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A MATLAB-BASED PROGRAM FOR THE PARAMETRIC STUDY OF DISTILLATION COLUMN IN A BINARY MIXTURE SYSTEM: EFFECT OF REFLUX RATIO, FEED COMPOSITION AND FEED QUALITY

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ABSTRACT

This paper presents the application of a GUI developed in Matlab® for a binary distillation column simulation, where the diameter, height, tray number, feed tray location and the heat flux in the condenser and reboiler were calculated for a given operational condition set by the user, like the feed condition, distillation and bottom molar fraction, reflux ratio, top, bottom and subcooling temperature of distillate. The program, called *DTMB-UA v1.0* (Design of a distillation Tower for Binary Mixture-Universidad del Atlántico), uses the combination of material and energy balances, experimental equations of phase equilibrium and constant relative volatility, reported in the literature. The general procedure to calculate the outputs in the program start by selecting the type of phase equilibrium curve calculation, between the constant volatility and the experimental data; in the case of constant volatility, the vapor and liquid mean temperature, mean tower pressure and densities are estimated based on a set of empirical equations for the column diameter, column height, theoretical tray numbers, and energy requirement on the condenser and reboiler. The same steps are applied when using experimental data for the equilibrium curve, consisting in inputs of temperatures and molar fractions of the component with higher volatility in the liquid and the vapor phase. The last step is to select a binary mixture from the given by the software. The material balance is represented as the operation lines on the x-y diagram according to the McCabe-Thiele method. It was found the exact composition of the bottom molar fraction, the effect of reflux ratio on the distillation molar fraction under different tray numbers and the effect of feed quality variation on condenser and reboiler duties under different reflux ratio.

Keywords: *Distillation column, Reflux ratio, Distillation feed composition, Graphical user interface, Engineering education.*

1. INTRODUCTION

The advances in technology in the industry that involve chemical process around the world had an exponential increase in the last decade, creating a challenge to junior engineers when working with the main unit operations, especially distillation which has several variables that affect the product separation and is used in chemical and petrochemical plants, petroleum refineries, food industry, etc. The distillation phenomenon has to be completely understood when designing distillation towers to take advantage of the maximum heat and mass transfer rate between the two phases to obtain the required product with the highest concentration. To accomplish this purpose, it is necessary to employ highly capacitated personnel in all the phenomena involved inside the process with a high understanding of the technology used. Workers with that knowledge are capable to develop troubleshooting procedures to solve many process problems in several industries.

Most of the engineering academies try to prepare good professionals with specific training by introducing in their core curriculum laboratory practices, where the student can operate and study the behavior of tray and packed distillation columns, in order to compare the theory with the practice. However, there are lots of variables involved when operating a distillation tower that are extremely difficult to analyze experimentally and the effect of all of them in the efficiency of a tower.

It is necessary to complement the experimental practices with the help of a computer based technology that help the students to analyze the effect of more variables on the final product. There are some important software that use computational fluid dynamic (CFD) such as COMSOL Multiphysics, ANSYS Fluent, etc., (1-10) where the user can create a distillation systems by sections and study the internal behavior in a tower, e.g. flow, temperature and concentration profiles. Excellent results are obtained with these programs, however, the physic used in them is highly complex for an undergraduate student due to the numerical solutions employed to solve the governing differential equations of the systems.

There are some other robust programs capable to simulate processes in chemical plants and equipment that help to determine the highest efficiency of a tower or the highest quality of a product (11-15). These strong commercial programs such as Aspen, Pro/II, etc., (11, 16, 17) are so essential for the wide industry in general because they are used to select the best process or equipment design, all the way through a complete study of the necessary operating conditions which involve a deep former knowledge of the user. The mentioned programs generally lack of tutorials that help students to get specific academy training because they are so extensive that embrace a huge amount of different unitary operations and individual equipment.

Considering the degree of difficulty of the study of a distillation process, due to all the variables involved when operating a tower (18-22), it is necessary to complement the knowledge obtained theoretically and experimentally in the academy by including in their core program a user friendly software (23), where the student can be able to understand and explain the phenomena happening inside a tower using the most accepted equations and assumptions in a distillation process when different conditions are changed.

A new interactive graphical user interface in Matlab to simulate tray binary distillation towers is presented in this article, where the undergraduate students can handle different variables that let them to understand the phenomena happening inside a distillation column. The students can see the effect of the operational conditions set by the user, like feeding condition, distillation and bottom molar fraction, reflux ratio, top, bottom and subcooling temperature of distillate, etc., on the diameter, height, trays number, feed tray location and the heat flux in the condenser and reboiler to finally compare the results with laboratory experiences and give a better explanation of the obtained profiles with the variable chosen to be studied. It can help the creativity of the users by proposing different ways to increase the efficiency of the tower. The software was developed under criteria-based assessment ISO/IEC 25010:2011 which consider the product quality and include usability, sustainability and maintainability

2. ALGORITHM PRESENTATION

2.1. General aim of the GUI algorithm

The program *DTMB-UA v1.0*, which is a creative and original graphical user interface, is a type of interface that allows users, undergraduate engineering students and junior engineers, to have a significant learning experience through case studies in a binary distillation column process.

The software is based on some educational components to improve the knowledge and skill-based learning process on the users, which are presented as follow:

- The software was created in such a level of complexity that let undergraduate students to visualize and understand easily and quickly the mass and energy balances applied to a distillation column in a binary mixture. In addition, the evaluation of the educational objective through the software can be applied in any time and place by the professor.

- For engineers working for a chemical and petrochemical company, the software is a powerful and user friendly tool that does not require robust knowledge on informatics and mass transfer process to simulate and identify faults associated with abnormal operating conditions.

- The software allows the professor to change the methodology of the theory and practice of a distillation course by implementing simulation letting the students to become more involved in the development of distillation concepts that help them to perform and understand experiments so much easier supported in the *DTMB-UA v1.0.* graphical user interface.

- For designers, the software is a friendly application that determine the number of stages required, the feed tray in the column, the diameters and height of column, the required condenser and bottom duty, the distillate and bottom mass flow selecting from experimental, theoretical correlative and volatility constant data, a set of inputs parameter such as: inlet flow, feed quality, desired fractions, reflux ratio, distance between plates and liquid height plates, based on the McCabe-Thiele graphical method, mass balance and experimental equations applied to a distillation column in a binary mixture system.

This software was registered in the D.N.D.A. Dirección Nacional de Derechos de Autor (National Leadership Copyright), with register 13-44-284 at the 30 October 2014.

Figure 1-a is a screen capture of one of the views of the *DTMB-UA v1.0*, which shows the inputs given by the user. Furthermore, figure 1-b, is a screen capture of an additional view of the program that shows the column diameter and height, tray numbers, flows, the number of equilibrium stages and the location of the feed tray according to the McCabe-Thiele plot.

Figure 1. Main View of the DTMB-UA v1.0 software. (a) Inputs data; (b) Operation condition

2.2. Flowchart of the GUI

The *DTMB-UA v1.0* was developed and tested with Matlab®7.0. The system requirements depend heavily on the version of Matlab. *DTMB-UA v1.0* run on any Microsoft 32/64-bit Windows PC. All the *DTMB-UA v1.0* files use less than 577 MB disk space. The computational steps involved on the software are shown on Figure 9.

Figure 2. Flowchart of the DTMB-UA v1.0

2.3 Relations used in the algorithm

The fundamental equations involved in the software are organized as follows, (24):

The equilibrium curve using constant relative volatility, see equation 1

$$y = \frac{\alpha x}{1+(\alpha-1)x}, \quad (1)$$

The overall material balance, see equation 2.

$$L' = L + F\phi, \quad (2)$$

The feed quality, see equation 3.

$$\phi = \frac{H_V - H}{H_V - H_L}, \quad (3)$$

The operating line, see equation 4.

$$y = \frac{L}{V}x_n + \frac{D}{V}x_D, \quad (4)$$

The operating line in R terms, see equation 5.

$$y = \frac{R}{R+1}x + \frac{1}{R+1}x_D, \quad (5)$$

The stripping line, see equation 6.

$$y = \frac{L'}{V'}x + \frac{B}{V'}x_B, \quad (6)$$

The feed line, see equation 7.

$$y = -\frac{\phi}{1+\phi}x + \frac{1}{1-\phi}x_F, \quad (7)$$

The distilled flow in rectification zone, see equation 8.

$$D = F\frac{(xF - xB)}{(xD - xB)} \quad (8)$$

The bottom flow in stripping section, see equation 9.

$$B = F - D, \quad (9)$$

The liquid flow in rectification zone, see equation 10.

$$L = RD, \quad (10)$$

The vapor flow in rectification zone, see equation 11.

$$V = (R+1)D, \quad (11)$$

The vapor flow in stripping section, see equation 12.

$$V' = V + (\phi - 1)F, \quad (12)$$

The column diameter, see equation 13.

$$d = \sqrt{\frac{4\,V\,22.4\,(273+t)\,760}{\pi\,u\,3600\,p\,273}}, \quad (13)$$

The vapor velocity, see equation 14.

$$u = k\sqrt{\frac{\rho_L - \rho_v}{\rho_L}}, \quad (14)$$

The column height, see equation 15.

$$h = npG, \quad (15)$$

The cooling water flow used in the condenser, see equation 16.

$$\dot{m}_{water} = \frac{V[\lambda_1 x_D + \lambda_2(1-x_D)]}{Cp_{H2O}(T_{out}-T_{in})}, \quad (16)$$

The steam flow used as the heating medium in the boiler, see equation 17.

$$\dot{m}_{steam} = \frac{V'[\lambda_1 x_D + \lambda_2(1-x_D)]}{\lambda_{water}}, \quad (17)$$

The heat transfer in the condenser, see equation 18.

$$\dot{Q}_C = \dot{m}_{water}\, Cp_{water}(T_{out} - T_{in}), \quad (18)$$

The heat transfer in the reboiler, see equation 19.

$$\dot{Q}_R = \dot{m}_{steam}\lambda_{water}. \quad (19)$$

3. RESULT AND DISCUSSION

According to the software quality requirements and evaluation guide ISO/IEC 9126-1 (25), some factors were evaluated with the support of an academic panel on the area, such as the usability, sustainability and maintainability criteria as shown on Table 1.

Table 1. Software Evaluation Rubric

The assessment of the previous criterion was carried out under three different case studies in the mass transfer course at the Universidad del Atlantico, where 45 undergraduate engineering students used the software DTMB-UA v1.0 under a given set of operating conditions, the effect of reflux ratio on the distillation molar fraction under different tray numbers, the effect of feed composition on column dimension under different reflux ratio and finally the effect of feed quality variation on condenser, and reboiler duties under different reflux ratio. The average score given by the academic panel to the results of the tests done by the students shown on figure 3, were the usability with 4.3, the sustainability with 3.9 and the maintainability with 3.8.

Figure 3. Average score for the academic panel

In addition, the case study where the feed quality variation on condenser and reboiler duties under different reflux ratio is studied was the best evaluated for the expert with a global score of 4.5, which is a satisfactory evidence to ensure the quality of software as a powerful tool for support the learning process on undergraduate students. There was another case study that was not evaluated by the panel area because of the complexity of the iteration applied, though, it is mentioned due to the high importance on real distillation results. The case studies developed for the students are explained as follow.

3.1. Bottom Fraction Value - Accurate Selection

In order to get the exact bottom molar fraction value, first, it is necessary to introduce to the program the following input parameters: binary mixture (Methanol – water), tower pressure (*3atm*), feed flow (*1000 kmol/h*), feed quality *(φ=1*), feed molar fraction of the volatile component (*xF=0.3*), bottom molar fraction of the volatile component (*xB=0.05*), distillate molar fraction of the volatile component (*xB=0.97*), distance between trays (*60 cm*), liquid hold up on the trays (*25mm*), reflux ratio (*R=1.22*), density of the liquid mixture (*780 kg/m^3*) and the density of the vapor (*2.8 Kg/m^3*).

As soon as the parameters of the tower are chosen, the results show a new value of the bottom molar fraction which is different from the initial given value as can be seen in figure 4a. on the left-inferior side of the stripping line (green line) compared with the composition that leaves the last tower tray corresponding to the reboiler. Generally, the bottom molar fraction value is given by the user; however, this value is then calculated by the equations again. There is a small difference between the given and the calculated value producing a small error in the rest of the variables obtained. Usually, engineers work with that error when they try to make design and simulations. Considering that the McCabe-Thiele method uses an initial assumption regarding the enthalpies in all the trays resulting in an error in the output variables, then, if the user introduces another error during the process, the total error increases considerably making real experimental data differ from simulation. For that reason, it is necessary that users employ a trial and error

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method to find the exact composition of the bottom molar fraction which consists of giving initial values of the bottom composition until the value of the last tray matches with the given initial value (see figure 4b) minimizing the error produced by the McCabe-Thiele method letting to make better comparison with experimental data.

Figure 4. McCabe-Thiele operating line for rectifying and stripping section a) Composition with deviation of the real bottom molar fraction value b) Exact composition of the bottom molar fraction.

3.2. Effect Of Reflux Ratio On The Distillation Molar Fraction Under Different Tray Numbers.

On this section, it will be developed a parametric study by looking briefly the effect of reflux ratio on distillation molar fraction by changing the number of trays. It can be inferred from the relations used in the algorithm section that the number of trays and reflux radio will influence the degree of separation on the column. This is demonstrated in the following example, supported by the *DTMB-UA v1.0* software.

Consider a base case, where the feed flow (*F*) is *700kmol/hr* for a binary mixture of ethanol-water that has a composition of *0.4* molar fraction in terms of the more volatile component (*xF*), a feed quality (φ) of *0.5* and a bottom fraction (*xB*) of 0.05. The reflux ratio (*R*) as a function of distilled molar fraction (*xD*) under different tray numbers is presented on figure 5 where it can be seen that an increase in a specific distilled molar fraction at a constant reflux ratio, result in an increase in the number of trays. This plot presents an asymptotic trend between reflux ratio and the distilled molar fraction for all the different trays which means that it necessary to find an equilibrium between the fixed costs and the operating costs to choose if it is convenient to work with additional plates or to work with higher reflux ratio (*R*). Adding more plates would increase the fixed costs but adding higher reflux ratio would increase the operating costs. This happens due to the increase of larger quantities of recycled liquid and vapor per unit quantity of feed which implies to create larger pumps in the reboiler and the reflux. The making of this plot can help the student to understand the importance of obtaining a high-quality product at low cost.

Figure 5. Effect of reflux ratio (R) on distilled molar fraction (XD) under different tray number

3.3. Effect Of Feed Composition On Column Dimension Under Different Reflux Ratio.

In this case, it will be developed a parametric study by looking briefly the effect of feed molar fraction (*xF*) on column diameter and column height by changing the reflux ratio (*R*). The following parameters were used: binary mixture (Methanol – water), tower pressure (*3atm*), feed flow (*1000 kmol/h*), feed quality ($\varphi=1$), bottom molar fraction of the volatile component (*xB=0.05*), distilate molar fraction of the volatile component (*xB=0.97*), distance between trays (*30 cm*), liquid hold up on the trays (*50mm*), density of the liquid mixture (*780* kg/m^3) and the density of the vapor (*2.8* Kg/m^3).

The importance of figure 6 lies on the economy achieved when designing a tower because of the construction material area. It is necessary to use a distillation column with a high efficiency with the lowest diameter and height. Figure 6 shows that an increase on the feed molar fraction indicates the use of a tower with higher diameter and lower height.

Regarding an increase in reflux ratio at a constant feed molar fraction, it is necessary to increase the tower diameter and decrease its height. Comparing the column diameter with its height we can see that one increases while the other decreases causing a small significant effect on the construction material area.

One more thing that can be appreciated in figure 5 is that an increase in the reflux ratio at high feed molar concentrations requires the use of a higher increment in diameter than those that have to be used working at low feed molar concentrations. The same pattern can be seen with the height but inversely with the feed fraction.

Figure 6. Effect of feed composition (xF) on column dimension (d, h) under different reflux ratio (R).

3.4. Effect Of Feed Quality Variation On Condenser And Reboiler Duties Under Different Reflux Ratio.

Figure 7. Effect of feed quality variation on condenser and reboiler duties under different reflux ratio

To plot Figure 7 the following parameters where used as input: binary mixture (Methanol – water), tower pressure (3atm), feed flow (*1000 kmol/h*),feed molar fraction of the volatile component (*xF=0.3*), bottom molar fraction of the volatile component (*xB=0.05*), distillate molar fraction of the volatile component (*xB=0.97*), distance between trays (*60 cm*), liquid hold up on the trays (*25mm*), reflux ratio (*R=1.22*), density of the liquid mixture (*780* kg/m^3) and the density of the vapor (*2.8* Kg/m^3).

Figure 7 is highly important because it shows the relation of the duty required in the condenser and reboiler with changes in the feed quality and reflux ratio. This duty is directly related with the operational costs for a same amount of production. The lower the duty of the heat exchangers, the lower the expenses of the process. In Figure 7, we can see that an increase in the feed quality (Sub-cooled liquid) has no effect on the duty of the condenser but produce an increase in the energy required in the reboiler which makes sense because more energy is needed to evaporate the liquid inside the tower. This shows the importance of the use of a heat exchanger in the inlet stream (feed) to increase its quality. Generally, when a distillation tower is used in a process there are many other streams at high temperatures that can be used to transfer the energy to the feed stream. On the other hand, we have the effect of the reflux ratio on the duty of the condenser and reboiler. The higher the value of the reflux ratio, the higher the duty of the heat exchangers. Obviously, it is necessary to choose the lowest reflux ratio for better economy, however, there must be a balance with the values chosen because when the reflux ratio decreases, the distillate molar fraction decreases as well, becoming an inconvenient for the production. So, it is necessary to know the lowest working value of concentration of the distillate without affecting the production.

The limitation of the program is that only use the McCabe–Thiele method. However, it is the most used method to design distillation towers. A more advanced version will be created using Ponchon-Savarit including reactive distillation.

4. CONCLUSIONS

A mathematical tool for process, chemical, and mechanical engineers aimed at the design of distillation columns "*DTMB-UA v1.0*" has been presented with the application of four examples where the user can see its capacity by making a simple analysis of distillation column designs. The program makes use of mass and energy balances with a given set of distance between plates, liquid height plates and operating conditions such as the inlet flow, feed quality, desired fractions, reflux ratio and relative volatility to finally obtain outputs such as the number of stages required, the tray of feed, the diameter and height column, and the condenser and reboiler duties which are necessary for the energy requirements of the column.

The program was designed user-friendly to get a set of experimental data of equilibrium or select from theoretical data and use them as an input to later compare the concentration of the distillate with other results obtained with different operating conditions. These help users to go beyond a simple experiment and analyze different distillate columns at the same time.

The exact composition of the bottom molar fraction value was obtained by iteration so that engineers can see that the initial given value, is not always the right molar composition of the column bottom.

The relation of distillate molar fraction (*xD*) as a function of the reflux ratio (*R*), for different tray numbers (*N*) shows the importance to work with a high number of plates or to work with more reflux ratio (*R*) to obtain the needed distillate molar fraction.

It was obtained the effect of feed composition (*xF*) on column diameter (*d*) and column height (*h*), as a function of different reflux ratio (*R*). With the help of the software users can see how sensitive are these parameters to changes in feed molar fraction. With the comprehension of these parameter calculations, users can see the importance of the costs achieved when designing a distillation column due to the relation between the construction material and the diameter and height of the column.

It was determined the variation of condenser duty (*QC*) and reboiler duty (*QR*) as a function of different reflux ratio (*R*) and feed quality (φ). This let to understand the effect of the feed quality and reflux ratio in the operational costs because of the total energy required and the mass flow involved.

The use of the Graphical User Interface (GUI) would increase the efficiency of a mass transfer class since it makes students to get a better

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comprehension of what happen inside a distillation column by correlating all the different variables found on them.

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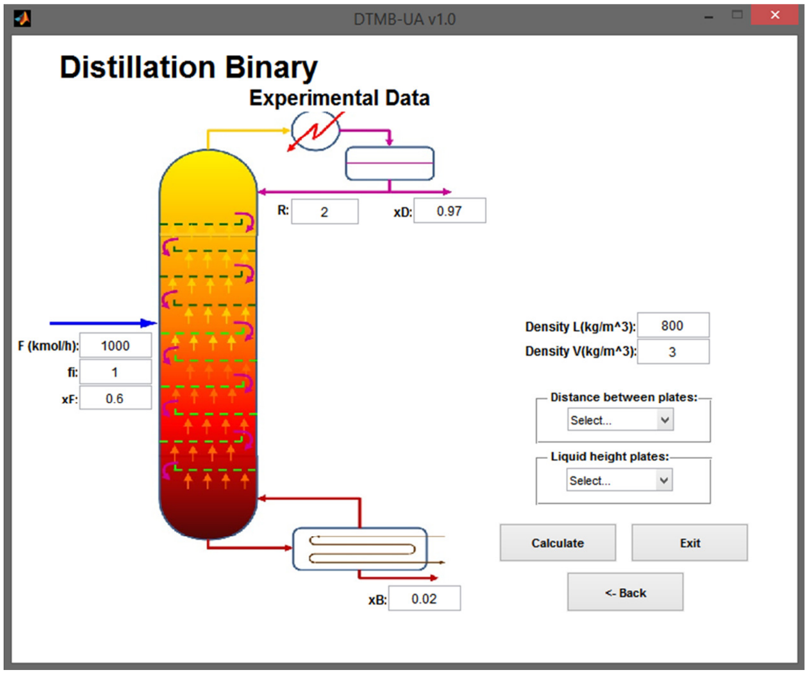
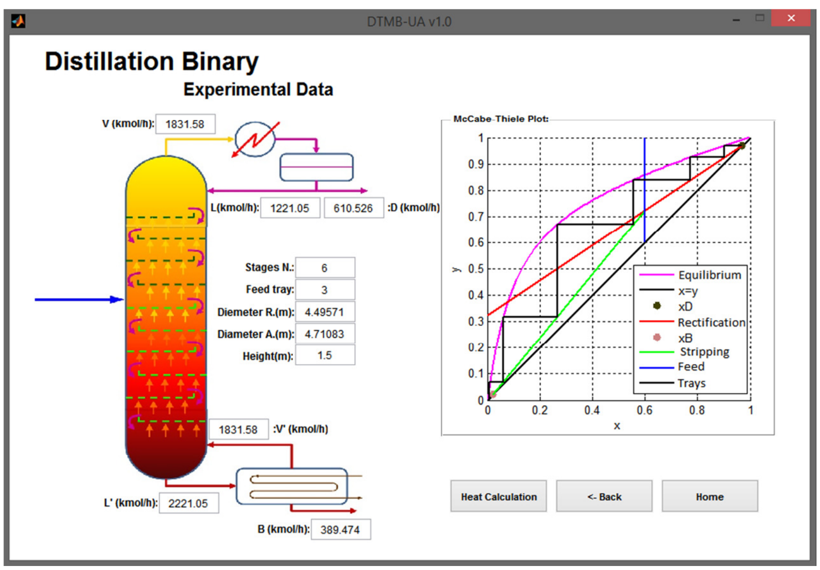
NOMENCLATURE

Symbols		*Units*
B	Bottom flow	[kmol/h]
Cp	Specific heat	[kJ/kg-°C]
D	Distillate flow	[kmol/h]
d	Column diameter	[m]
F	Inlet flow	[kmol/h]
G	Distance between plates	[cm]
H	Enthalpy	[kJ]
h	Column height	[m]
k	Coefficient height	[mm]
L	Liquid top flow	[kmol/h]
L'	Liquid bottomflow	[kmol/h]
ṁ	Mass flow rate	[kg]
N	plate numbers	[dimensionless]
p	Average absolute pressure	[mm Hg]]
Q	Heat flow rat	[kW]
R	Reflux ratio	[dimensionless]
t	Average temperature of vapors	[°C]
u	Vapor velocity	[m/s]
V	Vapor top flow	[kmol/h]
V'	Vapor bottom flow	[kmol/h]
x	Fraction of the volatile component in the liquid face	[dimensionless]
x_D	Distillate fraction of the volatile component	[dimensionless]
x_B	Bottom fraction of the volatile component	[dimensionless]
x_F	Feed fraction of the volatile component	[dimensionless]
y	Vapor fraction of the volatile component	[dimensionless]
Greek letters		
α	Constant relative volatility	[dimensionless]
λ	Heat of vaporization	[kcal/kg-mol]
ϕ	Feed quality	[dimensionless]
ρ	Density	[kg/m3]
Subscripts		
1	More volatile component	[dimensionless]
2	Less volatile component	[dimensionless]
B	Bottom	[dimensionless]
C	Condenser	[dimensionless]
D	Distillate	[dimensionless]
F	Feed	[dimensionless]
in	Inlet	[dimensionless]
L	Saturated liquid	[dimensionless]
np	Plate number	[dimensionless]
out	Outlet	[dimensionless]
R	Reboiler	[dimensionless]
V	Saturated vapor	[dimensionless]



(a)



(b)

Figure 8. Main View of the DTMB-UA v1.0 software. (a) Inputs data; (b) Operation condition

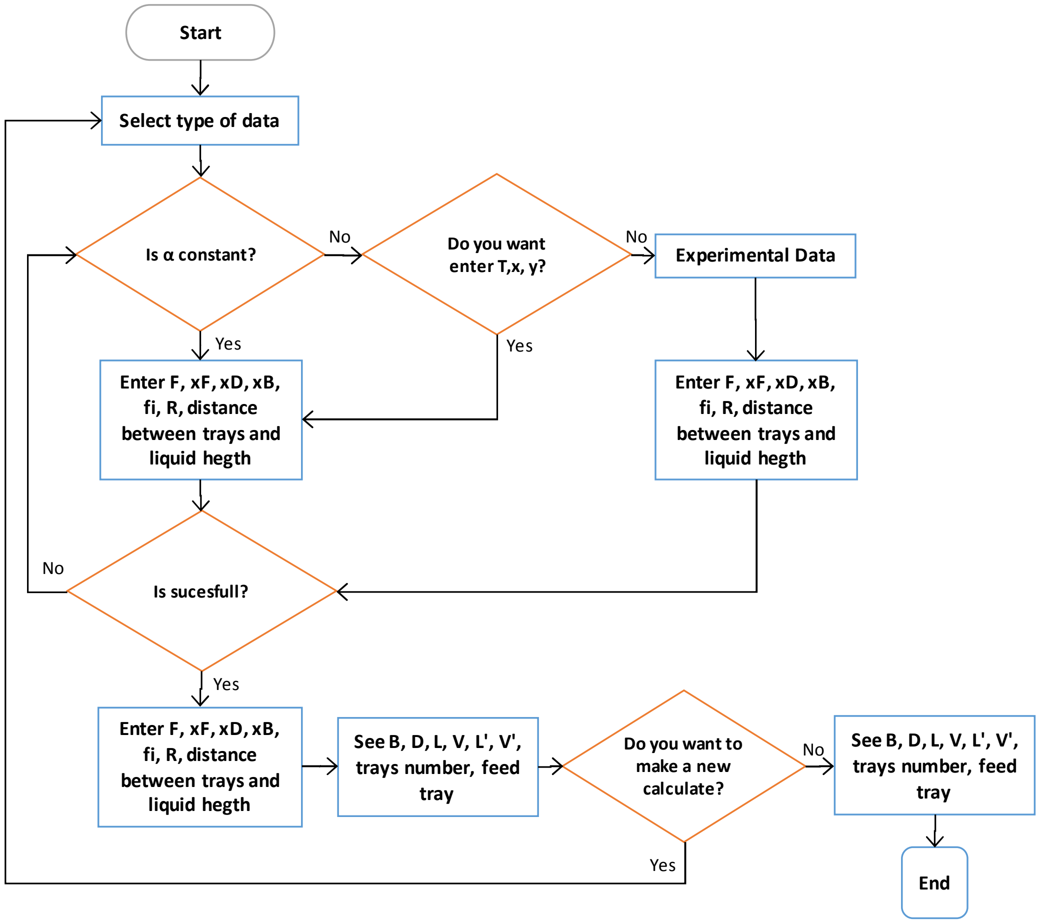


Figure 9. Flowchart of the DTMB-UA v1.0

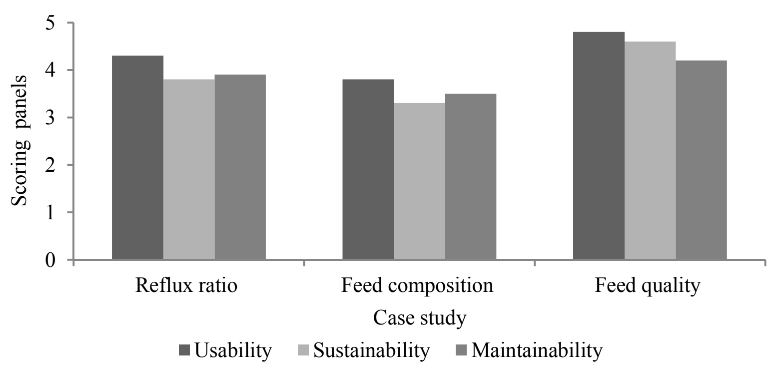


Figure 10. Average score for the academic panel

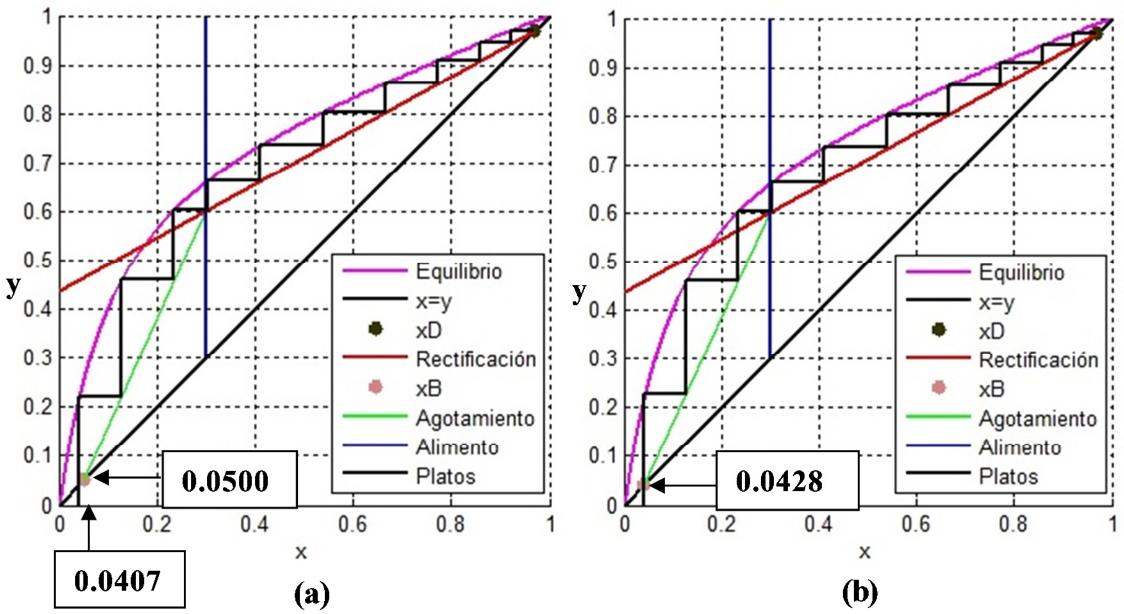


Figure 4. McCabe-Thiele operating line for rectifying and stripping section a) Composition with deviation of the real bottom molar fraction value b) Exact composition of the bottom molar fraction.

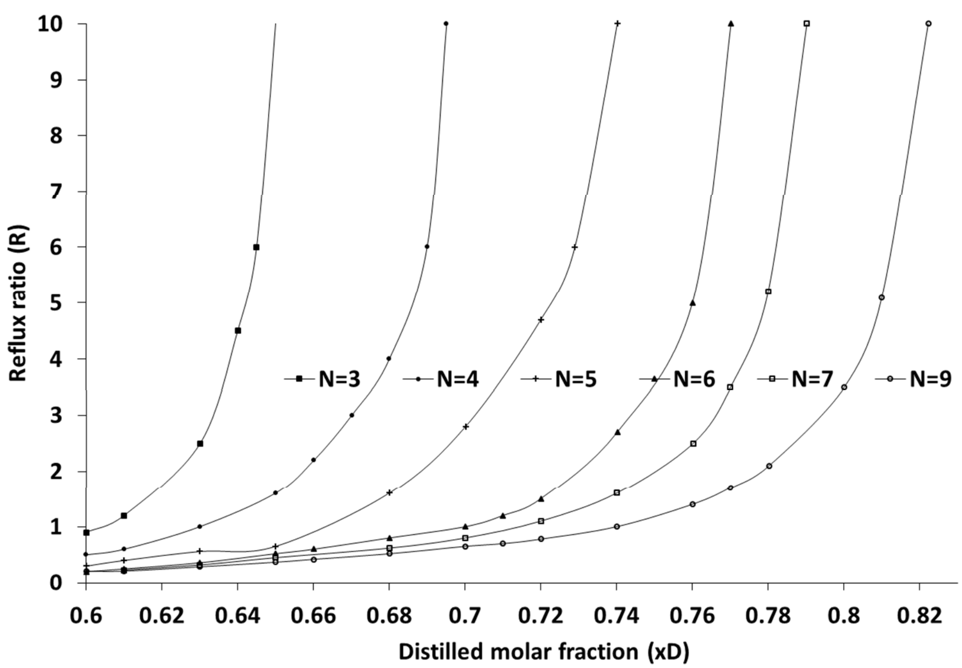


Figure 5. Effect of reflux ratio (R) on distilled molar fraction (XD) under different trays number

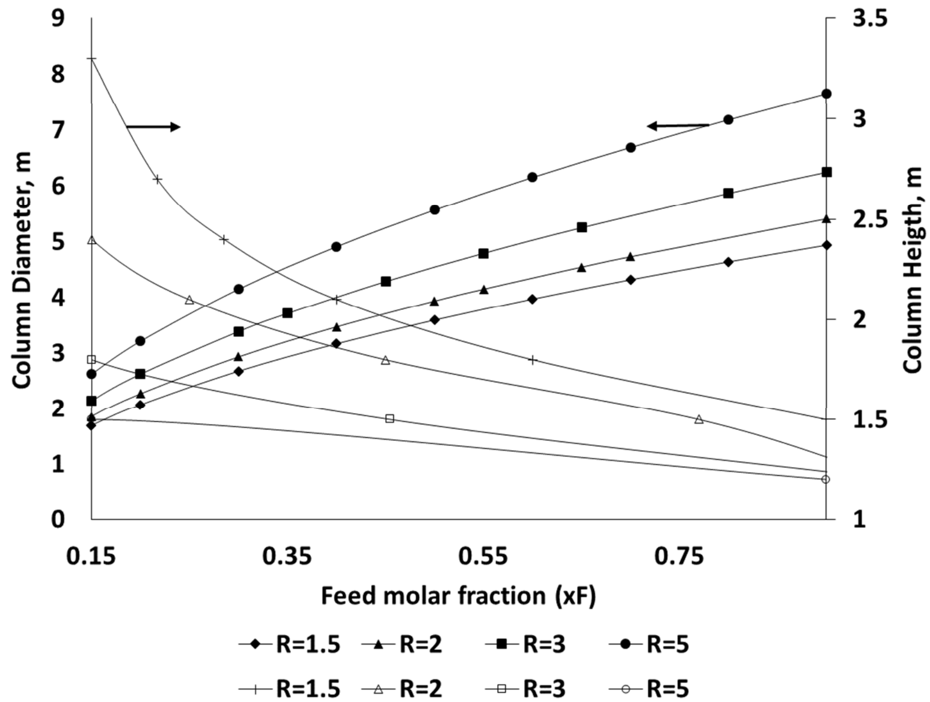


Figure 6. Effect of feed composition (xF) on column dimension (d, h) under different reflux ratio (R).

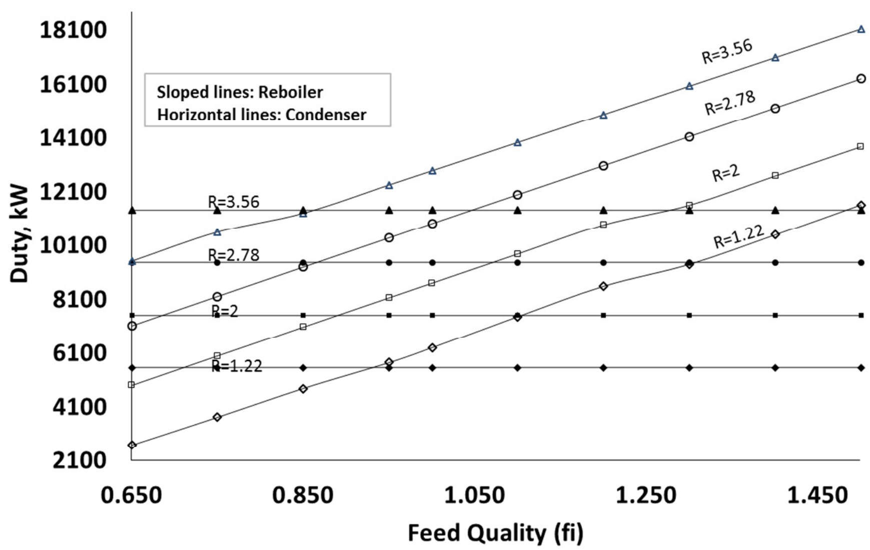


Figure 7. Effect of feed quality variation on condenser and reboiler duties under different reflux ratio

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Table 1. Software Evaluation Rubric

Criterion	Descripction	Outstanding (5,0 -4,5)	Good (4,5 - 3,5)	Satisfactory (3,5-3,0)	Unsatisfactory (1,0 - 0)
Usability	The software is perfect or near-perfect understood, very good comprehensive, appropriate, well-structured user guide and easy to learn how to use its commands.				
Sustainability	Is easy to see who owns the software, is easy to understand how the project is run and the development of the software managed and the software identity is clear and unique.				
Maintainability	The sotware is easy to modify and contribute changes to developers, is usable on multiple platforms and interoperable with other required software.				