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Excel as an optimization tool applied to multicomponent distillation column sizing

Excel como uma ferramenta de otimização aplicada ao dimensionamento de colunas de destilação multicomponente

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Resumo

A operação unitária de destilação é um método de grande importância para os processos de separação industrial, pois permite o fracionamento de uma mistura com base nas diferenças de volatilidade entre seus componentes. Considerando que uma mistura inicial típica geralmente contém três ou mais produtos de interesse, estudos que visam a otimização da destilação multicomponente, embora escassos na literatura, são cada vez mais imperativos para garantir a eficiência e reduzir os custos operacionais e energéticos associados ao processo. Como o dimensionamento de colunas de destilação multicomponentes usando os métodos Fenske-Underwood e Gilliland (FUG) e Kirkbride envolve cálculos extensos e complexos para obtenção de parâmetros operacionais, o objetivo deste trabalho foi desenvolver um método computacional usando o software Microsoft Excel® para torná-los mais práticos e aumentar a precisão dos resultados obtidos. A funcionalidade da planilha desenvolvida foi verificada através da resolução de um exemplo de aplicação, tanto manualmente quanto eletronicamente. Em ambos os casos, os resultados obtidos foram idênticos, porém com consumo de tempo e probabilidade de erro significativamente menores pelo método eletrônico, demonstrando seu potencial de uso em ambientes acadêmicos e industriais.

Palavras-chave: Separação. Multicomponente. Método de Fenske-Underwood. Método de Gilliland. Excel.

Abstract

The unit operation of distillation is a method of significant importance for industrial separation processes, as it enables the fractionation of a mixture based on the differences in volatility among its components. Considering that a typical initial mixture generally contains three or more products of interest, studies aimed at optimizing multicomponent distillation, although scarce in the literature, are increasingly imperative to ensure efficiency and reduce operational and energy costs associated with the process. Since sizing multicomponent distillation columns using the Fenske-Underwood and Gilliland (FUG) and Kirkbride methods involves extensive and complex calculations to obtain operational parameters, the objective of this study was to develop a computational method using Microsoft Excel® software to make them more practical and enhance the accuracy of the results obtained. The functionality of the developed spreadsheet was verified through the resolution of an example of application, both manually and electronically. In both cases, the results obtained were identical, but with significantly lower time consumption and probability of error by the electronic method, demonstrating its potential for use in academic and industrial settings.

Keywords: Separation. Multicomponent. Fenske-Underwood method. Gilliland method. Excel.

Nomenclature

A', B', C'	Thermodynamic constants for Antoine equation
A	Light key-component
B	Heavy key-component
C	Non-key component
D	Flow in the top stream of the distillation column
F	Feed flow in the distillation column
FR_i	Recovery fraction of component *i* in the distillate or waste
K_i	Distribution coefficient of component *i*
N	Theoretical number of trays
N_{strip}	Number of trays in the stripping section
N_F	Optimal location of the feed tray
N_{min}	Minimum number of trays
N_{rectif}	Number of trays in the rectifying section
P_{i^*}	Vapor pressure of component *i*
P_i	Component pressure *i*
q	Mixture feed condition.
R	Reflux ratio
R_{min}	Minimum reflux ratio
T	Temperature of a given component
T_i	Temperature of component *i* in the feed
W	Flow in the bottom stream of the distillation column
x_i	Liquid composition of component *i*
y_i	Vapor composition of component *i*
Z	Flow rate in the distillation column feed
Z_i	Fraction of a given component in feed
α	Volatility
θ	Auxiliary parameter of the Underwood equation

1. Introduction

Distillation is a unit operation of heat and mass transfer aimed at separating mixtures based on the difference in volatility between their components. This process involves simultaneous stages of vaporization and condensation, taking place in equipment known as a distillation column. During the separation, the less volatile components are collected at the base of the column, while the more volatile ones tend to vaporize more easily and exit through the top. This separation method is widely used in the industry to produce alcohols, lubricating oils, perform petroleum fractionation, among other applications (GIRI & MAHAJAN, 2022).

Considering the high energy demand associated with the process, the design of a distillation tower must be done carefully to maximize productivity and minimize costs. Thus, construction aspects related to the column, such as the number of stages, diameter, fluid dynamics of the phases, as well as thermodynamic calculations of heat and mass transfer, should be evaluated. Additionally, the liquid-vapor equilibrium relationship of the mixture is an essential parameter for the sized column to have adequate characteristics, since the vapor concentration of a given component depends on the pressure, its concentration in the liquid, and the concentration of the other components (KORETSKY, 2013; FOUST et al., 1982). Given its broad industrial applicability, the sizing of distillation columns is the subject of various recent research studies, both in academic and industrial settings (ALVES, MACHADO, & MARANGONI, 2023; HUANG et al., 2023; MARTINEZ et al., 2023).

Many studies document distillation processes involving binary systems, such as mixtures of acetone-n-heptane, benzene-toluene, and ethanol-water, which are extensively found in the literature (KALE et al., 2023; GOOTY et al., 2021). However, the availability of data and research regarding multicomponent distillation is still limited, mainly due to the challenges involved in obtaining operational parameters for systems with more than two components, such as the number of theoretical stages and the reflux ratio, compared to binary systems (GÓMES-SIUNARA & FONT-ESCAMILLA, 2023). For example, when dealing with multicomponent mixtures, fixing the composition of one component does not determine a unique composition for the other constituents, nor does it allow for the direct determination of the equilibrium temperature. This characteristic makes it impossible to independently specify the compositions of the column's top and bottom, requiring the definition of key and non-key components, i.e., components of the initial mixture that will be separated at different times during the process due to their specific physicochemical properties (SINNOTT, 1994). However, research aimed at optimizing the multicomponent distillation process is of utmost importance, as a significant portion of industrial operations, including petroleum fractionation, involves separating a multicomponent mixture into three or more products of interest (GIRI & MAHAJAN, 2022).

When it comes to the methods available for sizing multicomponent distillation columns, the applicability of the Fenske-Underwood and Gilliland (FUG) method and the Kirkbride method stands out, for enabling the determination of the ideal number of trays for component separation, as well as the minimum reflux, actual reflux, and optimal feed tray location (AZEVEDO & ALVES, 2013). However, the calculations required to obtain these parameters are complex and extensive, making manual resolution laborious and prone to errors when employing the proposed equations. In this context, the use of computational tools, such as Microsoft Excel®, offers significant advantages, reducing the time spent on calculations and increasing the reliability of the results obtained. In contemporary times, for example, Excel has been widely used in academic, business, and industrial settings, as it enables the creation of spreadsheets, from simple to complex ones, enabling users to perform calculations, generate graphs, and execute various mathematical and comparative analyses (GÓMES-SIUNARA & FONT-ESCAMILLA, 2023, CARNEIRO et al., 2022).

The multicomponent distillation stands out as an industrial separation method, along with the inherent complexity of the numerical calculations required to determine fundamental operational parameters of this process. Therefore, the present study aimed to develop, through the Microsoft Excel® software, an electronic method to improve the practicality and accuracy of calculations indispensable for the sizing of multicomponent distillation columns. Thus, through this study, we provide a practical resource for a industry project and a didactic tool of significant value for the academic field of chemical engineering, capable of offering a more dynamic and precise approach to understanding the unit operation of distillation.

2. Materials and methods

2.1 Materials

Spreadsheets for determining operational parameters in multicomponent distillation were developed using Microsoft Excel® software, employing the Fenske-Underwood and Gilliland (FUG) and Kirkbride methods. Initially, it was necessary to ascertain the pressure of each key component in the top and bottom streams by applying Antoine's equation (1), which establishes a relationship between the vapor pressure and the temperature of pure substances. Subsequently, the temperature at the ends of the equipment was calculated using Equation 2, which is an algebraic manipulation of Equation 1 (KORETSKY, 2013).

$$ln\, P^{sat} = A' - \frac{B'}{C' + T} \tag{1}$$

$$T = \frac{B'}{A' - \ln(P)} - C' \tag{2}$$

Where: P^{sat} is the saturation vapor pressure, T is the temperature in Kelvin and A', B' e C' are empirical constants for each substance.

The distribution coefficient (K_i) is a key indicator that describes the equilibrium between the liquid phase and the vapor phase in a mixture, based on a relationship between the vapor pressure of a specific component and the total pressure of the system, as expressed in Equation (3). This parameter, when calculated for two distinct components, typically exhibits moderate dependence on temperature, reflecting variations in the relative volatility of these components.

$$K_i = \frac{P_i^*}{P} = \frac{y_i}{x_i} \tag{3}$$

Where: K_i is the equilibrium ratio (distribution coefficient) generally determined for the key component, P_i^* is the vapor pressure of component i, P is the vapor pressure of the component generally determined for the key component, x_i is the mole fraction of i, in the liquid phase, y_i is the mole fraction of i, in the vapor phase

Bubble and dew points are parameters that can be determined by Equation (4) and represent critical conditions of the distillation process, where the first vapor formation and the first liquid condensation occur, respectively. Furthermore, every specific stream that enters the distillation tower has an associated temperature, which can be determined by Equation (5) and allows for a more precise analysis of the behavior of the components along the column (MCCABE et al., 2005).

$$P = \frac{1}{\sum_{i=1}^{n} y_i / P_i^{sat}} \tag{4}$$

$$T_i = T \cdot z_i \tag{5}$$

Where: T_i and z_i are, respectively, the temperature and feed composition of one component i, P_i^{sat} is the pressure of saturation of one component.

Relative volatility, in turn, relates to the difference in volatility between two distinct components present in a mixture, expressed in terms of the more volatile relative to the less volatile, as represented by Equation 6. This parameter directly influences the flows and separation of components, playing a crucial role in the planning and optimization of distillation processes, enabling the identification of ideal conditions to achieve a required efficiency (GUTIÉRREZ-GUERRA et al., 2023).

$$\alpha_{A,B} = \frac{K_A}{K_B} \tag{6}$$

Where: $\alpha_{A,B}$ is the relative volatility between the components A e B, K_A e K_B are vapor equilibrium constants.

In a distillation column, there are internal sections called trays, which allow for contact between the liquid and vapor, both in equilibrium, facilitating mass transfer between phases and the purification of different components present in the mixture. The minimum number of trays required in a specific distillation process, considering the operational condition of total reflux, can be calculated using the Fenske equation (7), considering two components A and B, where A is the more volatile component.

$$N_{min} = \frac{ln\left[\frac{x_A}{x_B}\right]_{top} \cdot \left[\frac{x_B}{x_A}\right]_{bottom}}{ln\ \alpha_{A,B}} \tag{7}$$

Where: N_{min} is the number of minimum trays in relation to the top (distillate) and bottom (waste), and $\alpha_{A,B}$ is the relative volatility of component A in relation to component B.

Within this scenario, a strategy to simplify the calculation of the minimum number of trays is to assume a constant value for the relative volatility at all stages of the column, as indicated by Azevedo and Alves (2013). In various distillation problems, the recovery fraction of component *i* in the distillate or waste (equation 8) is employed instead of the molar fraction, according to the approach described by the same authors (AZEVEDO & ALVES, 2013).

$$F_{R_i} = \frac{moles\ of\ i\ in\ the\ stream}{moles\ of\ i\ in\ the\ feed} \tag{8}$$

Where: F_{R_i} is the recovery fraction of component *i* in the distillate or waste.

Therefore, equations (9) and (10) are applicable to determine, respectively, the recovery fractions of component i in the distillate and waste streams, considering its presence in both streams of the system (AZEVEDO & ALVES, 2013).

$$F_{R_{i,D}} = \frac{D \cdot x_{D,i}}{F \cdot z_i} \tag{9}$$

$$F_{R_{i,w}} = \frac{W \cdot x_{w,i}}{F \cdot z_i} \tag{10}$$

Where: $F_{R_{i,D}}$ is the distillate recovery fraction of a component *i*, $F_{R_{i,w}}$ is the recovery fraction of the waste of a component i, $x_{D,i}$ is the composition of the distillate of a component i, $x_{W,i}$ is the composition of the waste of a component i, z_i is the feed composition of a component i, D is the molar flow rate of the distillate, F is the molar flow rate of the feed e W the molar flow rate of the waste.

Furthermore, considering that the sum of the distillate and waste recovery rates is equal to 1 (100%), as described by Azevedo and Alves (2013), it is possible to infer equation 11:

$$F_{R_{i,w}} + F_{R_{i,D}} = 1 \tag{11}$$

Using the definition of equation 11, it can be obtaining equation 12, written as follows:

$$N_{min} = \frac{ln\left[\frac{(F_{R_A}/(F_{R_B})top}{(F_{R_A}/(F_{R_B})bottom}\right]}{ln\alpha_{A,B}} = \frac{ln\left[\frac{\left(F_{R_A}\right)_{top}\cdot\left(F_{R_B}\right)_{bottom}}{\left(1-F_{R_A}\right)_{top}\cdot\left(1-F_{R_B}\right)_{bottom}}\right]}{ln\alpha_{A,B}} \tag{12}$$

Where: F_{R_A} is the recovery fraction of component A and F_{R_B} is the recovery fraction of component B (both compositions for both the distillate and the waste).

In the multicomponent distillation process, the principle of minimum reflux according to the Underwood equation is based on minimizing the loss of desired components in the distillate. This principle takes into account the difference between the molar compositions of different components in the feed and the distillate, as well as the relationship between these compositions and the molar volumes of the components in the vapor phase, aiming to determine the minimum amount of reflux necessary to ensure efficient separation and the desired purity in the distilled products. The mathematical expressions representing the Underwood equations (13) and (14) are presented below.

$$\sum_{i=1}^{n}\frac{z_{i,F}\cdot\alpha_{i,B}}{\alpha_{i,B}-\theta} = 1 - q \tag{13}$$

$$\sum_{i=1}^{n}\frac{x_{i,D}\cdot\alpha_{i,B}}{\alpha_{i,B}-\theta} = 1 + R_{min} \tag{14}$$

Where: $z_{i,F}$ is the feed composition of a component i, $\alpha_{i,B}$ the volatility of the heavy key component of a given componente, θ the auxiliary variable (*thḗta*), q the feed condition, $R_{mín}$ the minimum reflux ratio and $x_{i,D}$ the distillate composition of a component i.

In equation 13, the summation of all components of the mixture, from *i* to n, is obtained in relation to the liquid fraction of the feed. In equation 14, on the other hand, the summation of all components of the mixture, from *i* to *n*, is obtained in relation to the $R_{mín}$. In equation 13, of degree n, n roots are obtained. However, a value of θ must be chosen between 1 and $\alpha_{A,B}$ (AZEVEDO & ALVES, 2013).

The consideration of minimum reflux, according to Underwood's premises, suggests that under specific circumstances, the minimum amount of reflux required for efficient separation can be zero or even negative. This, theoretically, would eliminate the need for the rectification section in the distillation column to separate the desired components. However, it is crucial to emphasize that, although theoretically the minimum reflux rate can be negative, in practice, negative reflux is impossible to achieve. Additionally, the observation that the minimum reflux is less dependent on the feed composition in a multicomponent system indicates that, even with variations in feed composition, there is still a minimum reflux rate required to ensure an ideal separation between specific components (such as A and B) (SEADER et al., 2011). From the determination of the minimum reflux, the actual reflux (or operational reflux), which uses a factor ranging from 1.2 to 1.5 (AZEVEDO & ALVES, 2013), is determined by equation 15.

$$R = (1{,}2 - 1{,}5)\cdot R_{mín} \tag{15}$$

Where: R is the real reflux and $R_{mín}$ is the minimum reflux ratio.

The Gilliland correlation is a method that relates the actual reflux ratio to the number of trays, allowing for the efficient determination of the minimum reflux ratio. Thus, both the actual reflux ratio and the number of trays must exceed their minimum values. The definition of the actual reflux ratio is guided by economic considerations and is generally established as a multiple of the minimum reflux (SEADER et al., 2011). This correlation is expressed by equation 16:

$$\frac{N - N_{min}}{N+1} = 0.75 - 0.75\left(\frac{R - R_{mín}}{R+1}\right)^{0.5668} \tag{16}$$

Where: N is the number of theoretical trays, $N_{mín}$ is the number of minimum trays, R is the real reflux and $R_{mín}$ is the minimum reflux ratio.

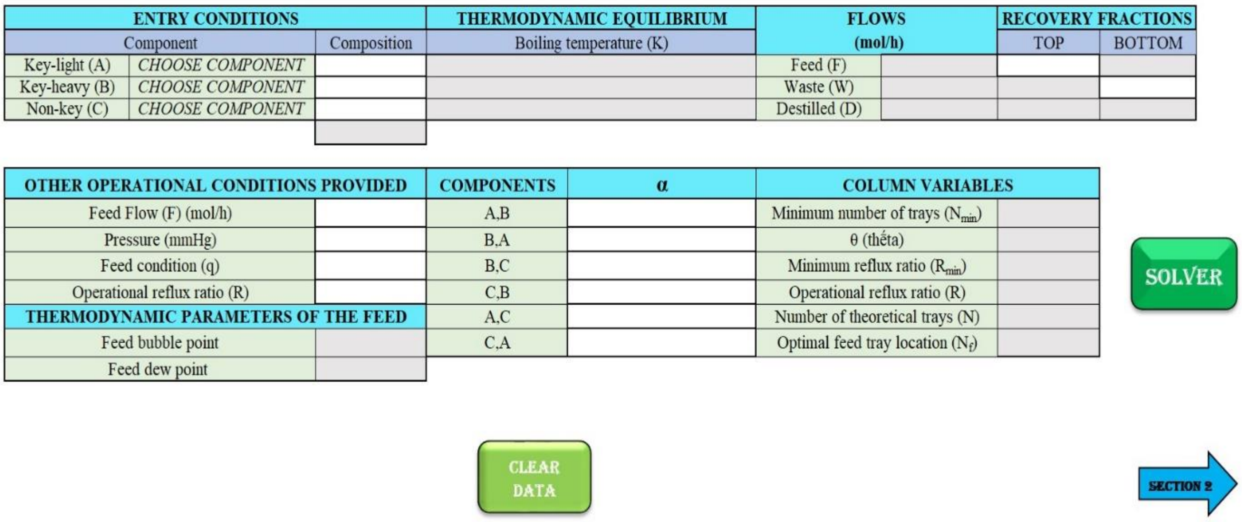
The Kirkbride correlation is employed to determine the optimal and actual position of the feed tray, aiming to achieve a finite total reflux condition and a more accurate approximation of the ideal feed tray location. This determination can be performed by applying equation (18) (AZEVEDO & ALVES, 2013).

$$\frac{N_F - 1}{N - N_F} = \frac{N_{rectif}}{N_{strip}} = \left[\frac{z_{B,F}}{z_{A,F}} \cdot \left(\frac{x_{A,W}}{x_{B,D}}\right)^2 \cdot \left(\frac{W}{D}\right)\right]^{0.206} \tag{17}$$

Where: N_{rectif} is the number of trays above the feed, N_{strip} is the number of trays below the feed, N_F is the optimal location of the feed tray, $z_{B,F}$ is the composition of the heavy key component feed, $z_{A,F}$ is the composition of the light key component feed, $x_{A,W}$ is the waste composition of the key light component, $x_{B,D}$ is the distillate composition of the key component heavy, W is the waste flow rate and D is the distillate flow.

2.2 Methods

The spreadsheet was developed according to each of the methods (FUG and Kirkbride) described in section 2.1. In Figure 1 is presented the layout of section 1 for the design of a multicomponent distillation tower.



ENTRY CONDITIONS			THERMODYNAMIC EQUILIBRIUM	FLOWS (mol/h)		RECOVERY FRACTIONS	
Component		Composition	Boiling temperature (K)			TOP	BOTTOM
Key-light (A)	*CHOOSE COMPONENT*			Feed (F)			
Key-heavy (B)	*CHOOSE COMPONENT*			Waste (W)			
Non-key (C)	*CHOOSE COMPONENT*			Destilled (D)			

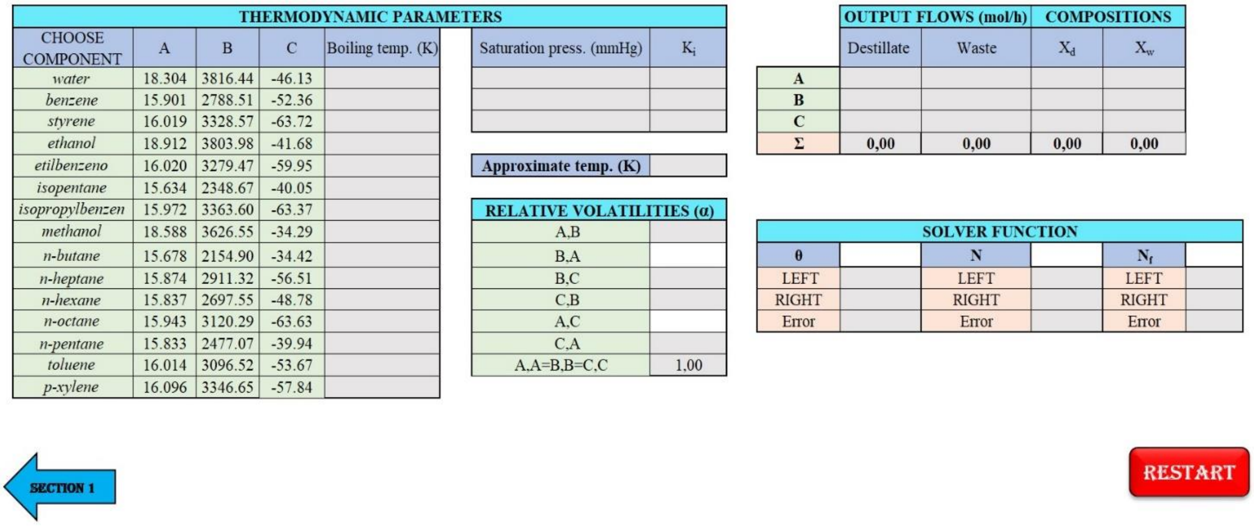
OTHER OPERATIONAL CONDITIONS PROVIDED		COMPONENTS	α	COLUMN VARIABLES	
Feed Flow (F) (mol/h)		A,B		Minimum number of trays (N_{min})	
Pressure (mmHg)		B,A		θ (théta)	
Feed condition (q)		B,C		Minimum reflux ratio (R_{min})	
Operational reflux ratio (R)		C,B		Operational reflux ratio (R)	
THERMODYNAMIC PARAMETERS OF THE FEED		A,C		Number of theoretical trays (N)	
Feed bubble point		C,A		Optimal feed tray location (N_f)	
Feed dew point					

Figure 1 - Layout of section 1 for designing a multicomponent distillation tower in the spreadsheet.

During the spreadsheet development process, data validations were implemented using the "SEERRO" function in Excel to ensure that users input only appropriate values. For example, for molar composition, only values between 0 and 1 are accepted; otherwise, the program will display an error message. Thus, experimental data should be provided in blank cells, while gray cells will display the obtained results. Additionally, the spreadsheet features the "CLEAR DATA" function and automatic navigation buttons between sections, making it an intuitive and easy-to-use program.

Firstly, in section 1, it is necessary to define the molar compositions of the top and bottom streams, as well as the light key (A), heavy key (B), and non-key (C) components, which must be present in both the top and bottom streams. Moreover, relative volatility and other operating conditions should be defined if applicable. Therefore, it is recommended to include components A, B, and C first to ensure accuracy in subsequent calculations.

In order to assist in this stage, section 2 includes a list of some of the main chemical compounds involved in distillation processes, as seen in Figure 2. This section displays the specific empirical parameters of each substance to determine its pressure and saturation temperature using Antoine's equation (1). These calculations are performed automatically and immediately after the user defines in section 1 which components are to be separated. Additionally, specific cells are provided for calculating the relative volatilities between the components, as well as the flow rates and compositions of the streams exiting the distillation tower. Section 2 also provides a sketch of using the "Solver" feature to solve the Underwood method, which incorporates the previously inserted equations 13, 14, 16, and 17, along with cells for viewing the possible error values encountered in attempts to determine the parameters θ, N e N_F.



THERMODYNAMIC PARAMETERS				
CHOOSE COMPONENT	A	B	C	Boiling temp. (K)
water	18.304	3816.44	-46.13	
benzene	15.901	2788.51	-52.36	
styrene	16.019	3328.57	-63.72	
ethanol	18.912	3803.98	-41.68	
etilbenzeno	16.020	3279.47	-59.95	
isopentane	15.634	2348.67	-40.05	
isopropylbenzen	15.972	3363.60	-63.37	
methanol	18.588	3626.55	-34.29	
n-butane	15.678	2154.90	-34.42	
n-heptane	15.874	2911.32	-56.51	
n-hexane	15.837	2697.55	-48.78	
n-octane	15.943	3120.29	-63.63	
n-pentane	15.833	2477.07	-39.94	
toluene	16.014	3096.52	-53.67	
p-xylene	16.096	3346.65	-57.84	

Saturation press. (mmHg)	K_i

Approximate temp. (K)	

RELATIVE VOLATILITIES (α)	
A,B	
B,A	
B,C	
C,B	
A,C	
C,A	
A,A=B,B=C,C	1,00

	OUTPUT FLOWS (mol/h)		COMPOSITIONS	
	Destillate	Waste	X_d	X_w
A				
B				
C				
Σ	0,00	0,00	0,00	0,00

SOLVER FUNCTION					
θ		N		N_f	
LEFT		LEFT		LEFT	
RIGHT		RIGHT		RIGHT	
Error		Error		Error	

Figure 2 - Layout of section 2 for designing of a multicomponent distillation tower in the spreadsheet

The determined saturation temperatures represent the point at which each component begins its vaporization at a specific pressure. Based on this data, the approximate temperature of all components will be automatically calculated by applying Equation 5 and summing these values to obtain an average temperature during the distillation process.

The subsequent analysis includes determining the bubble point and dew point pressures (Equation 4) in section 1 of the spreadsheet, which are crucial factors to ensure compliance of the inlet pressure with the optimal feeding conditions. Table 1 presents a synthesis of the values of q associated with different pressures. Thus, when the initial pressure is between the calculated pressures, partial vaporization of the feed is indicated, reflecting a value of q between 0 and 1. On the other hand, if the pressure corresponds exactly to the bubble point pressure, q will be 1; and for the pressure equivalent to the dew point, q will be 0 (KORETSKY, 2013; FOUST et al., 1982).

Table 1: Feed operating conditions

Feed condition	*Q*
Subcooled liquid	> 1
Liquid at the bubble point	1
Saturated vapor-liquid	$0 < q < 1$
Vapor at dew point	0
Superheated vapor	< 0

Thereafter, by conducting a distribution analysis of the components in the overhead and bottoms streams, automatically in section 2 the outlet flow rates for distillate and waste can be obtained through mass balance. In this context, it is important to note that components more volatile than A exit through the overhead stream of the distillation tower, while those less volatile than B exit through the bottoms stream. The distribution coefficient (K_i), is calculated for the key components (Equation 3). Upon obtaining the values of K_i, the individual relative volatilities are determined among the light key, heavy key, and non-key components (Equation 6).

After defining the relative volatilities, the Fenske equation (Equation 7) can be used to determine the minimum number of trays required for separation. Regarding recovery rates, Equation 8 is applicable to calculate the fractions of each component present in the distillate and waste streams, and Equations 9 and 10 enable the calculation of the recovery fractions of component i in the distillate and waste streams, respectively, considering their presence in both streams of the system. The remaining recovery fractions for the waste and distillate are determined using Equation 11, while Equation 12 allows the calculation of the minimum number of trays required in the distillation column.

The minimum number of trays necessary to carry out the separation is calculated with the relative volatilities and the Fenske equation (Equation 7). Moreover, the recovery rates are determined by Equation 8, which is applied for each component in both the distillate and the waste streams. On the other hand, recovery fractions of component i in the distillate and waste streams can be calculated by Equations 9 and 10, respectively (considering its presence in both streams). Finally, the other recovery fractions for the waste and distillate are determined using Equation 11. Besides, the minimum number of trays in the distillation column can be calculated by Equation 12.

To obtain the minimum reflux operational condition using the Underwood method (Equations 13 and 14), it is necessary to firstly determine the value of θ, obeying the conditions of being greater than 1 and less than the relative volatility between the key components (A and B). Once the necessary parameters for the summation are known, the calculation to obtain the minimum reflux will be automatically performed in section 1 of the spreadsheet.

Thus, still in section 1, it is also possible to determine the value of the actual reflux (Equation 15). When the values of $N_{mín}$, $R_{mín}$ and R are known, the ideal number of trays (N) is calculated using the Gilliland correlation (Equation 16). Through the Kirkbride equation (Equation 17), it is possible to determine the optimal location of the feed tray, considering the ratio between the number of trays in the rectification and stripping zones. A step-by-step description of the calculation procedures for the FUG and Kirkbride methods for sizing multicomponent distillation columns is presented in flowchart format in Figure 3.

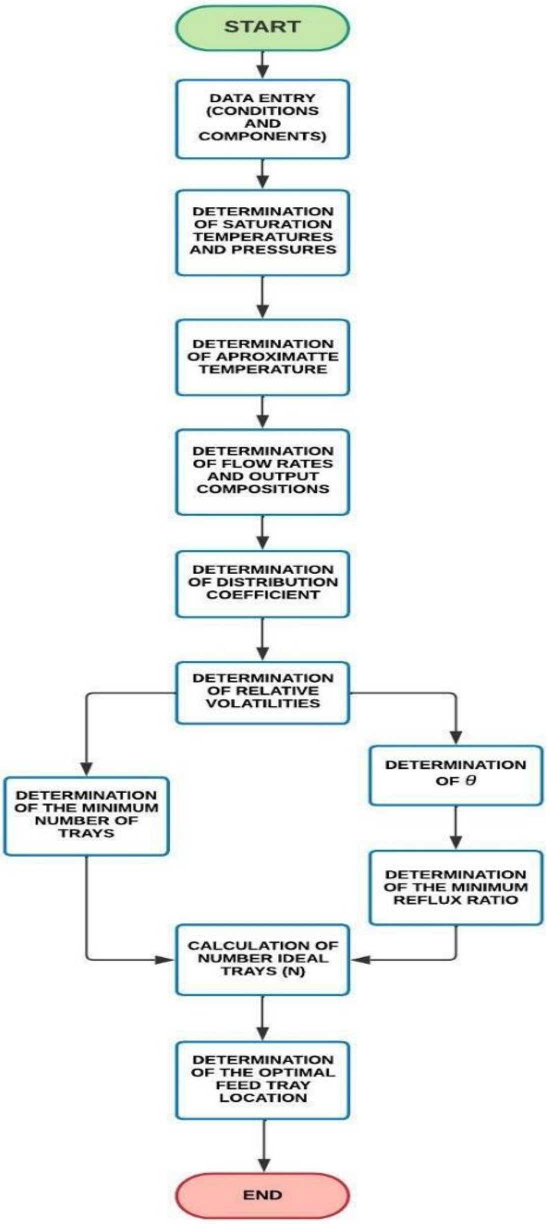


Figure 3 - Design procedures for multicomponent distillers using the FUG and Kirkbride methods.

3. Results and discussion

In this study, an electronic spreadsheet was developed for determining operational conditions in multicomponent distillation columns, including parameters such as flow rate and average volatility. A practical application exercise extracted from the book by Azevedo and Alves (2009), "Engenharia de Processos de Separação," page 259, was used to facilitate readers' understanding of the process and demonstrate the practical effectiveness of the developed spreadsheet.

3.1 Application example:

A distillation column is used with a total condenser and a partial reboiler to separate, at 1 atm, 100 mol/h of a gas mixture saturated with 40% benzene, 30% toluene, and 30% isopropylbenzene. It is intended to recover 95% of toluene in the distillate and a recovery of 95% of isopropylbenzene in the waste. The reflux is recycled to the column in the form of saturated liquid, and the liquid and vapor flow rates are approximately constant from tray to tray. The relative volatilities are constant,

and considering benzene as the reference, they are $\alpha_{benzene,toluene}$= 2.25 e $\alpha_{isopropylbenzene,toluene}$= 0.21. Thus, the following calculations are required:
a) Number of trays required for actual reflux, b) Recovery rate of benzene in the distillate, c) Minimum reflux ratio, and d) Number of theoretical trays and optimal feed tray location, considering that the operating reflux ratio is R = 2.

Manual Resolution: Using the example application from Azevedo and Alves (2009), the manual resolution of this exercise was performed first. Thus, the first step was the identification of the components described in the statement:

Light key: Toluene (A), Heavy key: Isopropylbenzene (B), Non-key light: Benzene (C).

$z_A = 0.3$, $z_B = 0.3$, $z_C = 0.4$

$\left(F_{R_A}\right)_{top}$ = 0.95, $\left(F_{R_B}\right)_{bottom}$= 0.95

F = 100 mol/h

$\alpha_{C,A} = 2.25 \;\; \alpha_{B,A} = 0.21$

a) The minimum number of trays can be calculated using equation 12:

$$N_{mín} = \frac{ln\left(\left(\frac{F_{R_A}}{1-F_{R_A}}\right)_{top}\left(\frac{F_{R_B}}{1-F_{R_B}}\right)_{bottom}\right)}{ln\,\alpha_{A,B}}$$

The relative volatility value between the light key component and the heavy key component was calculated by equation 6, obtaining the following result:

$$\alpha_{A,B} = \frac{k_A}{k_B} = \frac{1}{\alpha_{B,A}}$$

$$\alpha_{A,B} = \frac{1}{0.21} = 4.76$$

By substituting the values, it has:

$$N_{mín} = \frac{ln\left(\left(\frac{0.95}{1-0.95}\right)\left(\frac{0.95}{1-0.95}\right)\right)}{ln\,4.76}$$

$$\boldsymbol{N_{mín} = 3.84}$$

b) Applying equations 6 and 12 again, it was possible to determine respectively the relative volatility between the non-key component and the heavy key component, as well as the benzene recovery fraction in the distillate:

$$\alpha_{C,B} = \frac{k_C}{k_B} = \frac{k_C/k_A}{k_B/k_A} = \frac{\alpha_{C,A}}{\alpha_{B,A}}$$

$$\alpha_{C,B} = \frac{2.25}{0.21} = \mathbf{10.71}$$

The recovery fraction of benzene in the distillate was obtained using the relative volatility value:

$$(FR_C)_{top} = \frac{\left(\alpha_{C,B}\right)^{Nmín}}{\frac{(FR_B)_{bottom}}{(1 - FR_B)_{bottom}} + \left(\alpha_{C,B}\right)^{Nmín}}$$

$$(FR_C)_{top} = \frac{(10.71)^{3.84}}{\frac{0.95}{1 - 0.95} + (10.71)^{3.84}}$$

$$\boldsymbol{(FR_C)_{top} = 0.998}$$

c) To find the value of the minimum reflux ratio, first, θ is calculated (equation 13):

$$\sum_{i=1}^{c} \frac{\alpha_{i,B} \cdot z_{i,F}}{\alpha_{i,B} - \theta} = 1 - q$$

$$\frac{\alpha_{\mathrm{A,B}} \cdot z_A}{\alpha_{A,B} - \theta} + \frac{\alpha_{\mathrm{B,B}} \cdot z_B}{\alpha_{B,B} - \theta} + \frac{\alpha_{\mathrm{C,B}} \cdot z_C}{\alpha_{C,B} - \theta} = 1 - q$$

According to the statement, the feed enters in the form of saturated steam, with the feed condition equal to zero ($q = 0$). Therefore, substituting the values:

$$\frac{4.76 \cdot 0.3}{4.76 - \theta} + \frac{1 \cdot 0.3}{1 - \theta} + \frac{10.71 \cdot 0.4}{10.71 - \theta} = 1$$

$$\frac{1.428}{4.76 - \theta} + \frac{0.3}{1 - \theta} + \frac{4.284}{10.71 - \theta} = 1$$

$$\frac{1.428 \cdot (1 - \theta) \cdot (10.71 - \theta) + 0.3 \cdot (4.76 - \theta) \cdot (10.71 - \theta) + 4.284 \cdot (4.76 - \theta) \cdot (1 - \theta)}{(4.76 - \theta) \cdot (1 - \theta) \cdot (10.71 - \theta)} = 1$$

$$1.428 \cdot (1 - \theta) \cdot (10.71 - \theta) + 0.3 \cdot (4.76 - \theta) \cdot (10.71 - \theta) + 4.284 \cdot (4.76 - \theta) \cdot (1 - \theta) \\ = (4.76 - \theta) \cdot (1 - \theta) \cdot (10.71 - \theta)$$

Given that the calculations developed in this topic are extensive and complex, in order to facilitate the reader's understanding, it was decided to divide them into stages, with the following numerations I, II, III, and IV, from left to right respectively. This way, are obtained:

$$\mathbf{I} = 1.428 \cdot (1 - \theta) \cdot (10.71 - \theta) = (1.428 - 1.428\theta) \cdot (10.71 - \theta) \\ = 15.294 - 1.428\theta - 15.29\theta + 1.428\theta^2$$

$$\mathbf{I} = \mathbf{15.294 - 16.718\boldsymbol{\theta} + 1.428\boldsymbol{\theta}^2}$$

$$\mathbf{II} = 0.3 \cdot (4.76 - \theta) \cdot (10.71 - \theta) = (1.428 - 0.3\theta) \cdot (10.71 - \theta)$$
$$= 15.294 - 1.428\theta - 3.213\theta + 0.3\theta^2$$

$$\mathbf{II = 15.294 - 4.641\boldsymbol{\theta} + 0.3\boldsymbol{\theta}^2}$$

$$\mathbf{III} = 4.284 \cdot (4.76 - \theta) \cdot (1 - \theta) = (20.39 - 4.284\theta) \cdot (1 - \theta)$$
$$= 20.392 - 20.39\theta - 4.284\theta + 4.284\theta^2$$

$$\mathbf{III = 20.392 - 24.674\boldsymbol{\theta} + 4.284\boldsymbol{\theta}^2}$$

$$\mathbf{IV} = (4.76 - \theta) \cdot (1 - \theta) \cdot (10.71 - \theta) = (4.76 - 4.76\theta - \theta + \theta^2) \cdot (10.71 - \theta)$$
$$= (4.76 - 5.76\theta + \theta^2) \cdot (10.71 - \theta)$$
$$= 50.98 - 4.76\theta - 61.69\theta + 5.76\theta^2 + 10.71\theta^2 - \theta^3$$

$$\mathbf{IV = 50.98 - 66.45\boldsymbol{\theta} + 16.47\boldsymbol{\theta}^2 - \boldsymbol{\theta}^3}$$

How **I + II + III = IV** is replaced by the equations found.

$$15.294 - 16.718\theta + 1.428\theta^2 + 15.294 - 4.641\theta + 0.3\theta^2 + 20.392 - 24.674\theta + 4.284\theta^2$$
$$= 50.98 - 66.45\theta + 16.47\theta^2 - \theta^3$$

$$50.98 - 46.033\theta + 6.012\theta^2 = 50.98 - 66.45\theta + 16.47\theta^2 - \theta^3$$

$$\theta^3 - 10.458\theta^2 + 20.417\theta = 0$$

$$\boldsymbol{\theta}(\boldsymbol{\theta}^2 - \mathbf{10.458}\boldsymbol{\theta} + \mathbf{20.417}) = \mathbf{0}$$

$$\theta(\theta^2 - 10.458\theta + 20.417) = 0$$

$$\theta_1 = 0 \; ou \; \theta^2 - 10.458\theta + 20.417 = 0$$

Finding the roots of the quadratic equation described above, one obtains:

$$\theta_2 = 7.86 \qquad \theta_3 = 2.6$$

It is important to select a value for θ that meets the following conditions:

$$1 < \theta < \alpha_{CL,\, CP}$$

$$1 < \theta < 4.76$$

Finally:

$$\boldsymbol{\theta} = \mathbf{2.6}$$

Once the value of θ is found, the value of $R_{mín}$ is calculated using equation 14. However, this equation requires the values of $x_{i,D}$, which can be obtained first by defining the recovery fraction. Thus, for a component i, equation 9 is used:

$$(F_{R_i})_{top} = \frac{x_{i,D} \cdot D}{z_i \cdot F}$$

$$\boldsymbol{D_i = x_{i,D} \cdot D = (F_{R_i})_{top} \cdot z_i \cdot F}$$

$$D_A = x_{A,D} \cdot D = (F_{R_A})_{top} \cdot z_A \cdot F$$

$$D_A = 0.95 \cdot 0.3 \cdot 100\, mol/h$$

$$\boldsymbol{D_A = 28.5\, mol/h}$$

$$D_B = (F_{R_B})_{top} \cdot z_B \cdot F$$

$$D_B = 0.05 \cdot 0.3 \cdot 100\, mol/h$$

$$\boldsymbol{D_B = 1.5\, mol/h}$$

$$D_C = (F_{R_C})_{top} \cdot z_C \cdot F$$

$$D_C = 0.998 \cdot 0.4 \cdot 100\, mol/h$$

$$\boldsymbol{D_C = 39.92\, mol/h}$$

The distillate stream flow rate is given by the sum of the distilled flow rates of the light key, heavy key, and non-key components.

$$D = D_A + D_B + D_C$$

$$D = (28.5 + 1.5 + 39.92)\, mol/h$$

$$\boldsymbol{D = 69.92\, mol/h}$$

This allows for the calculation of the distillate fractions:

$$D_i = x_{i,D} \cdot D$$

$$x_{i,D} = \frac{D_i}{D}$$

$$x_{A,D} = \frac{D_A}{D} = \frac{28.5}{69.92}$$

$$\boldsymbol{x_{A,D} = 0.408}$$

Similarly:

$$\boldsymbol{x_{B,D} = 0.021}$$

$$\boldsymbol{x_{C,D} = 0.571}$$

From Underwood's equation (equation 14):

$$\sum_{i=1}^{c} \frac{\alpha_{i,B} \cdot x_{i,\,D}}{\alpha_{i,B} - \theta} = 1 + R_{min}$$

$$\frac{\alpha_{A,B} \cdot x_{A,D}}{\alpha_{A,B} - \theta} + \frac{\alpha_{B,B} \cdot x_{B,D}}{\alpha_{B,B} - \theta} + \frac{\alpha_{C,B} \cdot x_{C,D}}{\alpha_{C,B} - \theta} = 1 + R_{mín}$$

When substituting the data, the value of $R_{mín}$ is finally obtained:

$$\frac{4.76 \cdot 0.408}{4.76 - 2.6} + \frac{1 \cdot 0.021}{1 - 2.6} + \frac{10.71 \cdot 0.571}{10.71 - 2.6} = 1 + R_{min}$$

$$\boldsymbol{R_{mín} = 0,64}$$

d) The calculation of the theoretical tray number was conducted by applying Equation 16, considering the reflux ratio (R) to be 2.

$$\frac{N - N_{mín}}{N + 1} = 0.75 - 0.75\left(\frac{R - R_{mín}}{R + 1}\right)^{0.5668}$$

Given the reflux ratio (R = 2), the values are substituted:

$$\frac{N - 3.84}{N + 1} = 0.75 - 0.75\left(\frac{2 - 0.64}{2 + 1}\right)^{0.5668}$$

$$\frac{N - 3.84}{N + 1} = 0.27$$

$$\boldsymbol{N = 5.63}$$

For the calculation of the optimal feed tray location, Equation 17 was applied:

$$\frac{N_F - 1}{N - N_F} = \frac{N_{rectif}}{N_{strip}} = \left[\frac{z_{B,F}}{z_{A,F}} \cdot \left(\frac{x_{A,W}}{x_{B,D}}\right)^2 \cdot \left(\frac{W}{D}\right)\right]^{0.206}$$

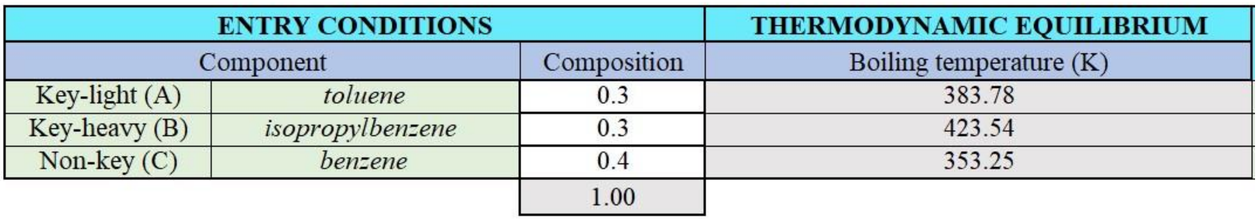
Substituting the values:

$$\frac{N_F - 1}{5.63 - N_F} = \left[\frac{0.3}{0.3} \cdot \left(\frac{0.05}{0.021}\right)^2 \cdot \left(\frac{30.08}{69.92}\right)\right]^{0.206}$$

$$\frac{N_F - 1}{5.63 - N_F} = 1.202$$

$$\boldsymbol{N_F = 3.52}$$

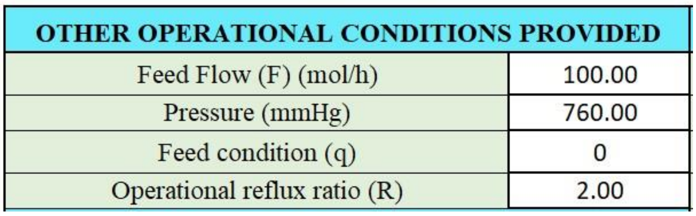
Electronic resolution: Initially, as depicted in Figure 4, the components of interest were defined, with toluene identified as the light key component (A), isopropylbenzene as the heavy key component (B), and benzene as the non-key component (C). Based on these fundamental data and the values of the constants A', B', and C' from Antoine's Law provided in Section 2, the spreadsheet automatically calculated the boiling temperature for each component, applying Equation 2.



ENTRY CONDITIONS			THERMODYNAMIC EQUILIBRIUM
Component		Composition	Boiling temperature (K)
Key-light (A)	*toluene*	0.3	383.78
Key-heavy (B)	*isopropylbenzene*	0.3	423.54
Non-key (C)	*benzene*	0.4	353.25
		1.00	

Figure 4 - Layout of section 1, where the feed input conditions were entered, and the respective boiling temperatures were calculated.

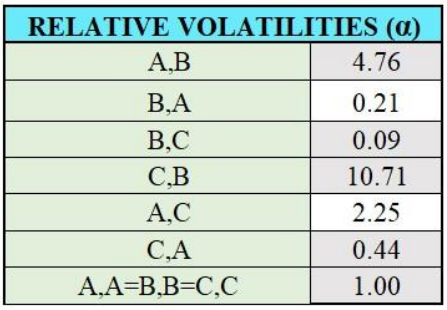
Following that, in Section 1 of the spreadsheet, under the 'other operational conditions provided' part, the remaining information provided in the exercise statement was inputted. This included the feed flow rate and condition, column pressure, and reflux ratio, as illustrated in Figure 5.



OTHER OPERATIONAL CONDITIONS PROVIDED	
Feed Flow (F) (mol/h)	100.00
Pressure (mmHg)	760.00
Feed condition (q)	0
Operational reflux ratio (R)	2.00

Figure 5 - Layout of section 1, the part to define other operational conditions.

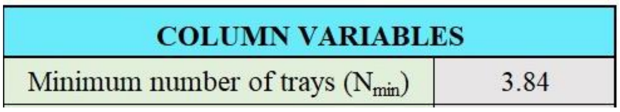
The relative volatility data $\alpha_{C,A}$ *and* $\alpha_{B,A}$ that appear in the exercise statement, were inserted in section 2 of the spreadsheet. Thus, the relative volatility between other components was automatically calculated, using equation 6, as shown in Figure 6.



RELATIVE VOLATILITIES (α)	
A,B	4.76
B,A	0.21
B,C	0.09
C,B	10.71
A,C	2.25
C,A	0.44
A,A=B,B=C,C	1.00

Figure 6 - Layout of section 2, the part to define the relative volatility of the components involved in the process.

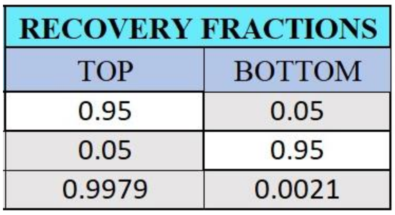
With this information available, considering $\alpha_{B,A}$ equal (0.21), the first parameter to be calculated is the minimum number of trays required for total reflux. Thus, in Section 1 under the "Column Variables" part, as depicted in Figure 7, the spreadsheet automatically determined $N_{mín}$ using the Fenske equation (13).



COLUMN VARIABLES	
Minimum number of trays (N_{min})	3.84

Figure 7 - Layout of section 1, a part for calculating column variables: Minimum number of trays.

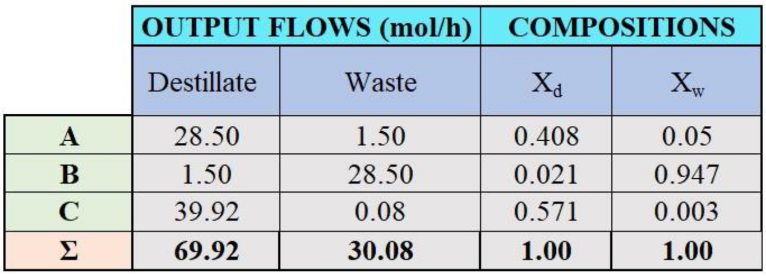
The exercise statement also specifies that the recovery fraction of toluene is 0.95 in the distillate ($\left(\left(F_{R_A}\right)_{top}\right)$) and 0.95 in the bottom for isopropylbenzene ($\left(\left(F_{R_B}\right)_{bottom}\right)$). Consequently, by difference, it is inferred that $\left(F_{R_A}\right)_{bottom}$ and $\left(F_{R_B}\right)_{top}$ are both equal to 0.05. Therefore, considering the relative volatilities between the components and the minimum number of trays required, the subsequent parameter calculated was the recovery fraction of benzene in the distillate ($\left(\left(F_{R_C}\right)_{top}\right)$), using Equation 12, as depicted in Figure 8.



RECOVERY FRACTIONS	
TOP	BOTTOM
0.95	0.05
0.05	0.95
0.9979	0.0021

Figure 8 - Layout of section 1, part for calculating recovery fractions.

In the penultimate topic, the determination of the minimum reflux ratio ($R_{mín}$) is requested, a parameter that initially requires the compositions of the distillate and the value of θ. In this context, the parameter q is considered equal to 0, given that the column feed is saturated vapor. Therefore, firstly, in Section 2 of the spreadsheet, the distilled and residual flow rates for each component were calculated (using Equation 9), and subsequently, the respective compositions of the distillate and waste streams (using Equations 9 and 10), as shown in the provided data in Figure 9.

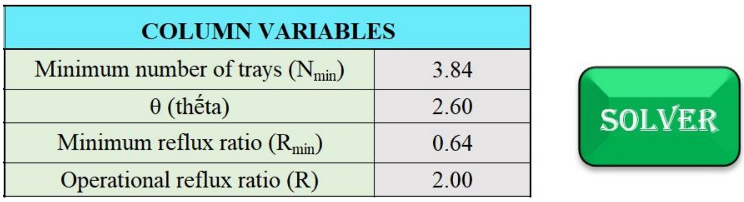


	OUTPUT FLOWS (mol/h)		COMPOSITIONS	
	Destillate	Waste	X_d	X_w
A	28.50	1.50	0.408	0.05
B	1.50	28.50	0.021	0.947
C	39.92	0.08	0.571	0.003
Σ	**69.92**	**30.08**	**1.00**	**1.00**

Figure 9 - Layout of section 2, part for calculating the flow rates and compositions of the distillate and waste.

The Solver, a resource available in Microsoft Excel, was employed to solve the Underwood method (Equations 13 and 14), which facilitates the determination of θ and other parameters using the trial-and-error method. Moreover, activating the 'Developer' and 'Solver' resources are two essential steps that must be followed to efficiently utilize this feature. Therefore, first, to activate the 'Developer' tab, the user must click on 'File', followed by 'Options', 'Customize Ribbon', and then select the 'Developer' checkbox in this window and click on 'OK.'

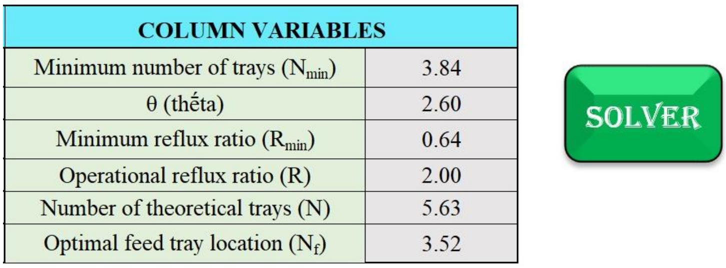
It is necessary to enable both the 'Developer' and the 'Solver' add-in. For that, the user must click on 'File', select 'Options', and then 'Add-ins'. Then, the user must select the 'Solver' checkbox and add it to the list of available add-ins. Once done, a click on the green "Solver" button can automatically calculate the values of θ and $R_{mín},$ as shown in Figure 10.



COLUMN VARIABLES	
Minimum number of trays (N_{min})	3.84
θ (thẽta)	2.60
Minimum reflux ratio (R_{min})	0.64
Operational reflux ratio (R)	2.00

Figure 10 - Layout of section 1, part for calculating column variables: θ, minimum reflux ratio and reflux ratio.

Finally, in the last topic, the determination of the theoretical tray number and the optimal feed tray location is requested, considering a reflux ratio (R) equal to 2. The determination of these parameters is also carried out in Section 1 under "Column Variables", utilizing the Gilliland correlation (Equation 16) to calculate the ideal number of trays and the Kirkbride equation (Equation 17) to determine the optimal feed tray location. Analogously to the determination of θ, given the complexity of the calculations involved in determining N and N_F, once again the Solver tool was used and the results obtained are presented in Figure 11.



COLUMN VARIABLES	
Minimum number of trays (N_{min})	3.84
θ (thẽta)	2.60
Minimum reflux ratio (R_{min})	0.64
Operational reflux ratio (R)	2.00
Number of theoretical trays (N)	5.63
Optimal feed tray location (N_f)	3.52

Figure 11 - Layout of section 1, part for calculating column variables: Feed tray and optimal location of this tray.

After solving the application example using manual and electronic methods, it was evident that both produced the same results. This consistency validates and reinforces the accuracy of the spreadsheets, which returned reliable results in a significantly shorter time. Furthermore, such uniformity strengthens confidence in the application of Microsoft Excel® for analysis, calculation resolution, and other complex problems similar to multicomponent distillation.

4. Conclusion

As evidenced throughout this study, distillation represents a unit operation of paramount importance for industrial separation processes. Therefore, the correct sizing of a distillation column is crucial to achieve required efficiency levels while maintaining the economic viability of the project. In this context, given the necessary knowledge about operational variables, often obtained through extensive and complex calculations, an electronic tool was developed using Microsoft Excel® software. This tool aims to assist in the sizing of multicomponent distillation columns. The functionality of the developed method was validated through a practical example, where the sizing of a separation column was conducted manually and using the electronic spreadsheet. Thus, obtaining identical results in both methods, along with the significant reduction in data processing time and error probability using the electronic method, demonstrates that the developed spreadsheet is a practical, didactic tool with great potential for use by students, teachers, and professionals in the field of chemical engineering and the industrial distillation sector.

5. Supplementary material

The spreadsheet developed for determining operational parameters in multicomponent distillation, applying the Fenske-Underwood and Gilliland (FUG) and Kirkbride methods, is the main structural element of this article. It is attached as supplementary material to facilitate readers' understanding, demonstrate the applicability of the developed electronic method, and allow its potential utilization to be explored. Therefore, the authors declare no conflicts of interest and permit the free availability of this material on the jCEC website.

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