produces unwanted waste, however, these residuals can be separated into a single column [7].

Following methods can be used to operate the batch distillation column [1]:

1) Constant reflux.

2) Variable reflux.

3) Optimal reflux.

4) Reflux profile.

Process behavior can be estimated by developing mathematical models based on mass and energy balance. The obtained mathematical models can be classified into [1, 8, 9]:

1) Simplified (shortcut method).

2) Semi rigorous.

3) Rough.

4) Order Reduction.

Currently, rigorous models are of great interest and require the use of computers with particularly high accuracy and processing capabilities; however, simplified methods can be applied with the use of devices such as tablets, smartphones, and/or laptops with small capacity for data processing, which enables search to predict the behavior of the process [2, 10]. In addition, using this type of method is a tool for obtaining initial data for mathematical optimization.

Rigorous methods consider the full dynamics of a column, but shortcut methods are mathematical models that take into consideration fewer equations and predict the behavior of the method, generally considering the general material balance and partial balance of any part. The most limiting factor of those shortcut methods is to seek out a functional relationship between the dome and therefore the lower densities. Shortcut methods are used because they require short calculus time and relatively fewer memory requirements, likewise as acceptable accuracy within the results obtained with relevancy the rigorous method. These are an appropriate tool for obtaining initial values for the mathematical optimization of some processes and need close data to unravel the complexity of the methods. The shortcut method is employed to get the minimum reflux ratio, Rmin, and a minimum number of phases Nmin for the

look and limit conditions of the columns. On the opposite hand, shortcut methods are easy to use and might be wont to program, therefore, a teaching alert process.

Two of the foremost important shortcut methods reported within the literature use the Fenskenderwood-Gilland (FUG) method for continuous distillation, but consider the feed changing at every moment; that's, the underside product at the present time is that the next time (phase) feed. The primary of the shortcut methods was developed by Diwekar [11] and reported within the literature by Diwekar and Madhavan [12]. This method is developed by considering both fixed and variable reflux patterns. This method used the Hengstbabek-Geddes equation. This method also makes comparisons between the values of Underwood's minimum reflux ratio and Gilliland's minimum reflux ratio, which increases the computational time because it uses an extra iteration process. The second method is reported by Sundaram and Evans [13] and is considered only as a continuing reflux approach and therefore the Fenske equation. The model obtains an answer in two parts; Solves the functional relationship between the dome and therefore the bottom composition using an external loop and FUG method that solves the fabric balance. The mathematical model developed is initially considered:

(1) Constant relative volatility.

(2) Constant molar flow.

(3) Low vapor and liquid accumulation in trays and condenser.

Based on the work of Sundaram and Evans [13], Norviz-Garcia et al. [10] using the variable reflux method developed a mathematical model for the batch distillation process. Current studies show the foremost important shortcut methods won't to assess the behavior of the batch distillation process.

2. Method followed

The mathematical model of the column is obtained by performing the total mass balance and fractional mass balances for the "I" portion. The functional relationship between the composition of the bottom and the dome of the column is found using the Fenske-Underwood-Gilliland method. Although it demonstrates the development of the model, considering only the operative modes of static and variable reflux, they can be demonstrated in only four studies for the shortcut method for variable reflux, considering the contribution of the authors to the state of the art. In each case, the mixture is boiled to a boiling temperature. The error tolerance is 10−4, the consolidation step is $\Delta t = 10^{-1}$ h and the production time is required to reduce the lighter component. It was considered a steam stream of 200 km feed and 110 km H - 1. In these cases, the relative volatility is considered constant throughout the process. The value of the vapor flow is established so that it can reduce the most volatile component during a short operation. Only the first cut is considered for ternary and quaternary alloys. For validation, the results of two

methods, Diwekar [11] and Norviz-Garcia et al. [10], compared the results using the rigorous method presented by Domenech and Engelbert [17]. This model is used because it is considered a low holdup.

3. Mathematical Models being simplified

The complete mathematical model of the batch distillation column, which considers the dynamics of the process, consists of a system of differential equations and algebra (DAEs) added by equations that allow the calculation of thermodynamic properties and hydraulic conditions of the column. The solution of the system is complicated by the state equations used to predict the behavior of the gas phase (Sow, Redlich-Quang Peng-Robinson, etc.) or by the models used to estimate the liquid phase behavior. Wilson, NRTL, UNIQUAC, UNIFAC, etc.) The equations in the rigorous mathematical model of batch distillation is the related in fact same as the number of the mixture of components NC and N trays (N + 2) (2nc + 1), where N + 2 is considered a reboiler and condenser-tank reflux according to Diwekar [9]

The equations consider the total limits of each step (Σ x = y = 1), the reflux ratio (R = L / D), and the expression of the liquid (L) and vapor (V) flows the calculations along the column. While calculating the other variables of interest, such as column hydraulic or thermodynamic efficiency, in turn increases the number of equations. The solution of this mobilization system is complex and requires intensive use of computers with enough processing capacity, which affects costs in the area of process simulation. Therefore, it is necessary to consider some simplifications to the mathematical model to reduce the data processing time. If this process is considered continuous, reductions to the mathematical model of batch distillation are possible, with the feed changing every moment as shown in Figure 1 [1, 10], which is Fenske [18], Underwood [19], and Gilliland [20] (FUG method) of continuous distillation.

The Gilland correlation can be replaced with the correlation of Edulliji [21] because the mathematical expression for numerical works is simpler. The shortcut method considers:

1) Constant molar flow along the column.

2) Constant relative volatility throughout the process.

3) Insufficient fluid and vapor accumulation within the column.

The enthalpy of evaporation is the same for all components of a constant molar flow, which is correct if the mixture contains many similar compounds. The simplification from the shortcut method is more limited to consider the relative volatility throughout the process. This observation significantly reduces the number of calculations in the model, especially if the iterative processes of the liquid-vapor equilibrium are not applicable. When the relative instability cannot be taken as a constant amount of time or along the column, the polynomial expressions or Win [22] equation can be used to estimate the changes; Therefore, Deveker [11] suggested that the relative volatility can be

used to calculate every moment of the process using the mean between the values of the bottom volatility and the dome. The vapor accumulation in the distillation column is neglected as it is less than the accumulated amount of liquid, moreover, the fluid accumulation in the column is neglected, which is less than the accumulated fluid in the reboiler. Under these conditions, two important shortcut methods for batch distillation in the literature have been reported by Diwekar [11], Sundaram, and Evans [13] and Narvaz-Garcia et al. [17].
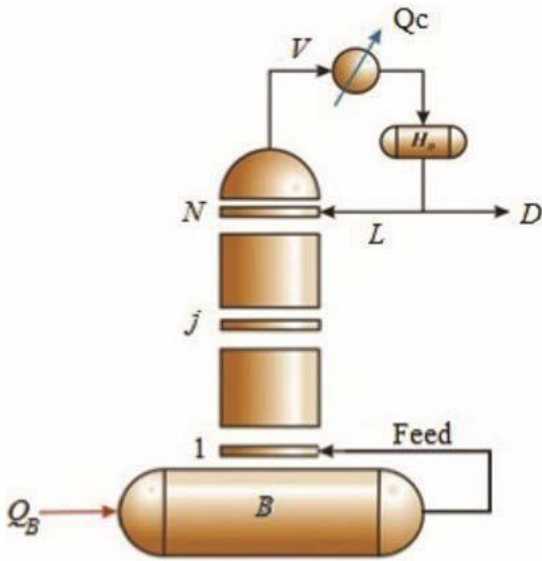
Fig -1: Scheme of a batch distillation column for the shortcut method.

3.1. Shortcut methods derived from FUG

Shortcut developed by Diwekar[11]. Diwekar developed the first shortcut method for batch distillation presented here. This method considers the global stability in the column and their partial equilibrium (part "i"); each of the equations used in the method are as follows: Mass balance:

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

$$\frac{dB}{dt} = -D; \qquad B_0 = -F \tag{2}$$

where D is the distillation obtained by mass balance in the dome of the column:

$$D = \frac{V}{R+1} \tag{3}$$

Where R is the reflux ratio:

The partial equilibrium with respect to a part is (i):

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

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

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

and substitution in Eq. (2) Received:

$$B \frac{dx_B^{(i)}}{dt} - Dx_B^{(i)} = -Dx_D^{(i)} \tag{8}$$

Substituting in Eq. (3) is obtained by:

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

$$\frac{dx_B^{(i)}}{dt} = \frac{V}{B[R+1]}[x_B^{(i)} - x_D^{(i)}]; \quad x_{B0}^{(i)} = x_{F0}^{(i)} \tag{10}$$

A material equilibrium also occurs for the ratio between the reference part (k) and the part (i) and part (k).

$$\frac{dx_B^{(k)}}{dt} = \frac{D}{B}[x_B^{(k)} - x_D^{(k)}] = \frac{V}{B[R+1]}[x_B^{(k)} - x_D^{(k)}]; \tag{11}$$
$$x_{B0}^{(k)} = x_{F_0}^{(k)}$$

$$\frac{dx_B^{(i)}}{dt} = \frac{D}{B}[x_B^{(i)} - x_D^{(i)}]; \tag{12}$$
$$\frac{dx_B^{(k)}}{dt} = \frac{D}{B}[x_B^{(k)} - x_D^{(k)}];$$
$$x_{B_0}^{(i)} = x_{F_0}^{(i)}; \qquad i=1,2,...,n; i \neq k$$

$$\frac{dx_B^{(i)}}{dx_B^{(k)}} = \frac{[x_B^{(i)} - x_D^{(i)}]}{[x_B^{(k)} - x_D^{(k)}]}; \tag{13}$$
$$x_{B_0}^{(i)} = x_{F_0}^{(i)}; \qquad i=1,2,...,n; i \neq k$$

$$dx_B^{(i)} = \frac{[x_B^{(i)} - x_D^{(i)}]}{[x_B^{(k)} - x_D^{(k)}]}dx_B^{(k)}; \tag{14}$$
$$x_{B_0}^{(i)} = x_{F_0}^{(i)}; \qquad i=1,2,...,n; i \neq k$$

Eqs. (2) and (14) consider the very small changes that can be obtained by considering Eq. (2), obtained from:

$$\frac{\Delta B}{\Delta t} = -D \tag{15}$$

$$\Delta B = -D \Delta t \tag{16}$$

$$B_{new} = B_{old} - D \Delta t \tag{17}$$

Eq. (3) is obtained by:

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

Considering Eq. (14) is obtained by: x

$$R = \frac{L}{D} \tag{4}$$

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

$$x^{(i)}_{B,new}=x^{(i)}_{B,old}+\frac{[x^{(i)}_B-x^{(i)}_D]_{old}}{[x^{(k)}_B-x^{(k)}_D]_{old}}\Delta x^{(k)}_B; \tag{20}$$
$$x^{(i)}_{B_0}=x^{(i)}_{F_0}; \qquad i=1,2,...,n; i\neq k$$

For this method, the functional relationship between the densities of the dome and the bottom is obtained using the equation Hengestebeck-Geddes:

$$x^{(i)}_D=(\frac{\alpha_i}{\alpha_k})^{C_1}[\frac{x^{(k)}_D}{x^{(k)}_B}x^{(i)}_B]; \qquad i=1,2,...,n; i\neq k \tag{21}$$

α is the relative instability and is equal to the minimum number of trays of the C1 Fenske equation. It is also necessary to use the equations of Underwood and Gilland or Edulzi:

$$\sum_{i=1}^{nc}\frac{\alpha_i x^{(i)}_B}{\alpha_i-\theta}=0 \tag{22}$$

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

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

The Eduljee correlation is
$$Y=0.75(1-X^{0.5668}) \tag{25}$$
being, in both cases:
$$X=\frac{R-R_{min}}{R+1} \tag{26}$$

$$Y=\frac{N-N_{min}}{N+1} \tag{27}$$

$$f_c=\frac{R_{minU}}{R}-\frac{R_{minG}}{R}=0 \tag{28}$$

$$\sum_{i=1}^{nc}x^{(i)}_D=\sum_{i=1}^{nc}(\frac{\alpha_i}{\alpha_k})^{C_1}[\frac{x^{(k)}_D}{x^{(k)}_B}x^{(i)}_B]=1 \tag{29}$$

$$\frac{x^{(k)}_D}{x^{(k)}_B}=\sum_{i=1}^{nc}(\frac{\alpha_i}{\alpha_k})^{C_1}x^{(i)}_B \tag{30}$$

$$f_v=\{\sum_{i=1}^{nc}[(\frac{\alpha_i}{\alpha_k})^{C_1}x^{(i)}_B]\}-\frac{x^{(k)}_D}{x^{(k)}_B} \tag{31}$$

$$x^{(k)}_D=\frac{x^{(k)}_D}{\sum_{i=1}^{nc}[(\frac{\alpha_i}{\alpha_k})^{C_1}x^{(i)}_B]} \tag{32}$$

$$dx^{(i)}_B=[x^{(i)}_D-x^{(i)}_B]\frac{dB}{B} \tag{33}$$

$$\Delta x^{(i)}_B=[x^{(i)}_D-x^{(i)}_B]\frac{\Delta B}{B} \tag{34}$$

$$x^{(i)}_{B,new}=x^{(i)}_{B,old}+[x^{(i)}_D-x^{(i)}_B]_{old}$$
$$\frac{(B_{new}-B_{old})}{B_{old}}; \quad x^{(i)}_{B_0}=x^{(i)}_{F_0}; \; i=1,2,...,n \tag{35}$$

$$dx^{(k)}_B=[x^{(k)}_D-x^{(k)}_B]\frac{dB}{B} \tag{36}$$

$$\frac{(B_{new}-B_{old})}{B_{old}}=\frac{\Delta x^{(i)}_B}{[x^{(i)}_D-x^{(i)}_B]_{new}} \tag{37}$$

$$N_{min}=\frac{ln[\frac{x^{(i)}_D}{x^{(k)}_D}\frac{x^{(k)}_B}{x^{(i)}_B}]}{ln(\alpha_i)} \tag{38}$$

$$R_{min}=\frac{[\frac{x^{(lk)}_D}{x^{(lk)}_B}]-\alpha_{lk,lk}[\frac{x^{(hk)}_D}{x^{(hk)}_B}]}{\alpha_{lk,lk}-1} \tag{39}$$

$$x^{(i)}_D=x^{(i)}_B[\frac{x^{(k)}_D}{x^{(k)}_B}]\alpha_i^{N_{min}}; \qquad i=1,2,...,n; i\neq k \tag{40}$$

$$\sum_{i=1}^{nc}x^{(i)}_D=\sum_{i=1}^{nc}x^{(i)}_B[\frac{x^{(k)}_D}{x^{(k)}_B}]\alpha_i^{N_{min}}=1 \tag{41}$$

$$x^{(k)}_D=\frac{x^{(k)}_D}{\sum_{i=1}^{nc}(\alpha_i^{N_{min}}x^{(i)}_B)} \tag{42}$$

3.2. Sundaram and Evans [13] solution algorithm

The mathematical model of Sundaram and Evans is made by the system of Eqs. (35), (37)–(42). to unravel this technique, follow subsequent steps:
1) Steady-state concentrations are calculated considering that Nmin=N.
   (a) The concentration of reference component (k) within 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 therefore the remaining amount within the reboiler (Eq. (37)) is calculated.
2) The Rmin and Nmin are calculated.
   (a) For Rmin Eq. (39) is employed.
   (b) For Nmin Eq. (38) is employed.
   (c) Eqs. (38) and (39) are solved using an iterative process.
3) Calculate the reference component concentration within the dome (Eq. (42)).
4) the opposite concentrations are calculated using the Fenske Eq. (40).
5) Back to step 2 until achieve the specified production time.

3.3. The short method developed by Narváez-García et al. [10] employing a variable reflux policy

This proposal is predicated on the concepts of Sundaram and Evans [13]. it's initiated by calculating the reflux ratio required to get the specified product; therefore, using Eq. (26) and solving it, the subsequent is obtained:

$$R=\frac{X+R_{min}}{1-X} \tag{43}$$

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

$$\sum_{i=1}^{nc}\frac{\alpha_i x^{(i)}_B}{\alpha_i-\theta}=0 \tag{45}$$

$$x^{(i)}_D = x^{(i)}_B \left[\frac{x^{(k)}_D}{x^{(k)}_B} \right] \alpha_i^{N_{min}}; \qquad i=1,2,\ldots,n; i \neq k \tag{46}$$

$$x^{(k)}_D = \frac{x^{(k)}_B}{\sum_{i=1}^{nc} (\alpha_i^{N_{min}} x^{(i)}_B)} \tag{47}$$

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

$$N_{min} = \frac{\log\left\{ [\frac{x^{(k)}_D}{x^{(k)}_B}] [\frac{x^{(lk)}_B}{x^{(lk)}_D}] \right\}}{\log(\alpha_{lk,k})} \tag{49}$$

$$x^{(lk)}_D = \left[\frac{x^{(k)}_D}{x^{(k)}_B} \right] x^{(lk)}_B \alpha_{lk,k}^{N_{min}} \tag{50}$$

$$\sum_{i=1}^{nc} x^{(i)}_D - x^{(lk)}_D = 1 - x^{(lk)}_D \tag{51}$$

$$\sum_{i=1}^{nc} \left\{ \left[\frac{x^{(k)}_D}{x^{(k)}_B} \right] (\alpha_{i,k}^{N_{min}}) x^{(i)}_B \right\} - x^{(lk)}_D = 1 - x^{(lk)}_D \tag{52}$$

$$\sum_{i=1}^{nc} \left\{ \left[\frac{x^{(k)}_D}{x^{(k)}_B} \right] (\alpha_{i,k}^{N_{min}}) x^{(i)}_B \right\} - \tag{53}$$

$$\left[\frac{x^{(k)}_D}{x^{(k)}_B} \right] x^{(lk)}_B \alpha_{LK,K}^{N_{min}} = 1 - x^{(lk)}_D$$

$$x^{(k)}_D = \frac{[1-x^{(lk)}_D] x^{(k)}_B}{\sum_{i=1}^{nc} \alpha_{i,k}^{N_{min}} x^{(i)}_B - x^{(lk)}_B \alpha_{lk,k}^{N_{min}}} \tag{54}$$

$$= \frac{[1-x^{(lk)}_D] x^{(k)}_B}{\sum_{i=2}^{nc} \alpha_{i,k}^{N_{min}} x^{(i)}_B}$$

$$N_{min} = \frac{\log\left\{ [\frac{x^{(lk)}_D \sum_{i=2}^{nc} \alpha_{i,k}^{N_{min}} x^{(i)}_B}{[1-x^{(lk)}_D] x^{(lk)}_B}] \right\}}{\log(\alpha_{lk,k}^{N_{min}})} \tag{55}$$

$$1 - x^{(lk)}_D = \left[\frac{x^{(lk)}_D}{x^{(lk)}_B} \right] \sum_{i=2}^{nc} \left(\frac{\alpha_{i,k}}{\alpha_{lk,k}} \right)^{N_{min}} x^{(i)}_B \tag{56}$$

$$f(N_{min}) = \left\{ \left[\frac{x^{(lk)}_D}{x^{(lk)}_B} \right] \sum_{i=2}^{nc} \left(\frac{\alpha_{i,k}}{\alpha_{lk,k}} \right)^{N_{min}} x^{(i)}_B \right\} - [1- \tag{57}$$

$$x^{(lk)}_D] = 0$$

$$f'(N_{min}) = \left[\frac{x^{(lk)}_D}{x^{(lk)}_B} \right]$$

$$\left\{ \sum_{i=2}^{nc} \left(\frac{\alpha_{i,k}}{\alpha_{lk,k}} \right)^{N_{min}} x^{(i)}_B \times \ln \left(\frac{\alpha_{i,k}}{\alpha_{lk,k}} \right) \right\} \tag{58}$$

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

The reflux ratio and other values can be calculated with respect to nmin. The solution to the method is solved in the following section Diwekar [11] and this model both

derive from the same material equilibrium (global and partial) and, in other words, both works are developed using the same methodology; However, the functional relationship between the dome and bottom densities are different equations. In fact, Underwood's and Gilland's equations are the same in each model, and the difference is the way in which the Nmin values are obtained. Norvis-Garcia et al. [10] used the Fenske equation, Diwekar [11], and Hengstek-Geddes equation. The calculation times in both models are similar, with Norwijk-Garcia et al. Using the simplified underwood equation (Eq. (39%)), the class I mixer has the advantage over the Diverker model when separating Class I mixtures.

Table -1 Comparison between two solution types

Diwekar
$f_v = \left\{ \sum_{i=1}^{nc} [x^{(i)}_B (\frac{\alpha_i}{\alpha_k})^{C_1}] \right\} - \frac{x^{(k)}_B}{x^{(k)}_D} = 0$
$x^{(i)}_D = x^{(i)}_B \left[\frac{x^{(k)}_D}{x^{(k)}_B} \right] (\frac{\alpha_i}{\alpha_k})^{C_1}; i=1,2,\ldots,n; i \neq k$
$x^{(k)}_D = \frac{x^{(k)}_B}{\sum_{i=1}^{nc} (\alpha_i^{N_{min}} x^{(i)}_B)}$ $B_{actual} = B_{anterior} - (\frac{V}{R+1}) \Delta t$
$x_{(i)B,actual} = x_{(i)B,anterior} + \frac{[x_{(i)B} - x_{(i)D}]_{anterior}}{[x^{(k)}_B - x^{(k)}_D]_{anterior}} \Delta x^{(k)}_B$; $x^{(i)}_B = x^{(i)}_F; \qquad i=1,2,\ldots,n; i \neq k$ $\sum_{i=1}^{nc} \frac{\alpha_i x^{(i)}_B}{\alpha_i - \theta} = 0; R_{min} = -1 + \sum_{i=1}^{nc} \frac{\alpha_i x^{(i)}_D}{\alpha_i - \theta'}$
Class II Not Considered
$Y = 1 - \exp\left[\frac{(1+54.4X)(X-1)}{(11+117.2X)\sqrt{X}} \right]$; $X = \frac{R-R_{min}}{R+1}$; $Y = \frac{N-N_{min}}{N+1}$

Narváez-García et al
$f(N_{min}) = \left\{ [\frac{x^{(lk)}_D}{x^{(lk)}_B} \sum_{i=2}^{nc} (\frac{\alpha_{i,k}}{\alpha_{lk,k}})^{N_{min}}] - [1-x^{(lk)}_D] = 0 \right\} x^{(lk)}_B$
$x^{(i)}_D = x^{(i)}_B \left[\frac{x^{(k)}_D}{x^{(k)}_B} \right] \alpha_i^{N_{min}}; \qquad i=1,2,\ldots,n; i \neq k$
$x^{(k)}_D = \frac{[1-x^{(lk)}_D] x^{(k)}_B}{\sum_{i=2}^{nc} \alpha_{i,k}^{N_{min}} x^{(i)}_B}$
$B_{actual} = B_{anterior} - \frac{\Delta x^{(k)}_B}{[x^{(k)}_B - x^{(k)}_D]_{anterior}} B_{anterior}$
$x^{(i)}_{B,actual} = x^{(i)}_{B,anterior} + [x^{(i)}_B - x^{(i)}_D]_{anterior} \frac{B_{actual} - B_{anterior}}{B_{anterior}}$;

$$R_{min} = \frac{\left[\frac{x^{(lk)}_D}{x^{(lk)}_B}\right] - \alpha_{lk,lk}\left[\frac{x^{(hk)}_D}{x^{(hk)}_B}\right]}{\alpha_{lk,lk} - 1};$$
Class I

The mathematical model of Norvis-Garcia et al. [10] is confirmed for the Eqs system. (22) and (23) or (39), (35), (37), (43), (48), (49), (54), (55), (57), (58) and (59).). The most objective of the system of those equations is to calculate the worth of the reflux ratio and for this Eq. (40) is employed. EQ. (43) requires the worth of X and Rmin. The worth of x is expounded to the minimum trays (Nmin) by Eqs. (48) and (49); Therefore, the primary Nmin is calculated, starting with the worth of the worth and iterating until it meets the proper value of Nmin. The Newton-Raphson iteration method used Eqs. (57) - (59). These equations are only a function of dome and bottom densities and relative instabilities.

The obtained value of x allows finding the worth of Rmin, which might be solved using the Underwood equation (39). However, to get the Rmin value before calculating the mole fractions of the dome (xD) using Eqs. (40) and (54). The reflux ratio R (Eq. (43%)) is calculated with the values of X and Rmin, and it's now possible to calculate the number remaining within the reboiler using Eq. (37) and therefore the lower concentration using Eq. (35).

3.4. Case Study

The mathematical models of the shortcut method presented in this work consider different combinations: binary, ternary, and quaternary. Since the variable reflux policy is more complex than the static reflux policy, only the instances where the variable reflux policy is considered are presented. The input conditions for the process are shown in Table 2. [23]

Table 2 gives the information about the input conditions for the case studies. The results that appear when these input conditions are given to the case studies is shown in the results section for each individual case study.

Table -2 Input conditions for cases of study.

Case	Feed molar fraction				Relatives volatilities (α)				N	k	$x^{(lk)}_D$
	1	2	3	4	1	2	3	4			
1	.4	.2	.3	.1	1.6	1.2	1	.8	5	3	.7
2	.3	.3	.3	-	1.3	1	.6	-	10	2	.8
3	.5	.5	-	-	2.4	1	-	-	9	2	.9

4. Results and discussion

The results of the study's cases are shown below. Taking that into account, the mole fraction of the desired component is obtained by a constant amount, reflux ratio profiles, the remaining residuals, and its concentrations.

The results were verified with the reflux rate obtained with the help of shortcut methods and a comparison was made with the profile of the reflux ratio obtained, also the profile obtained by the rigid method.

Case 1

Figures 2, 4, and 5 show the results obtained with the small methods of Diwekar [11] and Norviz-Garcia et al. [10]. Figure 3 shows the resulting comparison between the shortcut method and the stringent method. A comparison of results between the two shortcut methods (Figures 2, 4, and 5) allows for no significant differences. The maximum deviation for reflux is 1.5%, the rest of the reboiler is 0.55%, and the bottom concentrations are 2%. For a comparison between the shortcut method and the stringent method (Figure 3), the deviations are within the appropriate 9.7% range if the reflux ratio is calculated.
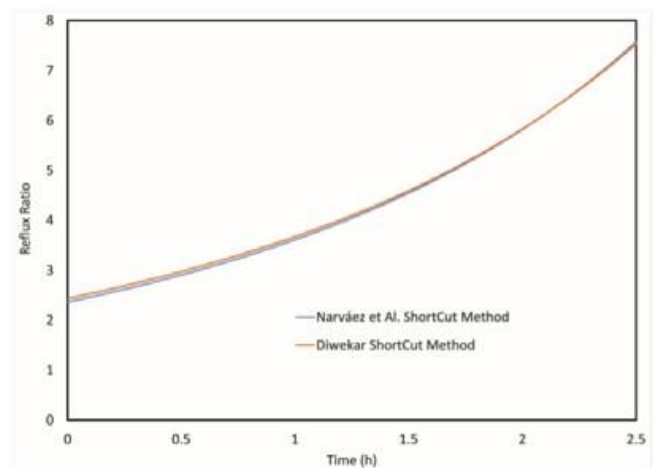

Fig -2: Reflux ratio profiles obtained with the shortcut methods.

Case 2

Figures 6, 8, and 9 show the results obtained with the little methods of Diwekar [11] and Norviz-Garcia et al. [10]. Figure 3 shows a comparison of the results between the shortcut method and the rigorous method.
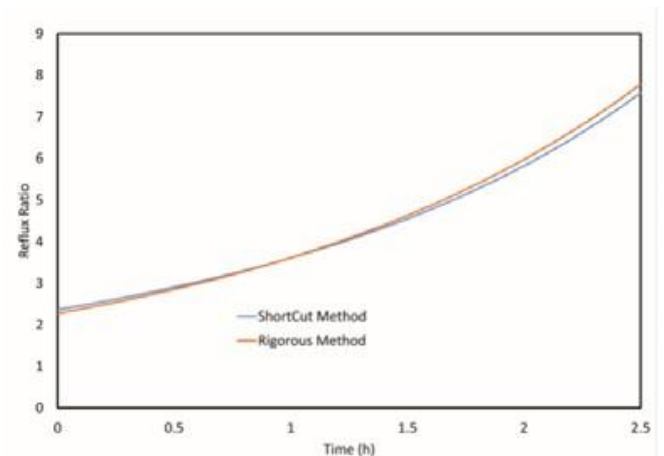

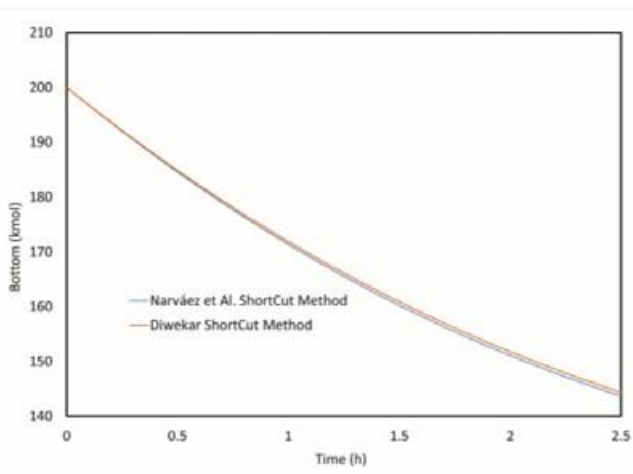**Fig -3**: Comparison of profiles of reflux ratio using the shortcut method and a rigorous method.

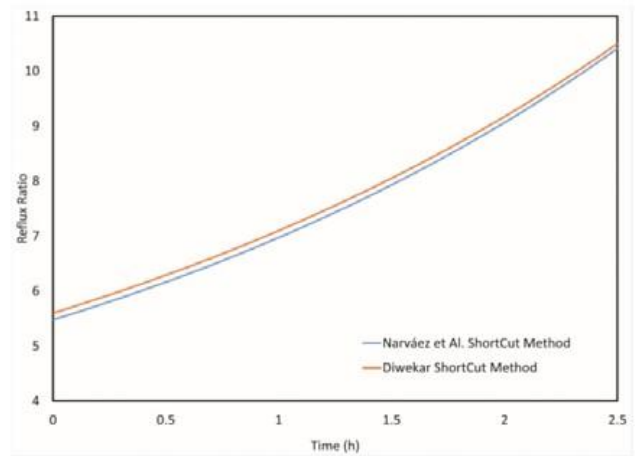**Fig -4**: Remaining amount in the reboiler obtained by shortcut methods.

The results of the 2 smaller methods (Figures 6, 8, and 9) leave no significant differences. The most deviation for the calculated reflux ratio is 2.2%, the number remaining within the reboiler is 0.29%, and the deviation at lower concentrations is 0.67%. For a comparison between the shortcut method and the stringent method (Figure 7), the deviations are within the appropriate 9.7% range if the reflux ratio is calculated.

Case 3

Figures 10, 12, and 13 show the results obtained with the small methods of Diwekar [11] and Norviz-Garcia et al. [10]. Figure 11 shows a comparison of the results between the shortcut method and the rigorous method. The results of the two smaller methods (Figures 10, 12, and 13) allow for no significant differences. For the calculated reflux ratio, the maximum deviation is 2.7%, and the remaining in the reboiler is 0.45%, also the deviation at lower concentrations is 0.63%. For a comparison between the shortcut method and the stringent method (Figure 11), the deviations are within the acceptable 3.8% range if the reflux ratio is calculated.
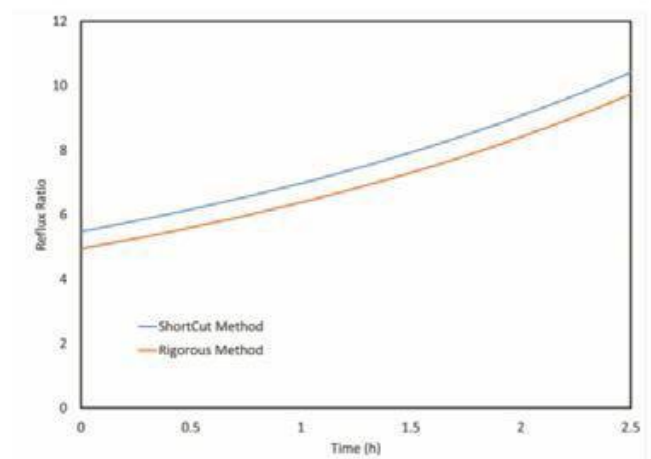

Fig -5: Concentration profiles in the reboiler obtained by shortcut methods.

Fig -6: Reflux ratio profiles obtained by shortcut methods.

Fig -7: Comparison of profiles of reflux ratio obtained using the shortcut method and a rigorous method.
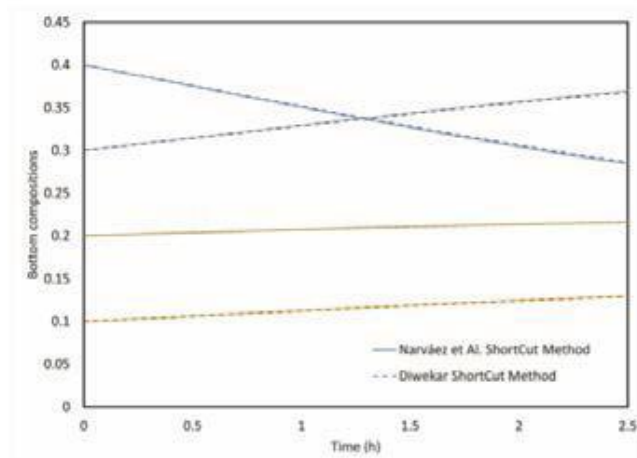
In general, as shown in each figure, the maximum deviation seen between the two shortcut methods considering the variable reflux method is less than 3%, and, in this sense, both of them depend on the ease of use of the method. In this case, the method developed by Norvis-Garcia et al. [10] This is good because it is adjusted to the original equations of the FUG method. Similarly, to validate the shortcut methods that take into account the variable reflux method, we have presented a comparison between the profiles of the reflux ratio, which shows that you can account for up to 9.7% difference between the shortcut method and the results of the rough method. , This difference is due to the simplifications of the small method, however, the difference falls within the acceptable range and it validates the presented shortcut methods. The maximum difference seen between the lower concentrations is less than 2%. In all cases, the behavior of the profiles is sufficient for the batch distillation process; In other words, more processing time is required for greater reflux and the more volatile component is depleted.
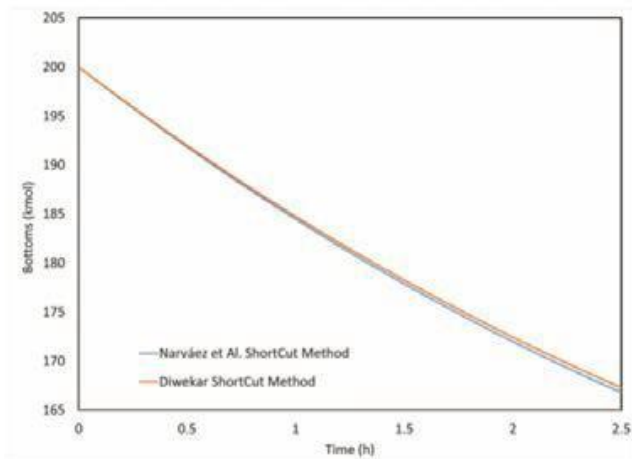
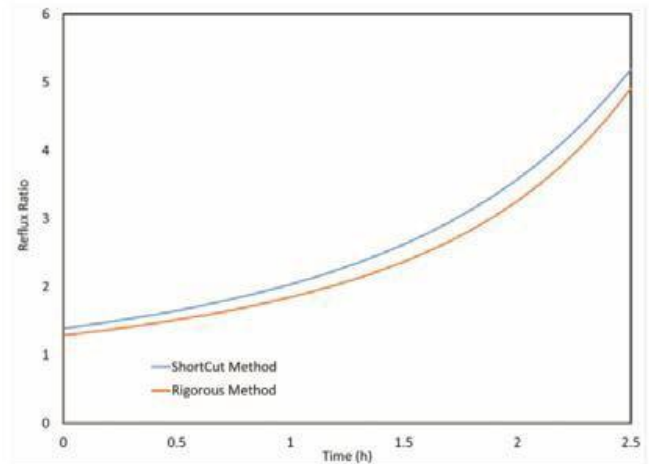**Fig -8**: Remaining amount in the reboiler obtained by shortcut methods.

Fig -11: Comparison of profiles of reflux ratio obtained
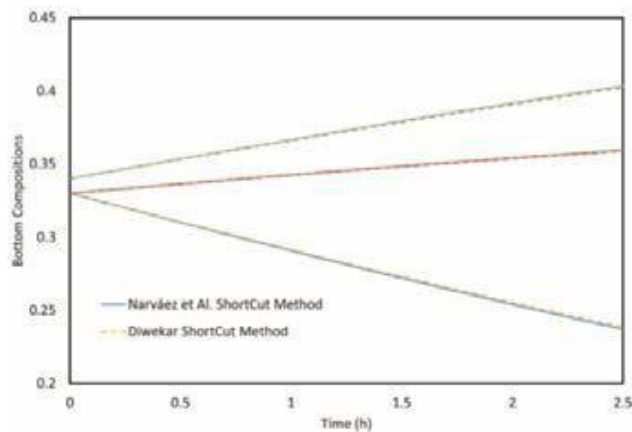

Fig -9: Concentration profiles in the reboiler obtained by shortcut methods.
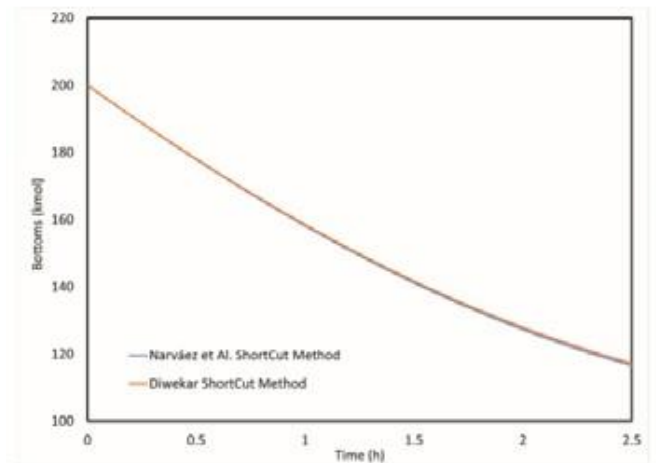

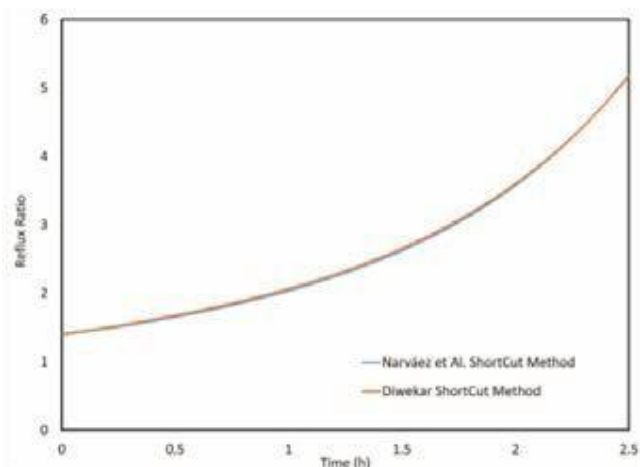**Fig -12**: Remaining amount in the reboiler obtained by shortcut methods.

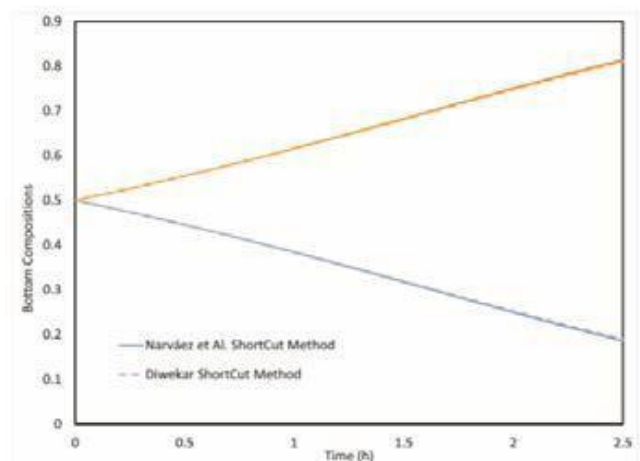**Fig -10**: Reflux ratio profiles obtained by shortcut methods.

Fig -13: Concentration profiles in the reboiler obtained by shortcut methods.

5. CONCLUSIONS

In this paper, we conclude with the shortcut methods developed by Divicar [11], Sundaram and Evans [13], and Norwicz-Garcia et al. [10]. Considering only the

complexity of the solution, the shortcut method can be solved with the variable reflux procedure. The results were verified using a rigorous method. The results of the shortcut methods are very close to the results of the rigorous method.

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