



# Trabajo Final de Grado

**Simulation software for batch binary distillation with Mathematica® code.**

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***El poder, no el saber, que proporciona la ciencia.*** *El valor que tiene el haberse dedicado con rigor a una ciencia rigurosa no radica en sus resultados: pues éstos, con el océano de cosas que valdría la pena saber, no son más que una gota infinitamente pequeña. Pero con dicha dedicación se consigue un aumento de energía, de capacidad de razonar y de tenacidad en el mantenimiento del esfuerzo: se ha aprendido a alcanzar un objetivo con los medios que se ajustan al mismo. En este sentido resulta muy valioso, con vistas a todo lo que se hará después, haber sido hombre de ciencia alguna vez en la vida.*

Friedrich Nietzsche, aforismo 256 de Humano, demasiado humano



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## SUMMARY

The distillation process is studied in this assignment, which is one of the most utilized unit operations in all the chemical industry.

With this intention, a simulation is carried out that explains the behaviour of a batch distillation column with a feed consisting of monoethylene glycol (MEG) and diethylene glycol (DEG). The computer programme used for this purpose is named Wolfram Mathematica®.

Nonetheless, the ultimate aim of this assignment constitutes the creation of an interface that allows a non-expert user to execute the simulation of any binary distillation without possessing programming knowledge. The obtention of said simulation is due to applying the McCabe-Thiele method which enables to calculate, among others, the number of theoretical trays required by the distillation column. However, it was necessary to carry out some previous calculations such as finding out the equilibrium curve or the relationship between pressure and the volatility of the mixture, to just give a pair of examples.

Finally, a similar distillation was carried out in the laboratory to evaluate how the already mentioned programme performs in a real situation. In both cases it has been concluded that the programme used is totally capable of meeting the requirements obtaining highly accurate results without saturating the kernel.

**Keywords:** Distillation column, simulation, McCabe-Thiele method.



## RESUMEN

En este trabajo se estudia el proceso de destilación, el cual es una de las operaciones unitarias más utilizadas en toda la industria química.

Para ello se simula el comportamiento de una columna de destilación discontinua cuyo alimento está compuesto de monoetilenglicol (MEG) y dietilenglicol (DEG). El programa informático empleado para dicho estudio corresponde a Wolfram Mathematica®.

No obstante, el propósito final de este trabajo representa la creación de una interfaz que permita a alguien no especializado llevar a cabo la simulación de una destilación binaria cualquiera sin poseer conocimientos de programación. La obtención de dicha simulación ha sido gracias a la aplicación del método McCabe-Thiele que permite calcular, entre otras cosas, el número de platos teóricos que necesitaría la columna de destilación. Sin embargo, fue necesario hacer unos cálculos previos hallando la relación entre presión y volatilidad de la mezcla o la curva de equilibrio, por poner un par de ejemplos.

Por último, se ha llevado a cabo una destilación similar en el laboratorio para evaluar cómo el ya mencionado programa informático opera ante una situación real. En ambos casos se ha podido concluir que el programa empleado es totalmente capaz de cumplir con las exigencias requeridas obteniendo resultados altamente exactos sin llegar a saturar el kernel.

**Palabras clave:** columna de destilación, simulación, método de McCabe-Thiele.



# 1. INTRODUCTION

Before delving into the actual distillation process, it is a wise thought to go over both compounds handled throughout the development of this assignment. These two substances are ethylene glycol and diethylene glycol and although they form an only phase, this simple binary mixture cannot be found in nature. Therefore, both chemical compounds will be discussed separately.

## 1.1. COMPOUNDS USED

### 1.1.1. Monoethylene glycol

Ethylene glycol, monoethylene glycol or ethane-1,2-diol, abbreviated as MEG is the simplest diol, thus classified as an organic compound. Diols contain a pair of hydroxyl groups (-OH), and MEG is no exception with a chemical formula of  $(\text{CH}_2\text{OH})_2$ .

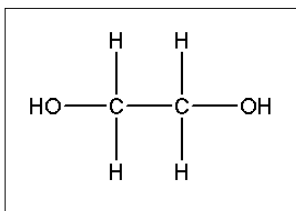


Figure 1. Lewis structure for MEG.

At room temperature remains in a viscous liquid state and boils at a temperature of around  $197.4^{\circ}\text{C}$  at 1atm. It is colourless, odourless and with a slight sweet flavour. Its density is  $1.116 \text{ g/cm}^3$ , which is superior to water and its molar mass is  $62.07 \text{ g/mol}$ . It is hygroscopic and totally miscible with a large quantity of polar solvents such as water or diethylene glycol.

MEG has a wide range of applications such as the production of polymers, ballpoint pens, cleaning products or lubricants. Nonetheless, its principal usage is to produce the anti-freezing fluid used for internal combustion engines or the de-icing fluid for aircrafts and boats. These two fluids operate optimally when the mixture contains water and MEG, achieving freezing points of around  $-55^{\circ}\text{C}$ . Since this compound does not attack metals or rubber, it is an excellent choice for these applications.

There are numerous ways of producing MEG, such as the chlorohydrin process in which ethylene oxide reacts with water, resulting in the production of only MEG. A lesser-known process in which formaldehyde and carbon monoxide react to produce MEG is also viable. Nonetheless, both processes are no longer used. Instead, ethylene suffers an oxidation in contact with oxygen or air and ethylene oxide is obtained. This same ethylene oxide is mixed with water at a temperature of around  $200^{\circ}\text{C}$  and the ethylene glycol is produced without the need of a catalyst. Other glycols are formed but in very reduced quantities.

MEG is easily biodegradable; it breaks down in air in around 10 days while in water or soil it takes a few weeks. It does not represent any problem regarding its transport or storage. Despite all this, it is toxic if exposed to large quantities. Due to this, hazard statements H302 (acute toxicity if ingested) and H373 (toxic to specific organs when exposed repeatedly or during a long period of time) are applied to it. Some precautionary statements are also applied such as P260 (do not inhale its vapours), P270 (do not eat, drink, or smoke during its manipulation). Every single container with MEG in its interior must display the pictograms which represent a health hazard and a serious health hazard.



Figure 2. Container with MEG.

### 1.1.2. Diethylene glycol

Diethylene glycol, ethylene diglycol, 2,2'-Oxydi(ethan-1-ol), abbreviated as DEG is also a diol, therefore an organic compound too. Its chemical formula is  $(\text{HOCH}_2\text{CH}_2)_2\text{O}$ .

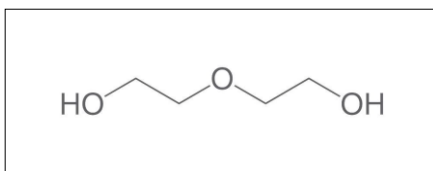


Figure 3. Skeletal structure of DEG.

Just as MEG, DEG remains in a liquid state at room temperature and is a colourless, sweet hygroscopic substance. It is odourless too, although at high concentrations some sweetness can be detected. It is also miscible in polar solvents such as water, alcohol, or MEG. The boiling point of this substance sits at around 244.9°C at 1atm, almost 50 degrees superior to MEG. Its density is 1.118 g/cm<sup>3</sup>, which is almost the same as MEG. However, its molar mass is much greater, being of 106.12 g/mol and this is the reason why it is considerably less volatile than MEG.

In regard to its applications, it has numerous uses such as a chemical intermediate in the production of unsaturated polyester resins, emulsifiers, lubricants or adhesives. Since it is a hygroscopic substance, it is also applied in the natural gas industry to remove the humidity in gas pipelines. Since it has lubricant properties, it is implemented in the process of cement grinding and mould releasing. Finally, it is also utilized to a much lesser extent in the production of anti-freezing and de-icing products since it is a secondary product of MEG synthesis.

The process used in the industry to produce DEG is very similar to the one applied to MEG obtention. In this case, ethylene is oxidized at elevated temperatures with a silver oxide catalyst. The resulting ethylene oxide is partially hydrolysed under certain conditions so that DEG is the main product and MEG and triethylene glycol the by-products.

Just like MEG, DEG is readily biodegradable in any environment, it does not bioaccumulate and its mobility in soil is very limited. Transporting or storing this substance does not imply any major risk. Nonetheless, it is still as toxic as MEG since it is extremely harmful to swallow it. As a result, the same hazard statements H302 and H373 and precautionary statements P260 and P270 are applied to it. Moreover, other precautionary statements are added such as P264 (wash thoroughly after handling) and P330 (rinse mouth). The same pictograms will be displayed in a container with DEG in its interior.



Figure 4. Container with DEG.

## 1.2. DISTILLATION PROCESS

Distillation is a separation operation in which two or more liquid compounds forming an only phase end up fairly separated in two mixtures with very different compositions when heated. Ideally one of the mixtures remains liquid whilst the other forms a vapour which is later condensed again and collected. Therefore, it is considered as a unit operation based in mass transfer and in fact it is the most utilized separation process in the chemical industry. It is important to remark that it is a physical process since there is no chemical reaction.



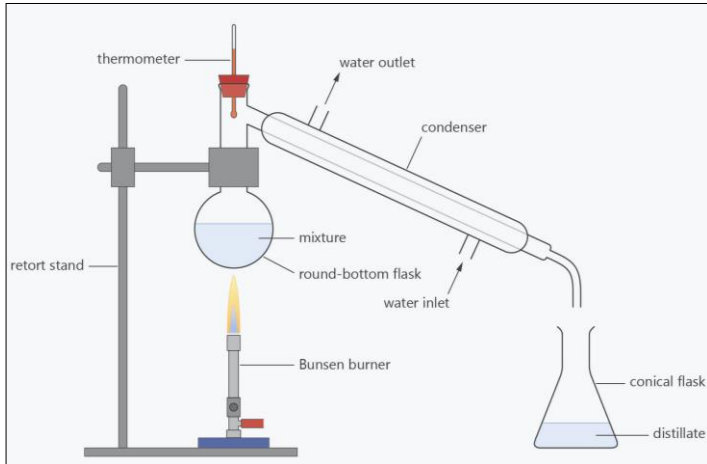


Figure 5. Basic setup of a distillation process.[14]

Distillation can be used for several purposes such as separating a liquid from non-volatile solids just as in the desalination process. However, it is normally applied to separate several liquids forming a unique phase. Some examples of this can be seen in the production of distilled beverages that contain a substantial percentage of alcohol or in the obtainment of perfumes.

### 1.2.1. Scientific foundation

Distillation occurs when heat is applied and thanks to the fact that the compounds present in the liquid mixture possess varied volatilities. Therefore, the most volatile substance will tend to evaporate with much greater ease than the heaviest one. In other words, the compound with a greater vapour pressure will have a lower boiling point in comparison to the rest. As a result, a vapour phase rich in the most volatile compound is formed. The greater the difference is in volatilities, the greater the separation between compounds will be. If volatilities are too similar, distilling the mixture will not be easy and alternative methods will be needed. However, if the vapour is not rich enough in the desired compound, the best way to proceed is by distilling it as

many times as necessary. Nonetheless, this is not efficient in terms of energy and time and here is where the rectification process comes into play.

### 1.2.2. Rectification

Rectification is one of the various ways of distilling, however it is widely used in the industry since it enables the obtention of a highly purified distilled. The aforementioned process takes place in a distillation column which operates with a counter current flow due to the difference in densities resulting in the vapour phase moving upwards and the liquid one downwards.

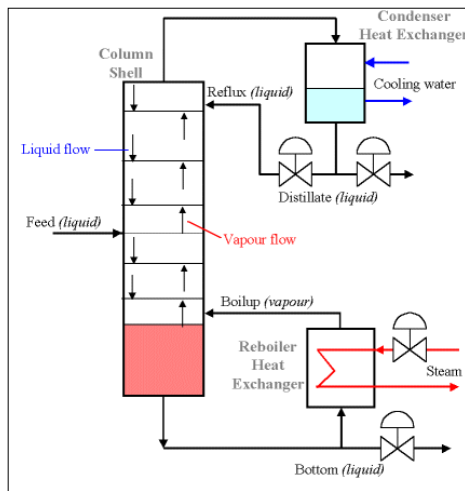


Figure 6. Basic scheme of a distillation column.[15]

#### 1.2.2.1. Reboiler

The liquid mixture is heated up in a reboiler located in the bottom part of the column and this is the reason why the lower part of the column is hotter than the upper one. Reboilers can be partial or total. In the first case, the liquid stream is partially vapourised and the steam generated is fed into the lowest stage of the column. The liquid mixture not vapourised is withdrawn as bottom product, nevertheless, both currents are in equilibrium with each other. These type of reboilers add up an ideal stage in the McCabe-Thiele method.

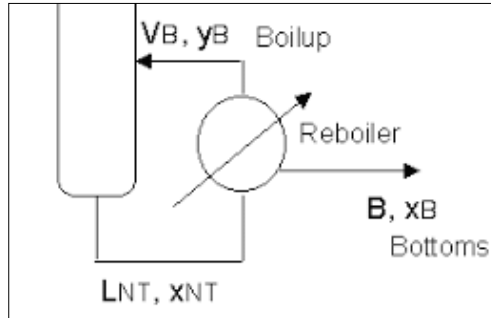


Figure 7. Scheme of a partial reboiler.[4]

In case of equipping the column with a total reboiler, the liquid current is firstly divided into two. One of these currents corresponds to the bottom product whilst the other one is entirely vapourised and sent to the last stage of the column, as a result, the streams entering and leaving the reboiler are in equilibrium. Since they are in equilibrium, these types of reboilers do not count as an extra ideal stage.

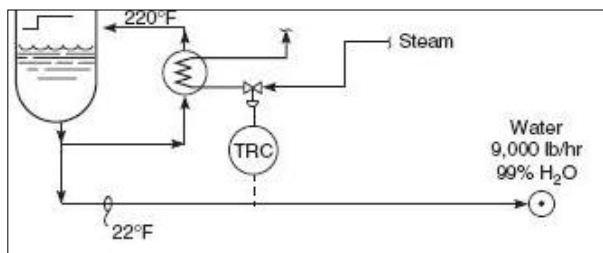


Figure 8. Diagram of a total reboiler.[4]

### 1.2.2.2. Condenser

Once it starts to evaporate, the vapour will rise to the top of the column where a condenser is located. A fraction of said vapour will be returned to the head of the column in a condensed state as reflux. A crucial variable when it comes to operating a distillation column corresponds to the reflux ratio which is basically defined as the ratio of the liquid returned to the head of the

column by the amount of liquid coming out as final distillate. The value of this ratio can range between zero and infinity since it is perfectly possible to not redirect any liquid to the column or to not extract anything as distillate.

$$R_D = \frac{L}{D} \quad (1)$$

There are two kinds of condensers, these being total and partial. In the first type, all the overhead product is completely condensed and later separated into the distilled and the reflux. As a result, the composition of both the overhead vapour and the liquid distillate is equivalent and therefore this sort of condenser does not count as an ideal stage in the McCabe-Thiele method.

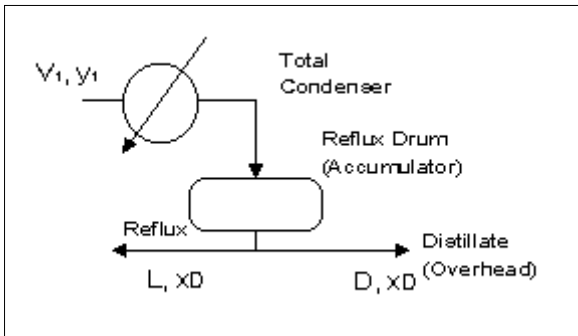


Figure 9. Scheme of a total condenser.[4]

Unlike total condensers, partial ones do not condense the top product completely. The vapour phase is taken out of the system whilst the liquid is reintroduced into the column. The compositions of the currents entering and exiting these condensers are different, however both leaving streams are normally in equilibrium. Nonetheless, operating with a partial condenser adds one more ideal stage to the system.

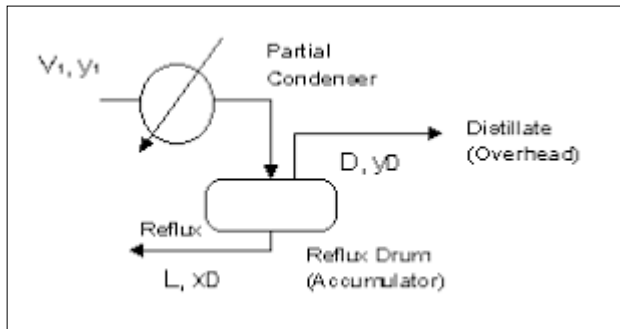


Figure 10. Diagram of a partial condenser.[4]

### 1.2.2.3. Trays

Although it may seem like in every section of the column there is an intimate contact between the vapour phase rising and the liquid one descending, originating a mass transfer between each other, truth is it is only in each of the ideal stages where an equilibrium between both phases is met. In practice, each of the ideal stages corresponds to a tray or plate and these are designed to enable an optimal contact between both phases. There are three main types of trays and the way of choosing one will depend on physical, chemical, and economic factors. However, all types of trays are disposed in such a way that forces the liquid phase to flow from one side to the other of every single plate. Liquid flows from one plate to another through a downcomer thanks to the action of gravity. Furthermore, plates include a weir to ensure that there is liquid on top of their surface at every moment.

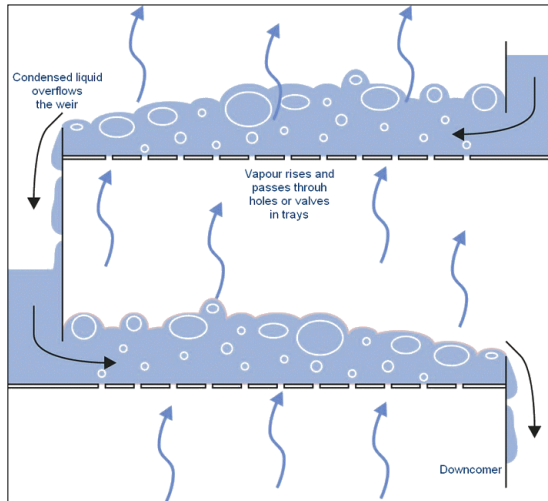


Figure 11. Disposition of trays in a distillation column.[6]

The first type corresponds to bubble cap trays, in which each of these trays corresponds to a perforated plate that includes risers. Those risers resemble a chimney and are covered by a cap leaving a space in between to allow the flow of vapour. Caps also include a series of slots to encourage even more the circulation of vapour. Once the vapour rises through one of those risers, it is forced to advance downwards due to the cap and exits through one of the slots. Finally, it bubbles through the liquid on the plate.

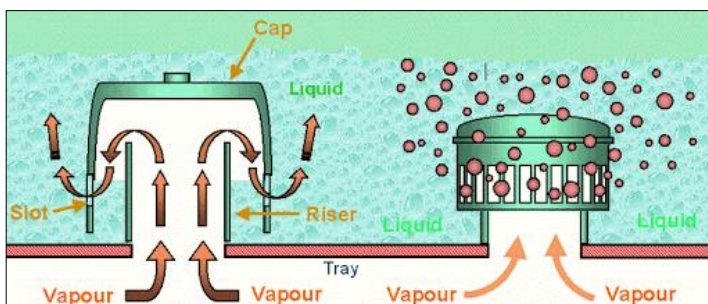


Figure 12. Representation of how a bubble cap plate operates.[5]



Figure 13. Bubble cap tray.[5]

Another variety is the sieve tray, which is just a flat metal plate that has been perforated many times. These holes are small with sizes ranging from  $\frac{1}{4}$ " to 1". The vapour rising prevents from the liquid falling through the holes, instead, it is forced to travel across the whole tray until it falls to the one immediately below. These kinds of trays are very simple to construct and because of this they are the cheapest option. Moreover, they do not require excessive maintenance and do not tend to foul as much as the rest of trays.

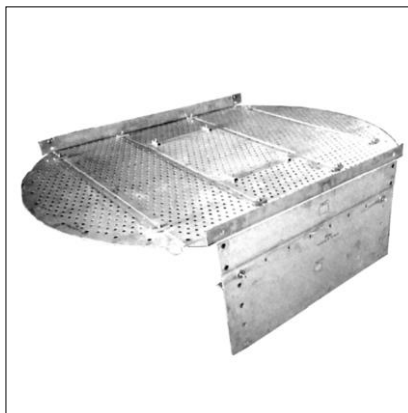


Figure 14. Sieve tray.[5]

Finally, the last option are valve trays, which have a design halfway between the other two varieties. They consist in a sieve tray covered by a valve in each of the perforations, being the valve fixed or movable. When the vapour collides with the valve, it is directed horizontally to the liquid phase and this contributes to a better contact in comparison with sieve plates. It is ideal if what is sought is a flexible tray that can operate in a wide range of conditions (pressure, flowrate, etc).

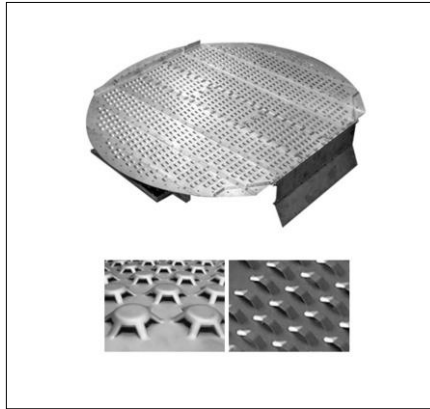


Figure 15. Valve tray with a closer look at the valves [5]

Reality is that plates do not have an optimal efficiency and because of this, perfect equilibrium between phases is not met in all the stages. This can occur due to the formation of froth which causes an incomplete interaction between both phases or due to the phases flowing too fast for them to have enough time to interact properly. Additional problems may take place such as vapour rising through the downcomers, liquid descending through the plate holes, liquid being dragged by the vapour to the upper plate or vapour being dragged by the liquid to the lower plate. None of the aforementioned problems should be too significant if the column is correctly sized and the trays displayed and designed in a proper way. When it comes to tray configuration, the disposition, number and size of the holes are design parameters. However, it is not a simple task. Considering all this, not a single distillation column will work in an ideal way and that is the reason why additional trays will be needed in comparison to what theory predicts. A ratio known as overall tray efficiency will define how effective the trays used are in terms of how well do they separate the compounds, assuming they all perform equally:



$$\eta_0 = \frac{N_t}{N_a} \quad (2)$$

Where  $\eta_0$  is the overall plate efficiency,  $N_t$  is the theoretical minimum number of trays and  $N_a$  is the actual number of trays. It is crucial that plates are efficient enough, not only to separate components optimally, but also to have less energy and construction costs. Despite of this being useful information to have an idea of how the distillation column will perform, it is important to consider that it is only an estimation because it is based on the premise that all trays will be equally efficient.

#### 1.2.2.4. Operating regime

There are two ways of operating a distillation column and these can be by introducing the feed in batches or continuously. If the column runs with a batch-wise regime, before initiating the process, the reboiler is charged with the feed. At first, during the start-up, it is very usual to operate with a total reflux to improve the contact between both phases. While the distillation is taking place, the distilled is taken out of the system progressively through the head of the column and the residue remains in the pot. This implies that the concentration of the most volatile compound in the reboiler will diminish as the process is being carried out. As a result, the evaporation temperature of the residue increases, resulting in a drop of the boiling rate unless more heat is applied to compensate. Operating with a pot still adds up one more theoretical stage to the system, just as if a partial reboiler was being used. Once it has come to an end, the column is emptied, and a fresh feed is introduced. Therefore, this type of process operates at a transient state from start to end. It is important to notice that it is very common to discard the first and last condensate since they do not meet the compositions required.

In contrast, carrying out the distillation continuously implies that the column is fed and discharged constantly. The feed enters the system in a point near the middle of the column. As a result, steady state is achieved in all the column as there is always the same mass and conditions in its interior. This is the most common way of operating since it enables to handle large quantities of product in a brief amount of time.

### 1.2.2.5. Feed

Regarding the feed entering the column, it can contain two components and in this case the distillation would be binary. If the feed contains several compounds, the distillation would be multicomponent such as in the separation of petroleum. In this last condition, fractional distillation would be applied since there are many compounds present in the mixture which have similar boiling points. This results in not separating pure compounds, but fractions. To achieve an excellent separation, the more trays used, the better.

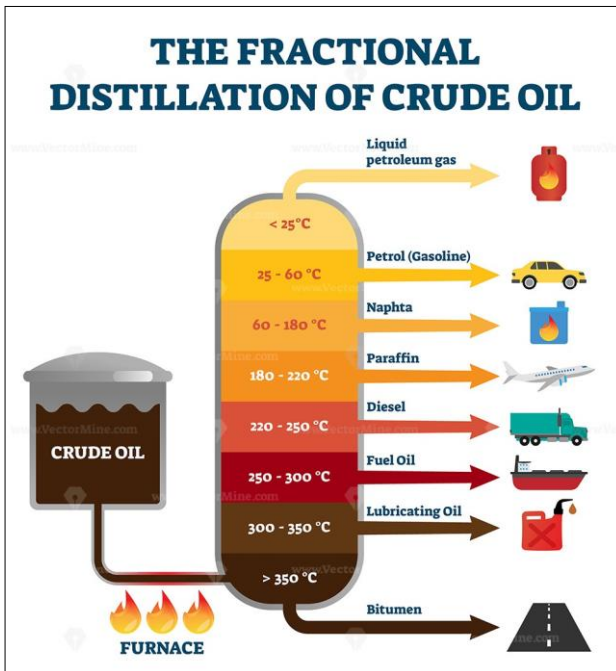


Figure 16. Representation of a fractional distillation.[8]

## 2. OBJECTIVES

The foremost objective of this assignment is to develop a computer program using Wolfram Mathematica® software which enables a non-expert user to simulate a binary batch distillation. Some other minor objectives aside from the above mentioned are:

- Develop some further knowledge regarding Wolfram Mathematica®.
- Consolidate what has been learnt about distillation processes, including the development of the mathematical model used to describe what should theoretically occur.
- Verify the fact that the mathematical model must provide results that match what would happen if the process were to be carried out physically.



## 3. MCCABE-THIELE METHOD

The McCabe-Thiele method is used to study binary distillations in a simple way to ease its understanding. This method allows to find out, among others, the number of theoretical trays needed to carry out the desired distillation. It was first published by Warren L. McCabe and Ernest Thiele in 1925 in an article called “Graphical Design of Fractionating Columns” while they were both working at MIT. It is based on plotting a vapour-liquid equilibrium curve, an operating line and all the required stages represented as triangles in between the previous two functions so that the distillate composition can be related to the reboiler composition. Although it is a useful and straightforward method to apply, some assumptions will be required to be made. Therefore, the results obtained will not always exactly match reality. Firstly, the heat of vapourisation of both compounds are equivalent. This implies that if one mole of compound A is vapourised, another mole of compound B will immediately condense. In addition, some thermodynamic effects are not taken into account such as the heat of dissolution. Finally, it is important to highlight again that it can only be used for binary distillations and that the number of trays obtained are theoretical. This means that tray efficiency is supposed to be of 100% but this does not occur in reality. Therefore, the number of plates required will always be superior, depending on the actual efficiency of the trays used.

### 3.1. POSED PROBLEM

McCabe-Thiele is a graphic method; hence the answer will be obtained by plotting the right functions and following some specific steps. However, there are multiple possibilities regarding known and unknown variables, operating conditions, and desired results. Therefore, not all problems will be solved with the exact same procedure, so this is the reason why it is necessary to determine what kind of problem is addressed in this case. To start with, the distillation carried

out is binary and the feed composition in weight is determined being in this case 50% of MEG. The molar masses for MEG and DEG are known values being 0.06207kg/mol and 0.10612kg/mol. Pressure inside the column and the amount of feed introduced are also known, being 100 000Pa and 0.50kg, respectively. The power of the reboiler is given being of 500W and the molar latent heat of the mixture is also known being of 61000J/mol. Moreover, it is stated that the final quantity of MEG in the reboiler must be of 5% w/w and that the distilled must always contain a 99.5% w/w of MEG. Since it is a batch distillation, the residue remains in the reboiler. Finally, it is stated that the distillation column is composed of 10 stages. However, because a pot still is being used, the total number of stages is increased to 11. To make things clear, stage number 1 corresponds to the upper plate and successive stages correspond to the lower trays until stage number 11 which is the reboiler. All these parameters will eventually be introduced into Wolfram Mathematica© alongside several equations which will be explained further ahead since they are all crucial to solve the problem. Nevertheless, the complete code used to solve this problem is included in the first appendix.

### 3.2. PREVIOUS CONSIDERATIONS

Before proceeding to do all the necessary calculations, it is essential to go over some concepts that will be required later. To begin with, vapour pressure corresponds to the pressure that a vapour phase exerts over its liquid phase (or solid in cases where sublimation takes place) in a closed system at a given temperature and with both phases being in dynamic equilibrium. This implies that the liquid's evaporation rate is the same as the vapour's condensation rate. Therefore, in this state both the vapour and liquid phases are saturated. It is an intensive property; this means it does not depend on the quantity of vapour or liquid present but only on the system's temperature. It gives an idea of how volatile a pure substance is because the lower the temperature at which the vapour pressure matches the external pressure, the easier it will evaporate. It is measured in the standard units of pressure and can be calculated with correlations such as the Antoine Equation:

$$\log_{10}P^0 = A - \frac{B}{C + T} \quad (3)$$

Where A, B and C correspond to constants specific to the pure compound and T is measured in Kelvin.

In a gaseous mixture, multiplying the vapour pressure of a pure substance by its mole fraction results in the partial pressure of said component. This statement corresponds to Raoult's law and is expressed in the following manner:

$$p_i = P_i^0 \cdot x_i \quad (4)$$

Combining it with Dalton's law which states that the total pressure exerted by a mixture of non-reacting gases is equal to the sum of the partial pressures of the individual gases:

$$P = \sum_{i=1}^n p_i \quad (5)$$

$$P = P_1^0 \cdot x_1 + P_2^0 \cdot x_2 \quad (6)$$

Partial pressures are obtained by multiplying the total system's pressure by the component's mole fraction in the vapour phase:

$$p_i = y_i \cdot P \quad (7)$$

It is also fundamental to talk about the latent heat, which corresponds to the amount of energy released or absorbed by a substance that is going through a phase shift such as vapourisation or condensation. This energy is indeed used to achieve said phase shift, therefore the substance's temperature will remain constant while its molecules are modifying their state of matter. Every single substance has a unique value of heat of fusion and of vapourisation. Latent heat is expressed as any heat unit per unit of mass (normally in J/mol) and can be calculated joining both Clausius-Clapeyron and derived Antoine equations:

$$\frac{d \log_{10} P^0}{dT} = \frac{\Delta H^{vap}}{RT^2} \quad (8)$$

$$\frac{d \log_{10} P^0}{dT} = \frac{B}{(C + T)^2} \quad (9)$$

Equalling both equations and reordering the terms it is possible to calculate the latent heat of vapourisation:

$$\Delta H^{vap} = RT^2 \frac{B}{(C + T)^2} \quad (10)$$

The next crucial concept is volatility, which has been discussed previously but not defined mathematically. It basically quantifies the tendency of a substance to evaporate itself. However, in this essay only relative volatility will be used, which will indicate how easy it is to achieve a separation through distillation. A binary system with a relative volatility very superior to one, will be completely viable to distillate. In contrast, distillation on a large scale does not usually occur if the relative volatility of the mixture is inferior to 1,05. Mixtures which are hard to distillate will need taller columns containing more plates. We define this magnitude as follows:

$$\alpha_{ij} = \frac{K_i}{K_j} = \frac{y_i/x_i}{y_j/x_j} = \frac{\gamma_i \cdot P_i^0}{\gamma_j \cdot P_j^0} \quad (11)$$

Where the sub-index i corresponds to the most volatile compound and the sub-index j to the least volatile one. K represents the equilibrium constant; y is the mole fraction in the vapour phase and x is the mole fraction in the liquid phase. This last equivalence is only true for pure compounds or ideal mixtures (mixtures in which the vapour phase obeys Raoult's law and both activity coefficients are equal to one) since the volatility of said compound and its vapour pressure are the same at a given temperature.

Doing some mathematical arrangements in equation 11, it is possible to obtain the function that represents the vapour-liquid equilibrium of the system. To start with, it is important to recall that mole fractions will add up to one in each phase, therefore:



$$\alpha_{ij} = \frac{\frac{y_i}{x_i}}{\frac{1-y_i}{1-x_i}} = \frac{y(1-x)}{x(1-y)} = \alpha \quad (12)$$

Notice how the sub-indexes have been removed for a better understanding. Reordering terms:

$$\alpha x(1-y) = y(1-x) \quad (13)$$

$$\alpha x - \alpha xy = y - xy \quad (14)$$

$$y(1-x + \alpha x) = \alpha x \quad (15)$$

$$y[1 + (\alpha - 1)x] = \alpha x \quad (16)$$

$$y = \frac{\alpha x}{1 + (\alpha - 1)x} \quad (17)$$

In some cases, it is useful to isolate x, obtaining an expression as follows:

$$x = \frac{y}{y + \alpha - \alpha y} \quad (18)$$

Another important aspect to cover is the mass balance applied to the entirety of the distillation column. Since there is no chemical reaction, the mass that enters the system will be equal to the one coming out. Therefore, the amount of mass fed into the column (F) will be the same as the sum of the mass remaining in the reboiler ® and the one leaving the head of the column as distillate (D).

$$F = D + R \quad (19)$$

This balance remains to be true if the mole fraction of the most volatile compound in each of these three mixtures is multiplied by its corresponding mixture.

$$F \cdot x_F = D \cdot x_D + R \cdot x_R \quad (20)$$

### 3.3. ADDRESSING THE PROBLEM

Before plotting anything, it is vital to ensure that both latent heats of vapourisation are alike in order to apply the McCabe-Thiele method. This has been calculated applying Antoine correlation with 2 parameters using data from NIST and DECHEMA and the Clausius-Clapeyron equation (equation 10). All these inputs are introduced into Wolfram Mathematica® separated by a semicolon so that the programme displays one unique output which is the print function that shows the value of both latent heats of vapourisation. The user will have to modify both Antoine equations to represent the vapour pressure of the compounds which he works with. Whatever name the user decides to give to both Antoine equations, they must be the same that appear inside the latent heat equation highlighted in yellow and respecting the fact that the variable T stands for temperature. Moreover, the user has the option to change the text in grey inside any print function so that the programme displays whatever he desires. Once the user has built these functions, he must press the shift and enter key at the same time to execute the programme (this is true for any function in Wolfram Mathematica®).

```
(*Vapour pressure equation for both compounds. Pressure is measured in pascals and temperature in kelvin*)
PvMEG[T_] := 1000 Exp[20.41 - 7377 / T];
PvDEG[T_] := Exp[25.66 - 7324 / T];
(*Latent heat of vapourisation using Clausius-Clapeyron equation in J/mol*)
ΔHvapMEG = 8.314 T2 ∂T Log[PvMEG[T]];
ΔHvapDEG = 8.314 T2 ∂T Log[PvDEG[T]];
Print["ΔHvapMEG = ", ΔHvapMEG, " J/mol", " ΔHvapDEG = ", ΔHvapDEG, " J/mol"]
ΔHvapMEG = 61332.4 J/mol ΔHvapDEG = 60891.7 J/mol
```

Figure 17. Code used to calculate both latent heats highlighted in light yellow.

Both values are clearly not identical but can be considered equal enough to proceed with the graphical method. In this case, both latent heats are alike due to both being chemically similar. Nevertheless, more calculations must be done to continue but will additionally help the user to identify if the data introduced in the Antoine equations is correct enough. With the following functions the programme generates a matrix showing the boiling temperature of the mixture at different pressures and compositions. The user can modify the variable  $xMEG_{inc}$  depending on the accuracy required. The matrix is created applying equation 6 so the user must modify it inserting the name given to his Antoine equations. The user also has the option to decide what pressures should be used by changing the values at the end of that same piece of code. Executing this function may take a few seconds since many calculations are being made to generate said matrix. Once the programme displays it, the user can check the boiling point of both pure compounds by going over the information at mole fraction 0 and 1 of the most volatile compound. If these values match the ones provided by official entities, the data introduced in the Antoine equations can be considered correct.

```
(*Molar fraction of MEG ranges from xMEGi to xMEGf and xMEGincr represents the increment*)
xMEGi = 0; xMEGf = 1; xMEGincr = 0.05;
points = (xMEGf - xMEGi) / xMEGincr + 1;
Print["Amount of points = ", points];
|describe
Amount of points = 21.
```

Figure 18. Code used to decide how many compositions the matrix will include.

```
(*Creation of a matrix that shows the boiling temperature of the mixture for different values of pressure and molar fraction of MEG*)
tb =
Quiet[
|silencioso
MatrixForm[Transpose[Table[{P, xMEG, T /. Solve[xMEG PvMEG[T] + (1 - xMEG) PvDEG[T] == P, T, Reals][[1]]], {xMEG, xMEGi, xMEGf, xMEGincr}],
|forma de mat (transposicor) (tabla) (resultado) (numeros reales)
{P, {101320, 80000, 60000, 40000, 20000}}]]]]]
|efor=

```

101320	101320	101320	101320	101320	101320	101320	101320	101320	101320	101320	101320	101320	101320	101320	101320
0.	0.05	0.1	0.15	0.2	0.25	0.3	0.35	0.4	0.45	0.5	0.55	0.6	0.65	0.7	0.75
518.185	511.988	506.827	502.416	498.572	495.172	492.128	489.374	486.864	484.558	482.428	480.449	478.603	476.87	475.24	473.71
80000	80000	80000	80000	80000	80000	80000	80000	80000	80000	80000	80000	80000	80000	80000	80000
0.	0.05	0.1	0.15	0.2	0.25	0.3	0.35	0.4	0.45	0.5	0.55	0.6	0.65	0.7	0.75
509.665	503.681	498.694	494.429	490.711	487.421	484.474	481.808	479.376	477.142	475.078	473.161	471.372	469.65	468.02	466.4
60000	60000	60000	60000	60000	60000	60000	60000	60000	60000	60000	60000	60000	60000	60000	60000
0.	0.05	0.1	0.15	0.2	0.25	0.3	0.35	0.4	0.45	0.5	0.55	0.6	0.65	0.7	0.75
499.662	493.923	489.136	485.04	481.467	478.304	475.469	472.904	470.564	468.413	466.426	464.579	462.856	461.24	459.63	458.02
40000	40000	40000	40000	40000	40000	40000	40000	40000	40000	40000	40000	40000	40000	40000	40000
0.	0.05	0.1	0.15	0.2	0.25	0.3	0.35	0.4	0.45	0.5	0.55	0.6	0.65	0.7	0.75
486.213	480.795	476.271	472.396	469.014	466.018	463.332	460.9	458.68	456.639	454.753	453.	451.363	449.82	448.29	446.76
20000	20000	20000	20000	20000	20000	20000	20000	20000	20000	20000	20000	20000	20000	20000	20000
0.	0.05	0.1	0.15	0.2	0.25	0.3	0.35	0.4	0.45	0.5	0.55	0.6	0.65	0.7	0.75
464.824	459.898	455.778	452.243	449.155	446.416	443.958	441.731	439.697	437.826	436.095	434.486	432.983	431.53	430.13	428.73

Figure 19. Code used to generate the displayed pressure-composition-temperature matrix.

```

(*Creation of a matrix that shows the boiling temperature of the mixture for different values of pressure and
molar fraction of MEG*)
tb =
Quiet[
MatrixForm[Transpose[Table[{P, MEG, T /. Solve[MEG PwMEG[T] + (1 - xMEG) PwDEG[T] = P, T, Reals][[1]]], {xMEG, xMEG1, xMEGf, xMEGincr},
{P, {101320, 80000, 60000, 40000, 20000}}]]]]

```

101320	101320	101320	101320	101320	101320	101320	101320	101320	101320	101320	101320	101320	101320	101320
0.35	0.4	0.45	0.5	0.55	0.6	0.65	0.7	0.75	0.8	0.85	0.9	0.95	1.	1.
489.374	486.864	484.558	482.428	480.449	478.603	476.874	475.248	473.715	472.264	470.888	469.58	468.334	467.144	466.000
80000	80000	80000	80000	80000	80000	80000	80000	80000	80000	80000	80000	80000	80000	80000
0.35	0.4	0.45	0.5	0.55	0.6	0.65	0.7	0.75	0.8	0.85	0.9	0.95	1.	1.
481.888	479.376	477.142	475.078	473.161	471.372	469.695	468.119	466.632	465.225	463.89	462.622	461.412	460.258	459.144
60000	60000	60000	60000	60000	60000	60000	60000	60000	60000	60000	60000	60000	60000	60000
0.35	0.4	0.45	0.5	0.55	0.6	0.65	0.7	0.75	0.8	0.85	0.9	0.95	1.	1.
472.904	470.564	468.413	466.426	464.579	462.856	461.241	459.721	458.288	456.932	455.646	454.422	453.256	452.142	451.074
40000	40000	40000	40000	40000	40000	40000	40000	40000	40000	40000	40000	40000	40000	40000
0.35	0.4	0.45	0.5	0.55	0.6	0.65	0.7	0.75	0.8	0.85	0.9	0.95	1.	1.
460.9	458.68	456.639	454.753	453.	451.363	449.828	448.385	447.023	445.734	444.51	443.347	442.238	441.179	440.164
20000	20000	20000	20000	20000	20000	20000	20000	20000	20000	20000	20000	20000	20000	20000
0.35	0.4	0.45	0.5	0.55	0.6	0.65	0.7	0.75	0.8	0.85	0.9	0.95	1.	1.
441.731	439.697	437.826	436.095	434.486	432.983	431.574	430.247	428.995	427.81	426.685	425.614	424.593	423.618	422.688

Figure 20. Figure showing the rest of the pressure-composition-temperature matrix.

The user can plot a graph showing the information laid out in the matrix with the next piece of code. The variable  $i$  stands for the pressure that will be used. In this case,  $i=1$  means that the data belonging to the atmospheric pressure will be plotted since it is the one corresponding to the first row of the matrix. The next pressure in the list will have a value of 2 for variable  $i$  and so on. The blue curve displays this data while the red one represents the lighter compound's mole fraction of the vapour phase in equilibrium with the liquid phase. Below the blue curve the mixture is totally liquid whereas above the red curve it is totally in vapour phase. In between the curves both phases coexist.

```

(*Construction of a graph showing the boiling temperature of the mixture against the mole fraction of the
lighter compound. The blue curve represents the liquid phase and the red curve represents the vapour phase
in equilibrium with the liquid one*)
i = 1;
Print["pressure = ", tb[[1]][4][[1]][1], " Pa"]
graf1 = ListPlot[Table[{tb[[1]][4][[5]][[2]], tb[[1]][4][[5]][[3]] - 273}, {j, 1, points}], Joined -> True, AxesLabel -> {"x, y of MEG", "T[°C]"},
GridLines -> Automatic];
graf2 = ListPlot[Table[{tb[[1]][4][[5]][[2]], PwMEG[tb[[1]][4][[5]][[3]]], tb[[1]][4][[5]][[3]] - 273}, {j, 1, points}],
Joined -> True, PlotStyle -> Red];
Show[graf1, graf2]

```

Figure 21. Code used to generate the boiling temperature against mole fraction graph.

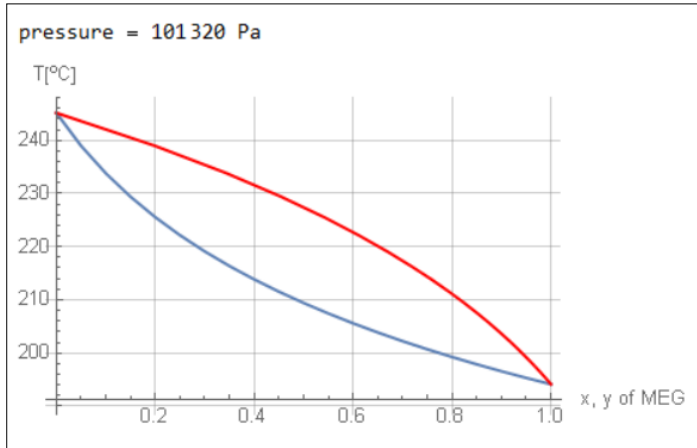


Figure 22. Graph showing the boiling temperature against the mole fraction of the most volatile compound.

The next piece of code uses all the data inside the matrix to find an equation that calculates the boiling temperature of the mixture in which variable  $x$  stands for pressure and variable  $y$  is the mole fraction in the liquid phase of the most volatile compound. The user will have to change the number 5 highlighted in green to match the number of pressures used in the matrix.

```
(*Development of an equation that calculates the boiling temperature of the mixture depending
on the pressure and the mole fraction in the liquid phase of the most volatile compound*)
data =
Partition[Flatten[Table[{tb[[1]][[j]][[1]][[1]], tb[[1]][[j]][[1]][[2]], tb[[1]][[j]][[1]][[3]]},
|particiona |aplana |tabla
{j, 1, 5}, {i, 1, points}], 3];
temperature = Fit[data, {1, x, x^2, y, x y, y^2}, {x, y}]
|ajusta
442.669 + 0.00118961 x - 4.70478 × 10-9 x2 - 73.0921 y - 0.000108049 x y + 36.3489 y2
```

Figure 23. Code used to generate the boiling temperature equation highlighted in red.

This temperature equation is essential to further obtain the temperature of every single plate that comprises the distillation column since these plates are supposed to be operating at the mixture's equilibrium.

The following code generates a graph representing the boiling temperature against mole fraction of the lighter compound for every single pressure the user is working with. These graphs compare the data in the matrix (shown in blue) with the data obtained thanks to the temperature equation (shown in red). The user will once again have to modify the number 5 highlighted in green to match the number of pressures used in the matrix.

```
(*Comparison between the values provided by the matrix in blue and the ones provided by the
above equation in red*)
Clear[x, y]
borra
p = 0;
Do[
  (repte
  p = p + 1;
  temperatura2[x_, y_] = temperature;
  j = tb[[1]][[p]][[1]][[1]];
  Print["pressure = ", j, " Pa"];
  (describe
  Print[Show[ListPlot[Table[{tb[[1]][[p]][[i]][[2]], tb[[1]][[p]][[i]][[3]] - 273}, {i, 1, points}],
  (describe (mue - (representa: |tabla
  ListPlot[Table[{i, temperatura2[j, i] - 273}, {i, xMEGi, xMEGf, xMEGincr}], PlotStyle -> Red)], {5})
  (representa: |tabla (estilo de repr: |rojo
```

Figure 24. Code used to generate the several graphs which show the boiling temperature against the mole fraction of the most volatile compound.

Taking a look at the several graphs plotted, the user should notice an important similarity between both dotted curves such as in the chart shown below. If this is true, the user can proceed to focus on obtaining the McCabe-Thiele diagram.

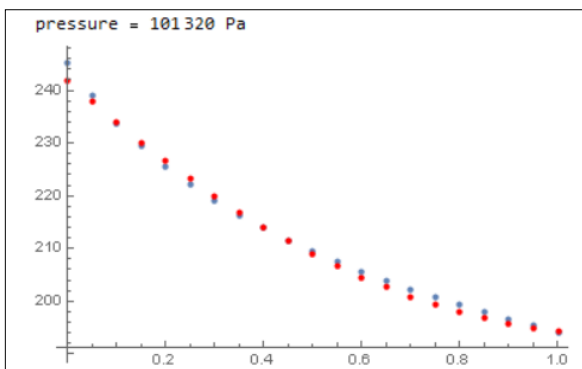


Figure 25. Graph showing the boiling temperature of the mixture at 101320Pa against the mole fraction of the most volatile compound.

To obtain this diagram, the first step consists in plotting a graph that represents the mole fraction of the most volatile component in both phases. The y-axis is used for the vapour phase and the x-axis for the liquid one. Once both axes are established, the function  $y=x$  must be drawn.

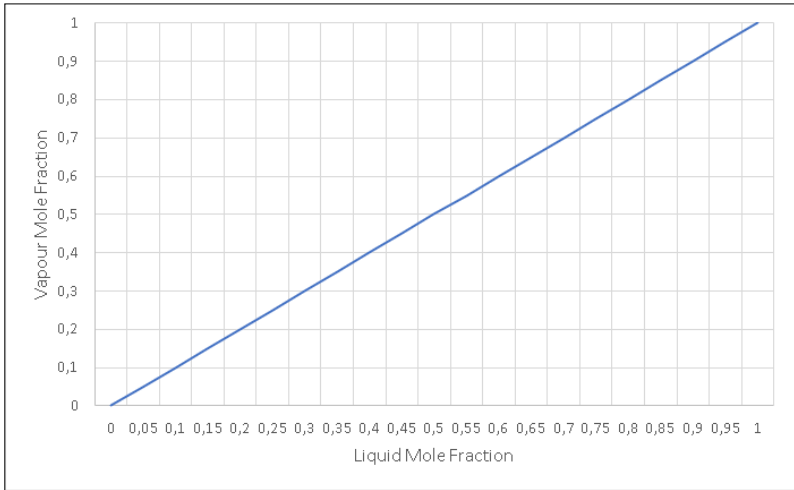


Figure 26. Graph in which the line  $y=x$  has been plotted.

The following step consists in plotting the vapour-liquid equilibrium of the mixture. Nonetheless, to obtain this curve it is necessary to know the value of the relative volatility at the working pressure. This is possible using Wolfram Mathematica© by calculating the mean value of the relative volatility at every single composition for the several pressures specified by the user. Relative volatilities have been obtained through equation 11. The user must introduce his own Antoine equations in the section highlighted in yellow and replace the variable  $T$  with `tb[[1]][[j]][[i]][[3]]` which represents the temperature for pressure  $j$  and composition  $i$  inside the matrix. Once again, the number 5 highlighted in green must be changed to match the number of pressures used in the matrix. Matching these values of  $\alpha$  with their respective pressures and adjusting them to a parabola, the function that explains the dependence of  $\alpha$  with pressure is found. Said function is shown highlighted in grey on top of the resulting curve and will be further used to obtain the McCabe-Thiele diagram.

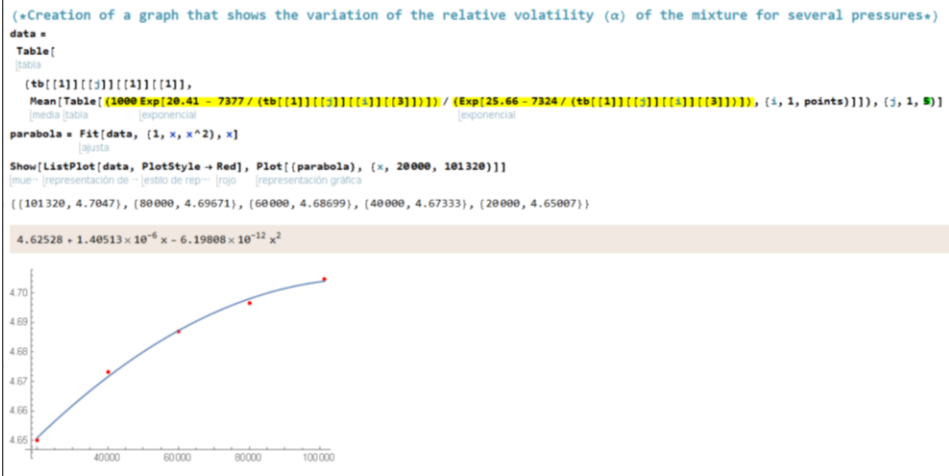


Figure 27. Code used to obtain the relative volatility equation highlighted in grey and the graph plotting this equation.

Observing the resulting graph, it is important to notice that the relative volatility is much greater than one, so this distillation process is totally feasible. It is crucial to check the variation of the relative volatility with pressure since if it is too big, the Antoine equations used are not accurate enough or the mixture is not ideal. In the second case the user will have to build a table that contains values of  $x$  and  $y$  in equilibrium and develop an equation that can relate both variables. Once the value of the relative volatility has been found out, the vapour-liquid equilibrium curve can be plotted using equation 17.



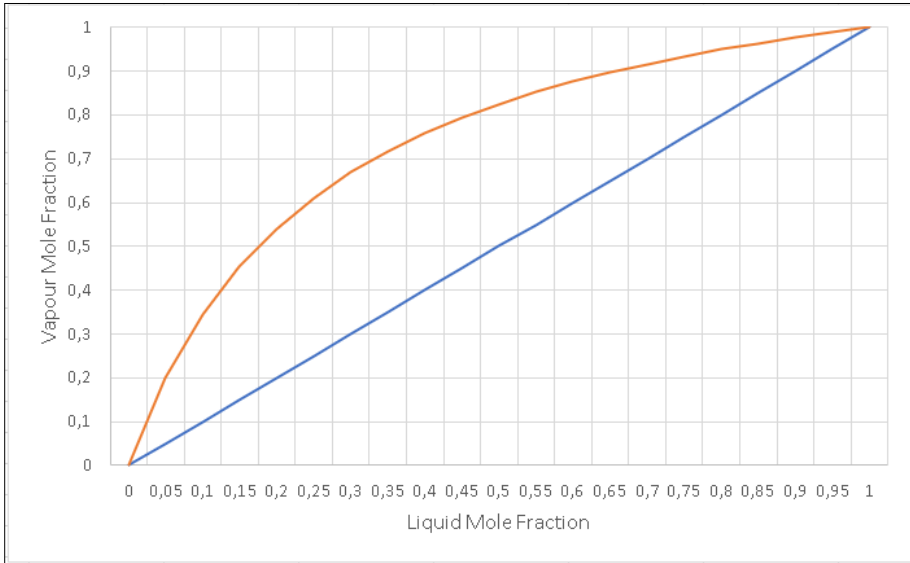


Figure 28. Graph showing the  $y=x$  line and the vapour-equilibrium curve in orange.

At this point it is important to consider which of the following two situations represents the problem faced. In the first case, the reflux ratio is maintained invariable at the expense of obtaining an increasingly poor distillate in the most volatile compound. However, if a distillate with a constant composition is desired, the reflux ratio must be incremented over time. Increasing the reflux ratio enables an enhanced contact between the liquid and vapour phase and as a result, purer distillates can be collected. A downside to this is that the distillate flow rate will diminish since more head product is being redirected into the column again, making the process last longer. Reality is that both cases are extreme since it is not always necessary to maintain one of those two variables intact during the whole process. Nevertheless, assuming that the column operates under one of the two situations greatly simplifies calculations. Having made these two possible conditions clear, it is time to state that the proposed problem corresponds to the second case since it is said that the distillate must constantly contain a 99,5% of MEG.

The operating line of the batch distillation is needed to proceed, although several new material balances must be applied. To start with, the one referred to all the plates forming the column will be developed.

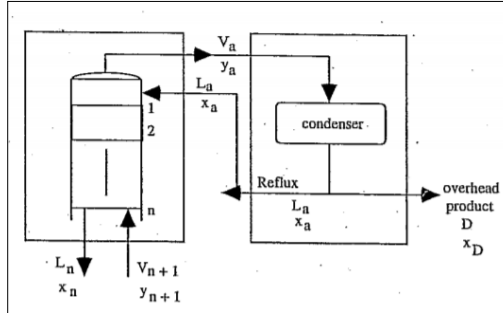


Figure 29. Simple scheme of a distillation column with its condenser.[7]

Observing the upper diagram and following the same notation, the total material balance is as follows:

$$L_a + V_{n+1} = L_n + V_a \quad (21)$$

This same balance referred to the most volatile compound is:

$$L_a \cdot x_a + V_{n+1} \cdot y_{n+1} = L_n \cdot x_n + V_a \cdot y_a \quad (22)$$

Reordering terms, it is possible to find out the operating line:

$$y_{n+1} = \frac{L_n}{V_{n+1}} \cdot x_n + \frac{V_a \cdot y_a - L_a \cdot x_a}{V_{n+1}} \quad (23)$$

However, it can be further simplified with the intention of operating with known variables. To achieve this the material balance on the condenser must be considered:

$$V_a = D + L_a \quad (24)$$

Rearranging terms and referred to the most volatile compound:

$$D \cdot x_D = V_a \cdot y_a - L_a \cdot x_a \quad (25)$$

The material balance applied to the distillation column in conjunction with the condenser must be developed too:

$$V_{n+1} = D + L_n \quad (26)$$

Reordering the equation and referred to the most volatile compound:

$$D \cdot x_D = V_{n+1} \cdot y_{n+1} - L_n \cdot x_n \quad (27)$$

Combining equations 23, 25 and 26 a new form of expressing the operating line is found:

$$y_{n+1} = \frac{L_n}{D + L_n} \cdot x_n + \frac{D \cdot x_D}{D + L_n} \quad (28)$$

Introducing the expression that describes reflux ratio it is possible to simplify the operating line equation to its final form. However, a last assumption must be made which states that there is a constant molar flow rate for both the liquid and vapour phases in the column's interior. Therefore, both currents travelling the entirety of the column can be considered uniform for every single plate. This results in the following equivalence:

$$R_D = \frac{L_a}{D} = \frac{L_n}{D} = \frac{L}{D} \quad (1)$$

Back to equation 28, if both the numerator and the denominator are divided by  $D$  in both sides of the equation, the final form of the operating line is obtained:

$$y_{n+1} = \frac{R_D}{R_D + 1} \cdot x_n + \frac{x_D}{R_D + 1} \quad (29)$$

Where  $\frac{R_D}{R_D + 1}$  corresponds to the slope and  $\frac{x_D}{R_D + 1}$  to the intercept with the  $y$  axis. Since the reflux ratio will constantly change to maintain the distillate composition constant, several operating lines with different slopes and intercepts with the  $y$  axis will be drawn. However, they all have a point in common which corresponds to  $(x_D, x_D)$ . This can be checked if  $x_n$  is substituted by  $x_D$ :

$$y_{n+1} = \frac{R_D}{R_D + 1} \cdot x_D + \frac{x_D}{R_D + 1} = \frac{R_D + 1}{R_D + 1} \cdot x_D = x_D \quad (30)$$

### 3.4. OBTENTION OF RESULTS

With the operating line defined, it is time to run the programme that will enable the user to find out the minimum reflux at any given time to operate the column with a constant distillate composition, the energetic demand of the reboiler, the amount of vapour generated by it and the time needed to carry out the distillation process. If these calculations were to be made by hand, it requires a trial-and-error process until the last stage drawn between the equilibrium curve and the operating line matches the value of the composition in the reboiler in that instant. Observing the interception of the operating line with the  $y$  axis it is possible to find out the reflux using equation 29 and replacing  $x_n$  by zero. However, as this reflux will continually increase, several operating lines that match the constant distillate composition and the decreasing composition at the reboiler must be found. This is simply too much work to be done correctly and in a reduced amount of time, therefore the programme will iterate by its own if some initial values are given and the right commands are typed in. The amount of vapour generated by the reboiler is obtained through integration using the trapezium method, therefore the programme needs at

least a pair of values to obtain said integral. However, using a single trapezium between the feed composition and the final composition in the reboiler is not accurate enough so the programme is built in such a way that will divide the distillation process in several intervals specified by the user. The larger the number of intervals used, the higher the accuracy obtained. Additional information regarding the equations used and the integration method applied to find out the amount of vapour will be discussed further in this essay's section.

To execute the programme, the user will need to introduce all the data mentioned in section 3.1. alongside the relative volatility and boiling temperature equations. The latent heat used in this case is a mean value between both compound's latent heat and rounded to the nearest thousandth. The number of stages that belong to the column and the number of intervals desired must be specified too. In this section of the programme, several relevant information is obtained and displayed in green such as the different mole fractions in the reboiler and the distillate and the amount of moles remaining in the reboiler at the end of the process. This last value has been calculated applying equations 19 and 20.

```
(* Input values *)
(* p = pressure [Pa]; Fm = kg of feed (F); Fp = % of MEG in the feed; Dp = Constant = % of MEG in the distillate (D);
Rp = % of MEG in the reboiler(R); λ = molar latent heat [J/mol]; Q = power of the reboiler [W];
MWMEG = molar mass of MEG;
MWDEG = molar mass of DEG *)

p = 100000;
Fm = 0.50; Fp = 50; Dp = 99.5; Rp = 5; λ = 61000; Q = 500;
MWMEG = 0.062; MWDEG = 0.106;

xF =  $\frac{Fp}{MWMEG}$ ; F =  $\frac{Fm}{MWMEG + (1 - xF) MWDEG}$ ; xD =  $\frac{Dp}{MWMEG}$ ; xR =  $\frac{Rp}{MWMEG}$ ;

Clear[R];
R = R /. NSolve[xR == F xF - (F - R) xD, R][[1]];

(*Introduce the previously calculated relative volatility equation highlighted in grey and replace x by p*)
α = 4.625282642123176 + 1.405129451139797 * 10^-6 p - 6.198082286842811 * 10^-12 p^2;
x[y_] :=  $\frac{y}{y + \alpha - y \alpha}$ 
y[x_] :=  $\frac{\alpha x}{1 + (\alpha - 1) x}$ 

(*Introduce the previously calculated boiling temperature equation highlighted in red*)
temp[x_, y_] := 442.6688229674054 + 0.0011896095099302557 x - 4.704782397480638 * 10^-9 x^2 - 73.09209593852118 y - 0.00010804948352970379 x y +
36.34886072394359 y^2
list = {xx, yy, temp[p, xx] - 273};
listz = {rd1, rd2, V, energy, time};
```

Figure 30. Code showing a part of the inputs introduced into the programme.

```

listv = {xx, int1};
listw = {xx, int2};
(*Introduce the number of intervals desired (INT) to carry out the calculations*)
INT = 10;
INCR = (Fp - Rp) / INT;
Print["Pressure = ", p, " Pa", "   α = ", α]
]escribe
Print["Fm = ", Fm, " kg of F", "   F = ", F, " mol"]
]escribe
Print["Fp = ", Fp, "% of MEG in F", "   xF = ", xF]
]escribe
Print["Dp = ", Dp, "% of MEG in D", "   xD = ", xD]
]escribe
Print["Rp = ", Rp, "% of MEG in R", "   xR = ", xR]
]escribe
Print["Rm = ", R (xR MWMEG + (1 - xR) MWDEG), " kg of R", "   R = ", R, " mol"]
]escribe
Print["λ = ", λ, " J/mol", "   Q = ", Q/1000, " kW"]
]escribe
Print["Increment = ", INCR, "% of MEG"]
]escribe
(*Introduce the desired amount of plates (ne) considering one more stage will be added during the calculations
since the column is operating batch-wise*)
ne = 10; rd1 = 0.5; rd2 = 2;
Rp = Fp - INCR;
int1 =  $\frac{1}{(xF - xD)^2 \left(1 - \frac{rd1}{rd1+1}\right)}$ ; int2 =  $\frac{1}{(xR - xD)^2 \left(1 - \frac{rd2}{rd2+1}\right)}$ ;

```

Figure 31. Code showing the rest of the inputs introduced.

$$V = F (xF - xD) \left( \frac{int1 + int2}{2} \right) (xR - xF); \text{ energy} = V \lambda / (3600000); \text{ time} = \left( \frac{V \lambda}{Q} \right) / 3600;$$

Pressure = 100000 Pa    α = 4.70381

Fm = 0.5 kg of F    F = 6.39075 mol

Fp = 50% of MEG in F    xF = 0.630952

Dp = 99.5% of MEG in D    xD = 0.997069

Rp = 5% of MEG in R    xR = 0.0825545

Rm = 0.261905 kg of R    R = 2.55847 mol

λ = 61000 J/mol    Q =  $\frac{1}{2}$  kW

Increment =  $\frac{9}{2}$  % of MEG

Figure 31. Code showing the final inputs and displaying the most relevant ones.

Once all the inputs have been entered and executed, the next piece of code shown in the appendix generates a list of values for all the intervals specified including the compositions and temperatures of each plate alongside the reflux ratio at which the column operates. It also displays the amount of vapour generated by the reboiler, the energetic demand required to make it operate and the time spent to cover that interval. It finally includes both values (named *int1* and *int2*) used to integrate and the amount of error made between the theoretical value of the composition in the feed or in the reboiler and the one obtained. Notice how the values belonging to the second part of an interval are the same to the ones belonging to the first part of the next interval. This makes sense since the trapeziums used to integrate are located one next to each other without leaving any space in between them. This explanation applied to this specific problem means that each interval is like a separate distillation in which the composition in the reboiler at the end of the process for one interval is the composition of the feed for the next interval. This long piece of code is hard to follow so the following block diagram is included for better understanding.

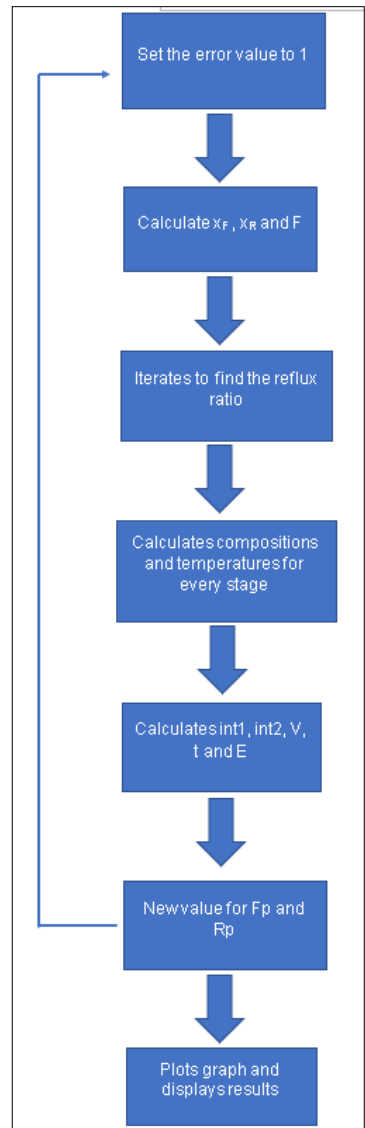


Figure 32. Block diagram describing how the code works.

The programme basically iterates until it finds the exact reflux ratio that gives a feed composition almost the same than its theoretical value. Once the reflux ratio is obtained, it calculates the composition of every stage alongside its temperature. The same procedure is repeated for the composition in the reboiler. Then the programme calculates the amount of vapour, the energy required and the time spent. With the first interval completed, the programme repeats the whole process with the next compositions in the feed and the reboiler as many times as intervals the user has set. Once the programme has reached the real composition in the reboiler at the end of the entire process, the calculations have come to an end. All the values calculated in this piece of code are displayed at once and in order alongside a McCabe-Thiele diagram showing the stages at the beginning and at the end of the process as a way of comparison. In figure 33 some results obtained are shown:

r/d1 = 0.468463			r/d1 = 1.77298		
1	xr = 0.986363	y = 0.997069 T(°C) = 194.193	1	xr = 0.986363	y = 0.997069 T(°C) = 194.193
2	x = 0.970835	y = 0.993654 T(°C) = 194.391	2	x = 0.955622	y = 0.990224 T(°C) = 194.602
3	x = 0.948982	y = 0.9887 T(°C) = 194.7	3	x = 0.875169	y = 0.970569 T(°C) = 195.998
4	x = 0.919503	y = 0.981729 T(°C) = 195.171	4	x = 0.707278	y = 0.919129 T(°C) = 200.427
5	x = 0.881924	y = 0.972325 T(°C) = 195.863	5	x = 0.478331	y = 0.811784 T(°C) = 209.768
6	x = 0.837326	y = 0.960336 T(°C) = 196.817	6	x = 0.297147	y = 0.6654 T(°C) = 219.862
7	x = 0.788685	y = 0.946109 T(°C) = 198.023	7	x = 0.205952	y = 0.549555 T(°C) = 225.845
8	x = 0.740282	y = 0.930591 T(°C) = 199.394	8	x = 0.170316	y = 0.491247 T(°C) = 228.347
9	x = 0.696319	y = 0.91515 T(°C) = 200.787	9	x = 0.1578	y = 0.468463 T(°C) = 229.248
10	x = 0.659579	y = 0.901125 T(°C) = 202.059	10	x = 0.153571	y = 0.46046 T(°C) = 229.555
11	x = 0.630951	y = 0.889405 T(°C) = 203.117	11	x = 0.152161	y = 0.457756 T(°C) = 229.658
xF = 0.630951 xF = 0.630952 (error = 0.00275691 %)			xF = 0.152161 xF = 0.152161 (error = 0.00283012 %)		
r/d2 = 0.499694			r/d2 = 3.26275		
1	xr = 0.986363	y = 0.997069 T(°C) = 194.193	1	xr = 0.986363	y = 0.997069 T(°C) = 194.193
2	x = 0.970153	y = 0.993502 T(°C) = 194.4	2	x = 0.949739	y = 0.988875 T(°C) = 194.688
3	x = 0.946392	y = 0.988101 T(°C) = 194.739	3	x = 0.83914	y = 0.960842 T(°C) = 196.776
4	x = 0.913161	y = 0.980184 T(°C) = 195.28	4	x = 0.600716	y = 0.876189 T(°C) = 204.3
5	x = 0.869622	y = 0.969111 T(°C) = 196.112	5	x = 0.324994	y = 0.693697 T(°C) = 218.155
6	x = 0.817202	y = 0.954604 T(°C) = 197.296	6	x = 0.165512	y = 0.482657 T(°C) = 228.692
7	x = 0.760152	y = 0.937138 T(°C) = 198.811	7	x = 0.107054	y = 0.360588 T(°C) = 233.017
8	x = 0.704501	y = 0.918129 T(°C) = 200.517	8	x = 0.0893731	y = 0.315844 T(°C) = 234.374
9	x = 0.655716	y = 0.899586 T(°C) = 202.198	9	x = 0.0843472	y = 0.30231 T(°C) = 234.764
10	x = 0.6168	y = 0.883331 T(°C) = 203.663	10	x = 0.0829442	y = 0.298463 T(°C) = 234.873
11	x = 0.588027	y = 0.870365 T(°C) = 204.817	11	x = 0.0825545	y = 0.297389 T(°C) = 234.904
xR = 0.588027 xR = 0.588027 (error = 0.00116035 %)			xR = 0.0825545 xR = 0.0825545 (error = 0.0000873998 %)		
$\text{int1} = \frac{1}{(x_F - x_D)^2 \left(1 - \frac{rd1}{rd1+1}\right)} = 10.9553$			$\text{int1} = \frac{1}{(x_F - x_D)^2 \left(1 - \frac{rd1}{rd1+1}\right)} = 3.88443$		
$\text{int2} = \frac{1}{(x_R - x_D)^2 \left(1 - \frac{rd2}{rd2+1}\right)} = 8.96328$			$\text{int2} = \frac{1}{(x_R - x_D)^2 \left(1 - \frac{rd2}{rd2+1}\right)} = 5.09692$		
V' = 1.00025 mol			V' = 1.32975 mol		
energetic demand = 0.0169488 kWh			energetic demand = 0.0225318 kWh		
time = $\frac{V\lambda}{Q} = 0.0338975$ h			time = $\frac{V\lambda}{Q} = 0.0450636$ h		

Figure 33. Displaying some of the results obtained.



Values on the left correspond to the first interval whilst the ones on the right belong to the last interval. Notice how the system consists of eleven stages and not ten since the reboiler in a batch distillation adds one more stage to the process. Regarding the error present in the calculations, it is so small that the values displayed can be considered almost exact. It is clear that the reflux ratio keeps increasing as the reboiler is getting poorer in the most volatile compound to maintain a constant distillate composition. This can be seen in figure 34.

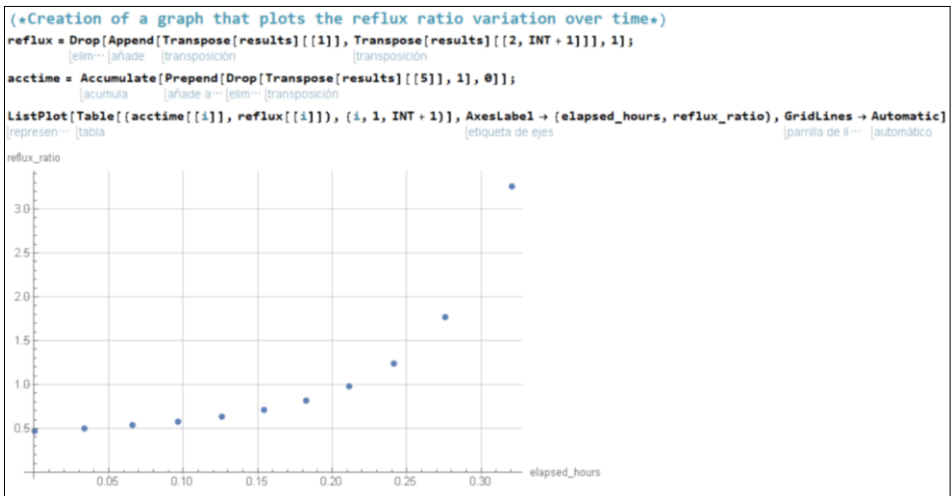


Figure 34. Code used to generate the graph plotting reflux ratio against time.

Observing the temperatures at which the stages operate, notice how they rise as they get poorer in the most volatile compound but never reach the boiling temperature of the least volatile compound in order to avoid its evaporation. These temperatures have been obtained applying the boiling temperature equation. However, stage 1 remains unchanged all along the process since a constant distillate composition is desired. The liquid composition labelled as  $x_r$  corresponds to the composition of the reflux that returns to the system through the head of the column. A comparison between the first and last stage through the whole process can be easily perceived in figure 35. The variables related to the last stage are shown to the right and it can be observed how the stage gets constantly warmer and poorer in the most volatile compound whilst the first stage shown to the left does not vary at all.

( x )	( 0.986363 )	( 0.630951 )
( y )	( 0.997069 )	( 0.889405 )
( T )	( 194.193 )	( 203.117 )
( x )	( 0.986363 )	( 0.588027 )
( y )	( 0.997069 )	( 0.870365 )
( T )	( 194.193 )	( 204.817 )
( x )	( 0.986363 )	( 0.542976 )
( y )	( 0.997069 )	( 0.84822 )
( T )	( 194.193 )	( 206.744 )
( x )	( 0.986363 )	( 0.495641 )
( y )	( 0.997069 )	( 0.822143 )
( T )	( 194.193 )	( 208.929 )
( x )	( 0.986363 )	( 0.445844 )
( y )	( 0.997069 )	( 0.790989 )
( T )	( 194.193 )	( 211.402 )
( x )	( 0.986363 )	( 0.393386 )
( y )	( 0.997069 )	( 0.753111 )
( T )	( 194.193 )	( 214.203 )
( x )	( 0.986363 )	( 0.33805 )
( y )	( 0.997069 )	( 0.706071 )
( T )	( 194.193 )	( 217.374 )
( x )	( 0.986363 )	( 0.279584 )
( y )	( 0.997069 )	( 0.646079 )
( T )	( 194.193 )	( 220.967 )
( x )	( 0.986363 )	( 0.217723 )
( y )	( 0.997069 )	( 0.566943 )
( T )	( 194.193 )	( 225.039 )
( x )	( 0.986363 )	( 0.152161 )
( y )	( 0.997069 )	( 0.457756 )
( T )	( 194.193 )	( 229.658 )
( x )	( 0.986363 )	( 0.0825545 )
( y )	( 0.997069 )	( 0.297389 )
( T )	( 194.193 )	( 234.904 )

Figure 35. Matrix comparing the first and last stage of the column throughout the whole process.

The resultant McCabe-Thiele diagram is as follows. Notice how the operating line in green has changed drastically due to the increase in the reflux ratio over time. The operating line with the least slope corresponds to the first instant of the distillation process and although the different stages cannot be distinguished clearly, it is possible to perceive how the last stage has the same composition as the feed entering the column. In contrast, the other operating line describes the end of the process and therefore the last stage has the same composition as the composition specified to remain in the reboiler. Taking a closer look at the last stages of the column, they all have compositions which are way too proximate to one another therefore some plates are redundant. This can be seen clearly by reading the values in figure 33. The user can determine how many theoretical stages are strictly necessary by running the programme with a lower number of stages. As long as the programme runs without giving an error message, the user can still try to reduce the number of plates. In this case five plates (six stages) are enough. Nevertheless, reducing costs in building a smaller column implies a higher investment in energy and a longer time to distillate.

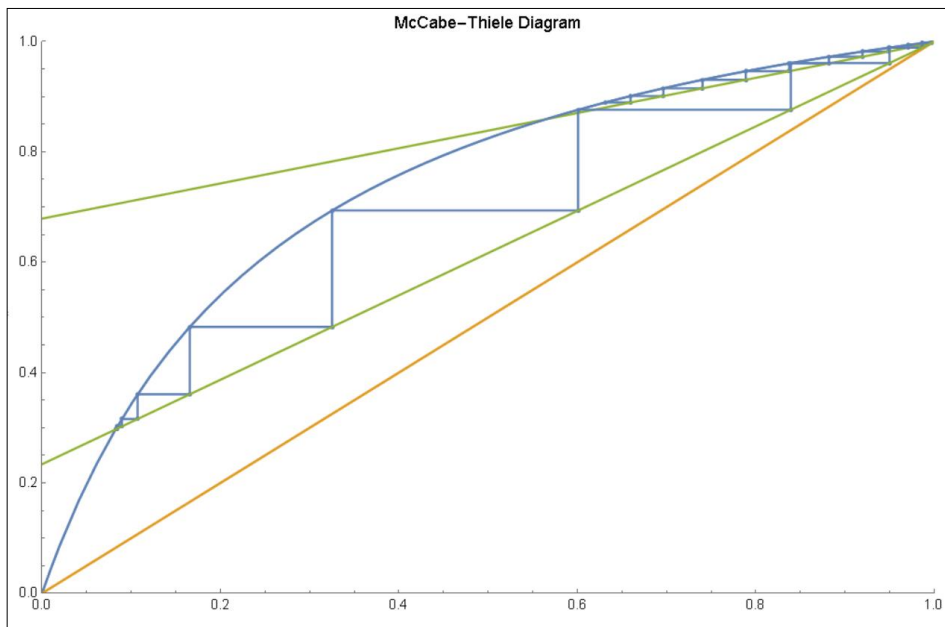


Figure 36. Resultant McCabe-Thiele diagram for the first and last interval.

The final step consists in processing the information obtained to calculate the amount of vapour generated by the reboiler during the whole distillation process, the amount of energy used and the time spent. However, to do this a new equation must be developed with the aid of three other expressions, the first of which is already known. Merging equations 19 and 20 the following is obtained:

$$x_D(F - R) = F \cdot x_F - R \cdot x_R \quad (31)$$

The following equation describes the variance in the residue's composition. Notice how the negative sign implies a decrease in the amount of the most volatile compound remaining in the residue.

$$dR = -D \cdot dt \quad (32)$$

Multiplying by their respective mole fractions:

$$-d(R \cdot x_R) = x_D \cdot D \cdot dt \quad (33)$$

Joining these two last equivalences and developing the product of both derivatives the next expression is obtained:

$$\frac{dR}{R} = \frac{dx_R}{x_D - x_R} \quad (34)$$

At this point, only one more equation is required to calculate the vapour generated by the reboiler. This can be expressed as:

$$dV' = V \cdot dt \quad (35)$$

Where  $V'$  represents the amount of vapour in mols and  $V$  in this case is the power expressed as the quantity of heat supplied to the reboiler per unit of time. Dividing the above expression by equation 32 results in the following equivalence:

$$\frac{dV'}{dR} = -\frac{V}{D} = -\frac{V}{V-L} \quad (36)$$

Isolating  $dV'$  and dividing both the numerator and the denominator by  $V$ :

$$dV' = -\frac{dR}{1 - L/V} \quad (37)$$

Bearing in mind that  $L/V$  corresponds to the slope of the operating line, this equation can finally be expressed as:

$$dV' = -\frac{dR}{1 - \frac{R_D}{R_D + 1}} \quad (38)$$

Combining equations 31, 34 and 38 the final equivalence to calculate the amount of vapour generated is obtained:

$$V' = F(x_F - x_D) \int_{x_F}^{x_R} \frac{dx_R}{(x_R - x_D)^2 \cdot \left(1 - \frac{R_D}{R_D + 1}\right)} \quad (39)$$

The way of integrating has been using trapeziums. This method is based in dividing the area below the curve into several trapeziums one next to each other. By calculating the area of all the trapeziums and adding them up, the value of the integral is obtained. As a reminder, the area of a trapezium is the following:

$$A = \left(\frac{a + b}{2}\right) \cdot h \quad (40)$$

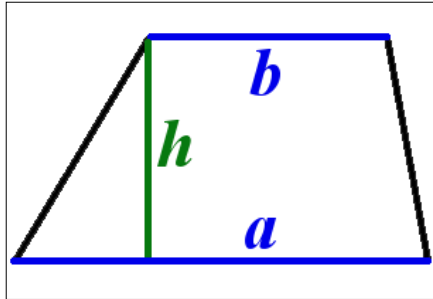


Figure 37. Diagram of a trapezium remarking its both bases and height.

Applying this to the addressed case and looking at figure 38, both trapezium's bases are  $int1$  and  $int2$  where the first one corresponds to the value inside the integral that relates the distillate with the feed while the latter stands for the one relating the distillate with the residue. The trapezium's height is the product resulting from subtracting the feed composition from the residue composition. Considering all the above stated and equation 39, the amount of vapour has been obtained in the following manner:

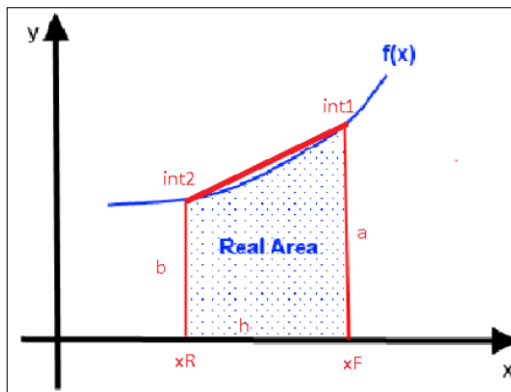


Figure 38. Diagram showing the trapezium formed by the curve.

$$int1 = \frac{1}{(x_F - x_D)^2 \left(1 - \frac{rd1}{rd1 + 1}\right)} \quad (41)$$

$$int2 = \frac{1}{(x_R - x_D)^2 \left(1 - \frac{rd2}{rd2 + 1}\right)} \quad (42)$$

$$V' = F(x_F - x_D) \left(\frac{int1 + int2}{2}\right) (x_R - x_F) \quad (43)$$

Now it is possible to obtain the amount of energy required to run the reboiler by applying the following simple equation:

$$E = V \cdot \lambda \cdot t \quad (44)$$

Where E is the energy demand in kWh and t stands for time in seconds. Applying the right conversion factors E is obtained in the desired units:

```
Print["energetic demand = ", Vλ / (3 600 000), " kWh"]
escribe
```

Finally, the total time required to run the whole distillation process can be calculated in the following way:

$$t = \frac{V \cdot \lambda}{Q} \quad (45)$$

Where Q is the power of the reboiler in W. Applying once again the precise conversion factors the duration of the process in hours is obtained:

$$\text{Print} \left[ \text{"time"} = \frac{V\lambda}{Q} = \text{"}, \left( \frac{V\lambda}{Q} \right) / 3600, \text{" h"} \right]$$

Since the programme operates using intervals, once all the results are obtained it is necessary to add them all up to know the total amount of vapour, energy and time. The following piece of code generates a matrix that includes all the reflux ratios alongside all the partial values of vapour, energy and time.

```
(*Generation of a matrix which contains all the different reflux ratios along with the
amount of vapour used, the energy needed and the time required in those lapses*)

list = Drop[list, 3]; listz = Drop[listz, 5];
results = Prepend[Partition[listz, 5], {"rd1", "rd2", "V", "energy", "time"}];
MatrixForm[Transpose[results]]

MatrixForm=
(
rd1 0.468463 0.499689 0.536266 0.580683 0.63693 0.711729 0.817158 0.976955 1.24458 1.77298
rd2 0.499694 0.536266 0.580683 0.63693 0.711729 0.817158 0.976955 1.24458 1.77298 3.26275
V 1.00025 0.943668 0.899015 0.865596 0.843935 0.836309 0.848197 0.892418 1.0042 1.32975
energy 0.0169488 0.0159899 0.0152333 0.014667 0.0143 0.0141708 0.0143722 0.0151215 0.0170157 0.0225318
time 0.0338975 0.0319799 0.0304666 0.0293341 0.0286 0.0283416 0.0287445 0.0302431 0.0340313 0.0450636
)
```

Figure 39. Code used to generate the matrix containing all the reflux ratios and partial values of vapour, energy and time.

The next piece of code sums up all the partial values and displays the definitive results in a clear way for the user. The fact that the amount of vapour moles generated is larger than the amount of moles introduced as feed makes sense since the condensed reflux will be vapourised again.



```
(*Addition to show the total vapour generated, energy demand and time*)
Total[Drop[Transpose[results][[3]], 1]]; Print["Total vapour generated = ", Total[Drop[Transpose[results][[3]], 1]], " mol"]
Total[Drop[Transpose[results][[4]], 1]];
Print["Total energy demand = ", Total[Drop[Transpose[results][[4]], 1]], " kWh"];
Total[Drop[Transpose[results][[5]], 1]];
Print["Total time = ", Total[Drop[Transpose[results][[5]], 1]], " hours"]

Total vapour generated = 9.46334 mol
Total energy demand = 0.160351 kWh
Total time = 0.320702 hours
```

Figure 40. Code used to display the values of total vapour generated, energy used and time spent.

Working with several intervals can be justified by plotting a graph showing  $int_1$  and  $int_2$  against the composition in the reboiler. Taking a look at the figure below, the function draws a parabola so using a single trapezium would increase the area used to integrate by a considerable amount thus obtaining bigger amounts of vapour, energy and time. This has an economical implication since the industry operating with this column would be wasting resources and time unnecessarily. Therefore, it is highly recommended to execute the programme with several intervals in order to improve efficiency.

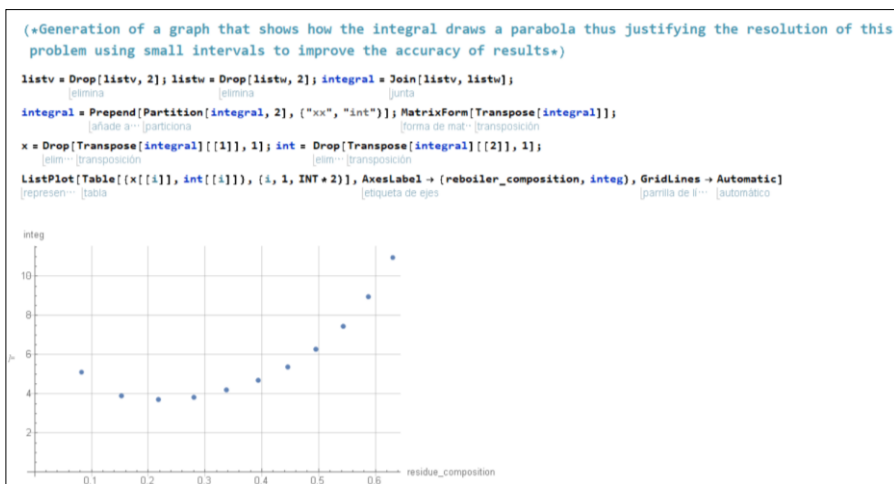


Figure 41. Code used to plot the graph showing how the value inside the integral varies with the composition.

### 3.5. ADDITIONAL SCENARIO

Apart from this previous case thoroughly addressed, an additional situation has been considered and solved. In this scenario, the distillation column is already built and the main issue to solve is the tray efficiency. Said column operates batch-wise at 100000Pa and consists of ten plates. The reboiler is connected to a vacuum to ensure that the pressure inside the column is as desired. However, the total number of stages is twelve since both the reboiler and the partial condenser included add one more stage to the system. In addition, the column has a total condenser where the distillate is really collected. The partial condenser operates with a tank filled with glycol and a pair of external refrigerators since the column is too hot whereas the total condenser is connected to a water refrigerator. The reboiler has a theoretical power of 700W but bearing in mind that some heat is lost, 500W is a more accurate value. Nonetheless, the column is covered with isolating material and aluminium foil to minimize the amount of heat dissipated. Temperatures inside the reboiler and at various plates can be tracked through the monitors. Both compounds used are the same as in the previous distillation though this time the percentage of MEG in the feed is of 13% in weight. The amount of mixture fed into the column is 2,09kg. The sample extracted from the partial condenser indicates a 96,8% w/w of MEG. Both compositions from the feed and the distillate have been obtained using a gas chromatograph and all the data has been provided by the tutor of this essay Dr. Llorens. These two mixtures from the partial condenser and the reboiler are supposed to be in perfect equilibrium whereas the trays inside the column operate at a limited efficiency.



Figure 42. Assemblage of the whole distillation column.

The way to calculate this value has been developing a programme in Wolfram Mathematica® and using the Murphree efficiency which is explained now. All the mentioned variables are introduced alongside the same relative volatility and temperature equations since the compounds are the same. A slight variation of equations 14 and 15 is applied where an efficiency factor (f) is multiplied by the relative volatility to represent the real vapour-liquid equilibrium curve followed by the plates. The programme then displays the values of the most important variables.

```
(* Input values *)
(* p = pressure [Pa]; Fm = kg of feed (F); Fp = % of MEG in the feed; Dp = Constant = % of MEG in the distillate (D);
Rp = % of MEG in the reboiler(R); λ = molar latent heat [J/mol]; Q = power of the reboiler [W]; MwMEG = molar mass of MEG;
MwDEG = molar mass of DEG; c = % of MEG in the last stage*)
p = 100000;
Fm = 2.09; Fp = 13; c = 96.8; f = 0.365;
MwMEG = 0.062; MwDEG = 0.106;
(*Introduce the previously calculated relative volatility equation highlighted in grey and replace x by p*)
α = 4.625282642123176 + 1.405129451139297 * 10^-6 p - 6.198082280842811 * 10^-12 p^2;
(*Introduce the previously calculated equilibrium temperature equation highlighted in red*)
temp[x_, y_] := 442.6688229674054 + 0.0011896095099302557 x - 4.704782397480638 * 10^-9 x^2 - 73.09209593852118 y - 0.00010804948392970379 x y + 36.348860722394359
x1[y_] :=

$$\frac{y}{y + \alpha - y\alpha}$$

y1[x_] :=

$$\frac{\alpha x}{1 + (\alpha - 1)x}$$

x2[y_] :=

$$\frac{y}{y + f\alpha - yf\alpha}$$

y2[x_] :=

$$\frac{f\alpha x}{1 + (f\alpha - 1)x}$$

Dp =

$$\frac{100 \text{ MwMEG } y1\left[\frac{c}{\text{MwDEG} + (100 - c)}\right]}{\text{MwDEG} \left(1 - y1\left[\frac{c}{\text{MwDEG} + (100 - c)}\right]\right) + \text{MwMEG } y1\left[\frac{c}{\text{MwDEG} + (100 - c)}\right]}$$

xF =

$$\frac{Fp}{\text{MwMEG}}$$
; F =

$$\frac{Fm}{xF \text{ MwMEG} + (1 - xF) \text{ MwDEG}}$$
; xD =

$$\frac{Dp}{\text{MwMEG}}$$

Print["Pressure = ", p, " Pa", " α = ", α]
Print["Fm = ", Fm, " kg of F", " F = ", F, " mol"]
Print["Fp = ", Fp, "% of MEG in F", " xF = ", xF]
Print["dp = ", Dp, "% of MEG in D", " xd = ", xD]
```

Figure 43. Code used to input all the key variables.

```
Print["Pressure = ", p, " Pa", " α = ", α]
Print["Fm = ", Fm, " kg of F", " F = ", F, " mol"]
Print["Fp = ", Fp, "% of MEG in F", " xF = ", xF]
Print["dp = ", Dp, "% of MEG in D", " xd = ", xD]
```

Pressure = 100000 Pa α = 4.70381

Fm = 2.09 kg of F F = 21.536 mol

Fp = 13% of MEG in F xF = 0.203485

dp = 99.3021% of MEG in D xd = 0.995906

Figure 44. Code used to display the key variables to the user.

The column operates at total reflux therefore no distillate is collected through the total condenser. To achieve a correct performance the mixture in the partial condenser is subcooled at first and then the refrigerating water flow rate is constantly decreased until the first droplet of distillate is collected in the total condenser. At this point the mixture inside the partial condenser is in equilibrium so the water flow rate is increased by a very small amount to avoid collecting any distillate at all. Both phases being in equilibrium enables the user to apply the McCabe-Thiele method with total confidence.

Since total reflux is being applied to the column, an incredibly high value (infinity is not possible) should be introduced into the programme as the reflux ratio. However, a value such as 200 is already high enough and because the reflux ratio is a known value, the programme does not need to iterate to obtain the compositions of the trays. Therefore, using the operation line and the temperature equation and applying equation 17 the programme displays the compositions and temperatures of all the stages bearing in mind that the first and last stage operate at a perfect equilibrium. Notice how the compositions are expressed in mole and weight fraction.

r/d1 = 200						
1	xr = 0.981031	y = 0.995906	T(°C) = 195.625	w/w% in liquid phase = 96.8	w/w% in vapour phase = 99.3021	
2	x = 0.967993	y = 0.981105	T(°C) = 196.719	w/w% in liquid phase = 94.6494	w/w% in vapour phase = 96.8123	
3	x = 0.946508	y = 0.968132	T(°C) = 198.522	w/w% in liquid phase = 91.1891	w/w% in vapour phase = 94.6721	
4	x = 0.911943	y = 0.946754	T(°C) = 201.421	w/w% in liquid phase = 85.8306	w/w% in vapour phase = 91.2281	
5	x = 0.858428	y = 0.912361	T(°C) = 205.911	w/w% in liquid phase = 78.0055	w/w% in vapour phase = 85.8939	
6	x = 0.7803	y = 0.859112	T(°C) = 212.466	w/w% in liquid phase = 67.5049	w/w% in vapour phase = 78.1021	
7	x = 0.6755	y = 0.781373	T(°C) = 221.258	w/w% in liquid phase = 54.9057	w/w% in vapour phase = 67.6422	
8	x = 0.549817	y = 0.677094	T(°C) = 231.803	w/w% in liquid phase = 41.6691	w/w% in vapour phase = 55.0859	
9	x = 0.417848	y = 0.552037	T(°C) = 242.875	w/w% in liquid phase = 29.5688	w/w% in vapour phase = 41.8873	
10	x = 0.297273	y = 0.420724	T(°C) = 252.99	w/w% in liquid phase = 19.8353	w/w% in vapour phase = 29.8153	
11	x = 0.200327	y = 0.300749	T(°C) = 261.124	w/w% in liquid phase = 12.78	w/w% in vapour phase = 20.1003	
12	x = 0.0517548	y = 0.204285	T(°C) = 273.589	w/w% in liquid phase = 3.09363	w/w% in vapour phase = 13.0559	

Figure 45. Compositions and temperatures of each stage displayed to the user.

The next instruction plots the McCabe-Thiele diagram and displays a comparison between the theoretical value of the composition in the reboiler and the one obtained through the calculations previously mentioned. Although it is extremely difficult to perceive, the operation line in red is almost overlapping the diagonal line in green. The orange curve represents the pseudo equilibrium present in the trays, while the blue curve is exclusive to the first and last stage due to them operating at the perfect equilibrium. To obtain the tray's efficiency, the

programme must be executed with different values of the efficiency factor until both feed compositions are similar enough. In this case, a value of  $f = 0,365$  gave the best results with a variation in both compositions of only 0,003. Therefore, the plates present in the distillation column operate at an efficiency of 36,5%.

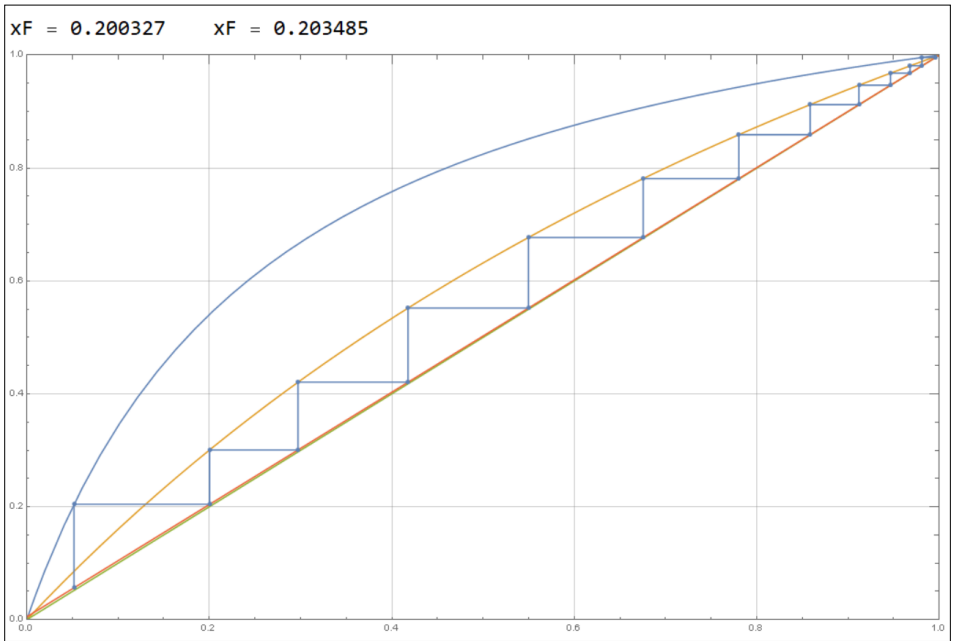


Figure 46. McCabe-Thiele diagram for all the stages forming the column and a comparison between the theoretical and calculated feed composition.



## 4. CONCLUSIONS

Several conclusions can be drawn from this assignment, the first and most fundamental being the fact that Wolfram Mathematica® is a powerful software which enables to simulate any binary distillation desired by the user, among infinitely other scenarios unrelated with a distillation process. In addition, it has been proven that Wolfram Mathematica® provides truly accurate results in both theoretical and practical problems. A non-expert user can feel overwhelmed at first when operating with this programme, but following the clear instructions given the interface becomes friendly. Finally, regarding my personal knowledge, this assignment has been useful in helping me apply everything I knew about distillation processes into Mathematica®, since I had never used it to solve this type of problems.





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## ACRONYMS

$\alpha$ : Relative volatility (-)

$\Delta H^{\text{vap}}$ : Latent heat of vapourisation (J/mol)

$\lambda$ : Latent heat of vapourisation (J/mol)

Atm: Atmospheres

°C: Degree Celsius

cm<sup>3</sup>: Cubic centimetre

D: Distillate flow rate (mol/s)

DEG: Diethylene glycol

E: Energy consumed (J)

F: Amount of feed (mol)

f: Murphree efficiency factor (-)

g: Grams

$\gamma$ : Activity coefficient (-)

h: Hours

J: Joules

K: Degree Kelvin or Equilibrium Constant

kg: Kilograms

kWh: Kilowatt-hour

L: Liquid flow rate (mol/s)

MEG: Monoethylene glycol

$N_a$ : Actual number of trays

$\eta_o$ : Overall tray efficiency (-)

$N_t$ : Theoretical number of trays

P: Total pressure (Pa)

p: Partial pressure (Pa)

P<sup>0</sup>: Vapour pressure (Pa)

Pa: Pascals

Q: Power of the reboiler (W)

R: Universal gas constant (J/K.mol)

R<sub>D</sub>: Reflux ratio (-)

s: Seconds

T: Temperature (°C)

t: Time (s)

V: Vapour flow rate (mol/s)

V': Amount of vapour the reboiler is generating (mol)

W: Watts

X<sub>D</sub>: Mole fraction of the distillate in the liquid phase (-)

X<sub>F</sub>: Mole fraction of the feed in the liquid feed (-)

X<sub>R</sub>: Mole fraction of the residue in the liquid phase (-)

X<sub>r</sub>: Mole fraction of the reflux in the liquid phase (-)

y: Mole fraction in the vapour phase (-)

# APPENDICES



# APPENDIX 1: THEORETICAL DISTILLATION COLUMN

(\*This function terminates the kernel losing all the current definitions. It is recommended to execute it at the beginning of the process\*)

```

In[7]= Quit[]
[deten núcleo del sistema]

(*Vapour pressure equation for both compounds. Pressure is measured in pascals and temperature
in kelvin*)

In[1]= PvMEG[T_] := 1000 Exp[20.41 - 7377 / T];
[exponencial]
PvDEG[T_] := Exp[25.66 - 7324 / T];
[exponencial]

(*Latent heat of vapourisation using Clausius-Clapeyron equation in J/mol*)
ΔHvapMEG = 8.314 T2 ∂T Log[PvMEG[T]];
[logaritmo]
ΔHvapDEG = 8.314 T2 ∂T Log[PvDEG[T]];
[logaritmo]

Print["ΔHvapMEG = ", ΔHvapMEG, " J/mol", " ΔHvapDEG = ", ΔHvapDEG, " J/mol"]
[describe]

ΔHvapMEG = 61332.4 J/mol ΔHvapDEG = 60891.7 J/mol

(*Molar fraction of MEG ranges from xMEGi to xMEGf and xMEGincr represents the increment*)

In[6]= xMEGi = 0; xMEGf = 1; xMEGincr = 0.05;
points = (xMEGf - xMEGi) / xMEGincr + 1;
Print["Amount of points = ", points];
[describe]

Amount of points = 21.

(*Creation of a matrix that shows the boiling temperature of the mixture for different
values of pressure and molar fraction of MEG*)

In[9]= tb =
Quiet[]
[silencioso]
MatrixForm[Transpose[Table[{P, xMEG, T /. Solve[xMEG PvMEG[T] + (1 - xMEG) PvDEG[T] == P, T, Reals][[1]]},
[forma de matriz [transposición] [tabla] [resuelve] [números reales]
{xMEG, xMEGi, xMEGf, xMEGincr}, {P, {101320, 80000, 60000, 40000, 20000}}]]]]

```



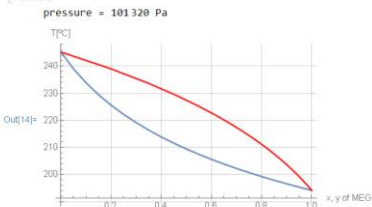


```
Out[9]/MatrixForm=
( 101 320 ( 101 320 ( 101 320 ( 101 320 ( 101 320 ( 101 320 ( 101 320 ( 101 320 ( 101 320 ( 101 320 ( 101 320
  0. ( 0.05 ( 0.1 ( 0.15 ( 0.2 ( 0.25 ( 0.3 ( 0.35 ( 0.4 ( 0.45 ( 0.5
518.185 511.988 506.827 502.416 498.572 495.172 492.128 489.374 486.864 484.558 482.428
( 80 000 ( 80 000 ( 80 000 ( 80 000 ( 80 000 ( 80 000 ( 80 000 ( 80 000 ( 80 000 ( 80 000 ( 80 000
  0. ( 0.05 ( 0.1 ( 0.15 ( 0.2 ( 0.25 ( 0.3 ( 0.35 ( 0.4 ( 0.45 ( 0.5
509.665 503.681 498.694 494.429 490.711 487.421 484.474 481.808 479.376 477.142 475.078
( 60 000 ( 60 000 ( 60 000 ( 60 000 ( 60 000 ( 60 000 ( 60 000 ( 60 000 ( 60 000 ( 60 000 ( 60 000
  0. ( 0.05 ( 0.1 ( 0.15 ( 0.2 ( 0.25 ( 0.3 ( 0.35 ( 0.4 ( 0.45 ( 0.5
499.662 493.923 489.136 485.04 481.467 478.304 475.469 472.904 470.564 468.413 466.426
( 40 000 ( 40 000 ( 40 000 ( 40 000 ( 40 000 ( 40 000 ( 40 000 ( 40 000 ( 40 000 ( 40 000 ( 40 000
  0. ( 0.05 ( 0.1 ( 0.15 ( 0.2 ( 0.25 ( 0.3 ( 0.35 ( 0.4 ( 0.45 ( 0.5
486.213 480.795 476.271 472.396 469.014 466.018 463.332 460.9 458.68 456.639 454.753
( 20 000 ( 20 000 ( 20 000 ( 20 000 ( 20 000 ( 20 000 ( 20 000 ( 20 000 ( 20 000 ( 20 000 ( 20 000
  0. ( 0.05 ( 0.1 ( 0.15 ( 0.2 ( 0.25 ( 0.3 ( 0.35 ( 0.4 ( 0.45 ( 0.5
464.824 459.898 455.778 452.243 449.155 446.416 443.958 441.731 439.697 437.826 436.095
```

```
( 101 320 ( 101 320 ( 101 320 ( 101 320 ( 101 320 ( 101 320 ( 101 320 ( 101 320 ( 101 320 ( 101 320
  0.55 ( 0.6 ( 0.65 ( 0.7 ( 0.75 ( 0.8 ( 0.85 ( 0.9 ( 0.95 ( 1.
480.449 478.603 476.874 475.248 473.715 472.264 470.888 469.58 468.334 467.144
( 80 000 ( 80 000 ( 80 000 ( 80 000 ( 80 000 ( 80 000 ( 80 000 ( 80 000 ( 80 000 ( 80 000
  0.55 ( 0.6 ( 0.65 ( 0.7 ( 0.75 ( 0.8 ( 0.85 ( 0.9 ( 0.95 ( 1.
473.161 471.372 469.695 468.119 466.632 465.225 463.89 462.622 461.412 460.258
( 60 000 ( 60 000 ( 60 000 ( 60 000 ( 60 000 ( 60 000 ( 60 000 ( 60 000 ( 60 000 ( 60 000
  0.55 ( 0.6 ( 0.65 ( 0.7 ( 0.75 ( 0.8 ( 0.85 ( 0.9 ( 0.95 ( 1.
464.579 462.856 461.241 459.721 458.288 456.932 455.646 454.422 453.256 452.142
( 40 000 ( 40 000 ( 40 000 ( 40 000 ( 40 000 ( 40 000 ( 40 000 ( 40 000 ( 40 000 ( 40 000
  0.55 ( 0.6 ( 0.65 ( 0.7 ( 0.75 ( 0.8 ( 0.85 ( 0.9 ( 0.95 ( 1.
453. ( 451.363 ( 449.828 ( 448.385 ( 447.023 ( 445.734 ( 444.51 ( 443.347 ( 442.238 ( 441.179
( 20 000 ( 20 000 ( 20 000 ( 20 000 ( 20 000 ( 20 000 ( 20 000 ( 20 000 ( 20 000 ( 20 000
  0.55 ( 0.6 ( 0.65 ( 0.7 ( 0.75 ( 0.8 ( 0.85 ( 0.9 ( 0.95 ( 1.
434.486 432.983 431.574 430.247 428.995 427.81 426.685 425.614 424.593 423.618
```

(\*Construction of a graph showing the boiling temperature of the mixture against the mole fraction of the lighter compound. The blue curve represents the liquid phase and the red curve represents the vapour phase in equilibrium with the liquid one\*)

```
In[10]= i = 1;
Print["pressure = ", tb[[1]][[i]][[1]][[1]], " Pa"]
(*escrito*)
graf1 = ListPlot[Table[{tb[[1]][[i]][[j]][[2]], tb[[1]][[i]][[j]][[3]] - 273}, {j, 1, points}], Joined -> True,
(*representa tabla *) (*unido *) (*verdadero*)
  AxesLabel -> {" x, y of MEG", "T[°C]"}, GridLines -> Automatic];
(*etiquetas de ejes *) (*parilla de lin *) (*automático*)
graf2 = ListPlot[Table[{tb[[1]][[i]][[j]][[2]], PVMEG[tb[[1]][[i]][[j]][[3]], tb[[1]][[i]][[j]][[3]] - 273},
(*representa tabla *)
  {j, 1, points}], Joined -> True, PlotStyle -> Red];
(*unido *) (*verdadero *) (*estilo de repr *) (*rojo*)
Show[graf1, graf2]
```



(\*Development of an equation that calculates the boiling temperature of the mixture depending on the pressure and the mole fraction in the liquid phase of the most volatile compound\*)

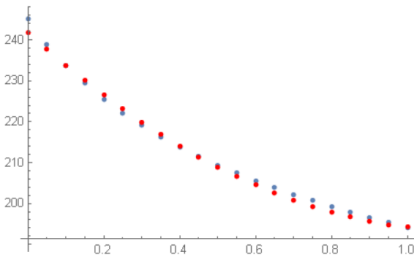
```
In[15]= data =
  Partition[Flatten[Table[{tb[[1]][[j]][[4]][[4]], tb[[1]][[j]][[4]][[2]], tb[[1]][[j]][[4]][[3]]},
  (*particiona *) (*opciones *) (*tabla *)
    {j, 1, 5}, {i, 1, points}], 3];
temperature = Fit[data, {1, x, x^2, y, xy, y^2}, {x, y}]
(*ajusta*)
```

```
Out[16]= 442.669 + 0.00118961 x - 4.70478 × 10-9 x2 - 73.0921 y - 0.000108049 x y + 36.3489 y2
```

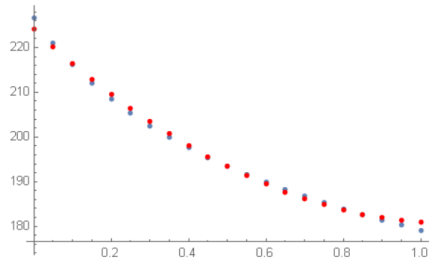
in[17]= (\*Comparison between the values provided by the matrix in blue and the ones provided by the above equation in red\*)

```
Clear[x, y]
borra
p = 0;
Do[
  repite
  p = p + 1;
  temperatura2[x_, y_] = temperature;
  j = tb[[1]][[p]][[1]][[1]];
  Print["pressure = ", j, " Pa"];
  describe
  Print[Show[ListPlot[Table[{tb[[1]][[p]][[1]][[2]], tb[[1]][[p]][[1]][[3]] - 273}, {i, 1, points}],
  describe |muev| |representa| |tabla
  ListPlot[Table[{i, temperatura2[j, i] - 273}, {i, xMEGi, xMEGf, xMEGincr}], PlotStyle -> Red]], {i}]]
  |representa| |tabla |esbilo de repr| |rojo
```

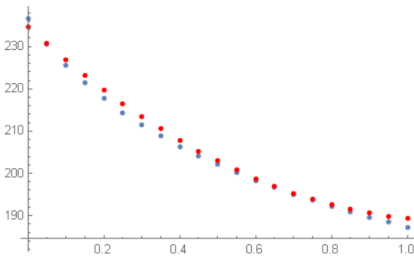
pressure = 101320 Pa



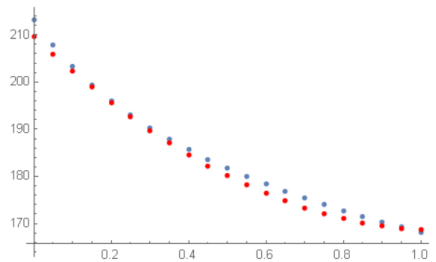
pressure = 60000 Pa



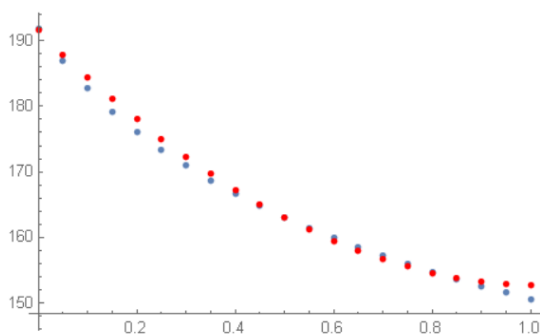
pressure = 80000 Pa



pressure = 40000 Pa



pressure = 20000 Pa



```

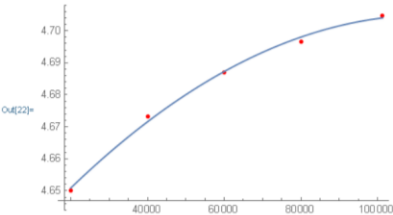
IN[20] := (*Creation of a graph that shows the variation of the relative volatility (α) of the mixture for several pressures*)
data =
Table[
{p},
{tb[[1]][[j]][[1]][[1]]},
Mean[Table[1000 Exp[20.41 - 7377 / (tb[[1]][[j]][[1]][[3]])] / (Exp[25.66 - 7324 / (tb[[1]][[j]][[1]][[3]])]), {i, 1, points}]], {j, 1, n}]]
parabola = Fit[data, {1, x, x^2}, x]
Show[ListPlot[data, PlotStyle -> Red], Plot[parabola], {x, 20000, 101320}]

```

```

OUT[20] := {{101320, 4.7047}, {80000, 4.69671}, {60000, 4.68699}, {40000, 4.67333}, {20000, 4.65007}}

```



```

(* Input values *)
(* p = pressure [Pa]; Fm = kg of feed (F); Fp = % of MEG in the feed; Dp = Constant = % of MEG in the distillate (D);
Rp = % of MEG in the reboiler(R); λ = molar latent heat [J/mol]; Q = power of the reboiler [W];
MWMEG = molar mass of MEG;
MWDEG = molar mass of DEG *)

```

```

IN[21] := p = 100000;
Fm = 0.50; Fp = 50; Dp = 99.5; Rp = 5; λ = 61000; Q = 500;
MWMEG = 0.062; MWDEG = 0.106;

```

$$x_F = \frac{F_p}{\frac{F_p}{MW_{MEG}} + \frac{(100-F_p)}{MW_{DEG}}}; F = \frac{F_m}{x_F MW_{MEG} + (1-x_F) MW_{DEG}}; x_D = \frac{D_p}{\frac{D_p}{MW_{MEG}} + \frac{(100-D_p)}{MW_{DEG}}}; x_R = \frac{R_p}{\frac{R_p}{MW_{MEG}} + \frac{(100-R_p)}{MW_{DEG}}}$$

```
Clear[R];
```

```

R = R /. NSolve[xR == F xF - (F - R) xD, R][[1]];

```

```

(*Introduce the previously calculated relative volatility equation highlighted in grey and replace x by p*)
α = 4.625282642123176 + 1.405129451139797 * 10^-6 p - 6.198082280842811 * 10^-12 p^2;

```

$$x[y_] := \frac{y}{y + \alpha - y \alpha}$$

$$y[x_] := \frac{x}{1 + (\alpha - 1) x}$$

```

(*Introduce the previously calculated boiling temperature equation highlighted in red*)

```

$$\text{temp}[x_, y_] := 442.6688229674054 + 0.0011896095099302557 x - 4.704782397480638 * 10^-9 x^2 - 73.09209593852118 y - 0.00010804948392970379 x y + 36.34886072394359 y^2$$

```
list = {xx, yy, temp[p, xx] - 273};
```

```
listz = {rd1, rd2, V, energy, time};
```

```
listv = {xx, int1};
```

```
listw = {xx, int2};
```

```

(*Introduce the number of intervals desired (INT) to carry out the calculations*)

```

```
INT = 10;
```

```
INCR = (Fp - Rp) / INT;
```

```
Print["Pressure = ", p, " Pa", " α = ", α]
```

```
Print["Fm = ", Fm, " kg of F", " F = ", F, " mol"]
```

```
Print["Fp = ", Fp, "% of MEG in F", " xF = ", xF]
```

```
Print["Dp = ", Dp, "% of MEG in D", " xD = ", xD]
```

```
Print["Rp = ", Rp, "% of MEG in R", " xR = ", xR]
```

```
Print["Rm = ", R (xR MWMEG + (1 - xR) MWDEG), " kg of R", " R = ", R, " mol"]
```

```
Print["λ = ", λ, " J/mol", " Q = ", Q / 1000, " kW"]
```

```
Print["Increment = ", INCR, " % of MEG"]
```

```

(*Introduce the desired amount of plates (ne) considering one more stage will be added during the calculations
since the column is operating batch-wise*)
ne = 10; rd1 = 0.5; rd2 = 2;
Rp = Fp - INCR;
int1 = \frac{1}{(xF - xD)^2 \left(1 - \frac{rd1}{rd1+1}\right)}; int2 = \frac{1}{(xR - xD)^2 \left(1 - \frac{rd2}{rd2+1}\right)};
V = F (xF - xD) \left(\frac{int1 + int2}{2}\right) (xR - xF); energy = V λ / (3600000); time = \left(\frac{V λ}{Q}\right) / 3600;

```

Pressure = 100000 Pa     $\alpha = 4.70381$

$F_m = 0.5$  kg of F     $F = 6.39075$  mol

$F_p = 50\%$  of MEG in F     $x_F = 0.630952$

$D_p = 99.5\%$  of MEG in D     $x_D = 0.997069$

$R_p = 5\%$  of MEG in R     $x_R = 0.0825545$

$R_m = 0.261905$  kg of R     $R = 2.55847$  mol

$\lambda = 61000$  J/mol     $Q = \frac{1}{2}$  kW

Increment =  $\frac{3}{2}$  % of MEG

(\*This instruction calculates the column's reflux ratio alongside the compositions and temperatures of all the trays until the desired reboiler composition ( $x_R$ ) is reached. The amount of vapour generated by the reboiler, its energetic demand, the time needed and the integral's value is also calculated for every single interval. It also plots the McCabe-Thiele diagram for the first and last set of data\*)

```

v(51): Print("number of stages = ", ne + 1, "    xD = ", xD)
|escribe

Do[ (
|repite
    error = 1; xF =  $\frac{Fp}{RmREG + (100-Fp)} + \frac{Fp}{RmDEG}$ ; xR =  $\frac{Rp}{RmREG + (100-Rp)}$ ; F =  $\frac{Fm}{xF RmREG + (1-xF) RmDEG}$ ; While[Abs(error) > 0.01,
|entre (valor absoluto)
    lista = {xD, xD};
    n = 0;
    yy =  $\frac{rd1}{rd1 + 1} xD + \frac{1}{rd1 + 1} xD$ ;
    xx = x[yy];
    n = n + 1;
    lista = Append[lista, xx];
|añade
    lista = Append[lista, yy];
|añade

    Do[ (
|repite
        yy =  $\frac{rd1}{rd1 + 1} xx + \frac{1 \times D}{rd1 + 1}$ ;
        lista = Append[lista, xx];
|añade
        lista = Append[lista, yy];
|añade
        xx = x[yy];
        lista = Append[lista, xx];
|añade
        lista = Append[lista, yy];
|añade
        n = n + 1; } , {ne} ];

    lista = Partition[lista, 2];
|particiona
    error = (lista[[2 ne + 2]][[1]] - xF) 100 / xF;
    rd1 = rd1 + error rd1 / 100; ];
    Print["r/d1 = ", rd1];
|escribe
    lista = {xD, xD};
    n = 0;
    yy =  $\frac{rd1}{rd1 + 1} xD + \frac{1}{rd1 + 1} xD$ ;
    xx = x[yy]; list = Append[list, xx]; list = Append[list, yy]; list = Append[list, temp[p, xx] - 273];
|añade |añade |añade
    n = n + 1; Print[n, " ", " xR = ", xx, "    y = ", yy, "    T(°C) = ", temp[p, xx] - 273];
|escribe
    lista = Append[lista, xx];
|añade
    lista = Append[lista, yy];
|añade

    Do[ (
|repite
        yy =  $\frac{rd1}{rd1 + 1} xx + \frac{1 \times D}{rd1 + 1}$ ;
        lista = Append[lista, xx];
|añade
        lista = Append[lista, yy];
|añade

```

```

xx = x[yy];
lista = Append[lista, xx];
lista = Append[lista, yy]; list = Append[list, xx]; list = Append[list, yy]; list = Append[list, temp[p, xx] - 273];
n = n + 1; Print["n", " ", "x = ", xx, " y = ", yy, " T(°C) = ", temp[p, xx] - 273], {ne}]; listv = Append[listv, xx];

lista = Partition[lista, 2];

Print["xF = ", lista[[2 ne + 2]][[1]], " xF = ", xF, " (error = ", error, " %)"];
error = 1;
Once[graf = Plot[{{ $\frac{\alpha x}{1 + (\alpha - 1)x}$ , x},  $\frac{rd1}{rd1 + 1}x + \frac{1 xD}{rd1 + 1}$ }, {x, 0, 1}, Frame -> True,
GridLines -> Automatic, PlotRange -> {{0, 1}, {0, 1}}, GridLines -> Automatic, DisplayFunction -> Identity];
graf1 = ListPlot[lista, PlotStyle -> PointSize[.005], PlotRange -> {{0, 1}, {0, 1}}, DisplayFunction -> Identity];
graf2 = ListPlot[lista, PlotJoined -> True, PlotRange -> {{0, 1}, {0, 1}}, DisplayFunction -> Identity]; While[Abs[error] > 0.01,
lista = {xD, xD};
n = 0;
yy =  $\frac{rd2}{rd2 + 1}xD + \frac{1}{rd2 + 1}xD$ ;
xx = x[yy];
n = n + 1;
lista = Append[lista, xx];
lista = Append[lista, yy];
Do[
yy =  $\frac{rd2}{rd2 + 1}xx + \frac{1 xD}{rd2 + 1}$ ;
lista = Append[lista, xx];
lista = Append[lista, yy];
xx = x[yy];
lista = Append[lista, xx];
lista = Append[lista, yy];
n = n + 1; ], {ne}];
lista = Partition[lista, 2];
error = (lista[[2 ne + 2]][[1]] - xR) 100 / xR;
rd2 = rd2 + error rd2 / 100;
Print["r/d2 = ", rd2];
lista = {xD, xD};
n = 0;
yy =  $\frac{rd2}{rd2 + 1}xD + \frac{1}{rd2 + 1}xD$ ;
xx = x[yy]; list = Append[list, xx]; list = Append[list, yy]; list = Append[list, temp[p, xx] - 273];

```

```

n = n + 1; Print[n, " ", " ", " xR = ", xx, " ", " y = ", yy, " ", " T(°C) = ", temp[p, xx] - 273];
lista = Append[lista, xx];
lista = Append[lista, yy];
Do[
  yy =  $\frac{rd2}{rd2 + 1} xx + \frac{1 xD}{rd2 + 1}$ ;
  lista = Append[lista, xx];
  lista = Append[lista, yy];
  xx = x[yy];
  lista = Append[lista, xx];
  lista = Append[lista, yy]; list = Append[list, xx]; list = Append[list, yy]; list = Append[list, temp[p, xx] - 273];
n = n + 1; Print[n, " ", " ", " x = ", xx, " ", " y = ", yy, " ", " T(°C) = ", temp[p, xx] - 273], {ne}]; listw = Append[listw, xx];
lista = Partition[lista, 2];
Print["xR = ", lista[[2 ne + 2]][[1]], " ", " xR = ", xR, " ", " (error = ", error, " %)"];
ggraf = Plot[ $\left\{ \frac{\alpha x}{1 - (\alpha - 1)x}, x, \frac{rd2}{rd2 + 1} x + \frac{1 xD}{rd2 + 1} \right\}$ , {x, 0, 1}, Frame -> True,
GridLines -> Automatic, PlotRange -> {{0, 1}, {0, 1}}, GridLines -> Automatic, DisplayFunction -> Identity];
ggraf1 = ListPlot[lista, PlotStyle -> PointSize[.005], PlotRange -> {{0, 1}, {0, 1}}, DisplayFunction -> Identity];
ggraf2 = ListPlot[lista, PlotJoined -> True, PlotRange -> {{0, 1}, {0, 1}}, DisplayFunction -> Identity];
int1 =  $\frac{1}{(xF - xD)^2 \left(1 - \frac{rd1}{rd1+1}\right)}$ ;
int2 =  $\frac{1}{(xR - xD)^2 \left(1 - \frac{rd2}{rd2+1}\right)}$ ;
V = F (xF - xD)  $\left(\frac{int1 + int2}{2}\right)$  (xR - xF); energy = V λ / (3600000); time =  $\left(\frac{V \lambda}{Q}\right) / 3600$ ; Print["int1 =  $\frac{1}{(xF - xD)^2 \left(1 - \frac{rd1}{rd1+1}\right)}$  = ", int1];
Print["int2 =  $\frac{1}{(xR - xD)^2 \left(1 - \frac{rd2}{rd2+1}\right)}$  = ", int2];
Print["V' = ", V, " mol"];
Print["energetic demand = ", V λ / (3600000), " kWh"];
Print["time =  $\frac{V \lambda}{Q}$  = ",  $\left(\frac{V \lambda}{Q}\right) / 3600$ , " h"]; listv = Append[listv, int1]; listw = Append[listw, int2];
listz = Append[listz, rd1];
listz = Append[listz, rd2];
listz = Append[listz, V];
listz = Append[listz, energy];
listz = Append[listz, time];
Fp = Fp - INCR; Rp = Rp - INCR;
}, {INT}];
Show[graf1, graf2, graf, ggraf1, ggraf2, ggraf, DisplayFunction -> $DisplayFunction, PlotLabel -> "McCabe-Thiele Diagram", LabelStyle -> {GrayLevel[0]}];
number of stages = 11 xD = 0.997069

```

r/d1 = 0.468463

```

1  xr = 0.986363  y = 0.997069  T(°C) = 194.193
2  x = 0.970835  y = 0.993654  T(°C) = 194.391
3  x = 0.948982  y = 0.9887  T(°C) = 194.7
4  x = 0.919503  y = 0.981729  T(°C) = 195.171
5  x = 0.881924  y = 0.972325  T(°C) = 195.863
6  x = 0.837326  y = 0.960336  T(°C) = 196.817
7  x = 0.788685  y = 0.946109  T(°C) = 198.023
8  x = 0.740282  y = 0.930591  T(°C) = 199.394
9  x = 0.696319  y = 0.91515  T(°C) = 200.787
10 x = 0.659579  y = 0.901125  T(°C) = 202.059
11 x = 0.630951  y = 0.889405  T(°C) = 203.117

```

xF = 0.630951 xR = 0.630952 (error = 0.00275691 %)

r/d2 = 0.499694

```

1  xr = 0.986363  y = 0.997069  T(°C) = 194.193
2  x = 0.970153  y = 0.993502  T(°C) = 194.4
3  x = 0.946392  y = 0.988101  T(°C) = 194.739
4  x = 0.913161  y = 0.980184  T(°C) = 195.28
5  x = 0.869622  y = 0.969111  T(°C) = 196.112
6  x = 0.817202  y = 0.954604  T(°C) = 197.296
7  x = 0.760152  y = 0.937138  T(°C) = 198.811
8  x = 0.704501  y = 0.918129  T(°C) = 200.517
9  x = 0.655716  y = 0.899586  T(°C) = 202.198
10 x = 0.6168  y = 0.883331  T(°C) = 203.663
11 x = 0.588027  y = 0.870365  T(°C) = 204.817

```

xR = 0.588027 xR = 0.588027 (error = 0.00116035 %)

$$\text{int1} = \frac{1}{(x_F - x_D)^2 \left(1 - \frac{rd_1}{rd_1 + 1}\right)} = 10.9553$$

$$\text{int2} = \frac{1}{(x_R - x_D)^2 \left(1 - \frac{rd_2}{rd_2 + 1}\right)} = 8.96328$$

V' = 1.00025 mol

energetic demand = 0.0169488 kWh

$$\text{time} = \frac{V \lambda}{Q} = 0.0338975 \text{ h}$$

r/d1 = 0.499689

```

1  xr = 0.986363  y = 0.997069  T(°C) = 194.193
2  x = 0.970153  y = 0.993502  T(°C) = 194.4
3  x = 0.946392  y = 0.988101  T(°C) = 194.739
4  x = 0.913162  y = 0.980184  T(°C) = 195.28
5  x = 0.869624  y = 0.969112  T(°C) = 196.112
6  x = 0.817205  y = 0.954605  T(°C) = 197.296
7  x = 0.760157  y = 0.937139  T(°C) = 198.811
8  x = 0.704506  y = 0.918131  T(°C) = 200.517
9  x = 0.655722  y = 0.899589  T(°C) = 202.198
10 x = 0.616807  y = 0.883334  T(°C) = 203.663
11 x = 0.588033  y = 0.870368  T(°C) = 204.817

```

xF = 0.588033 xF = 0.588027 (error = -0.00049044 %)

r/d2 = 0.536266

```

1  xr = 0.986363  y = 0.997069  T(°C) = 194.193
2  x = 0.969391  y = 0.993332  T(°C) = 194.411
3  x = 0.943408  y = 0.987408  T(°C) = 194.784
4  x = 0.905673  y = 0.978338  T(°C) = 195.414
5  x = 0.85487  y = 0.965165  T(°C) = 196.425
6  x = 0.793026  y = 0.947432  T(°C) = 197.909
7  x = 0.726345  y = 0.925844  T(°C) = 199.821
8  x = 0.663227  y = 0.902567  T(°C) = 201.928
9  x = 0.610432  y = 0.880535  T(°C) = 203.913
10 x = 0.570653  y = 0.862105  T(°C) = 205.543
11 x = 0.542976  y = 0.84822  T(°C) = 206.744

```

xR = 0.542976 xR = 0.542979 (error = 0.00288035 %)

$$\text{int1} = \frac{1}{(x_F - x_D)^2 \left(1 - \frac{rd_1}{rd_1 + 1}\right)} = 8.96325$$

$$\text{int2} = \frac{1}{(x_R - x_D)^2 \left(1 - \frac{rd_2}{rd_2 + 1}\right)} = 7.45042$$

V' = 0.943668 mol

energetic demand = 0.0159899 kWh

$$\text{time} = \frac{V \lambda}{Q} = 0.0319799 \text{ h}$$

$$r/d1 = 0.536266$$

1	xr = 0.986363	y = 0.997069	T(°C) = 194.193
2	x = 0.969391	y = 0.993332	T(°C) = 194.411
3	x = 0.943408	y = 0.987408	T(°C) = 194.784
4	x = 0.905673	y = 0.978338	T(°C) = 195.414
5	x = 0.85487	y = 0.965165	T(°C) = 196.425
6	x = 0.793026	y = 0.947432	T(°C) = 197.909
7	x = 0.726345	y = 0.925844	T(°C) = 199.821
8	x = 0.663227	y = 0.902567	T(°C) = 201.928
9	x = 0.610432	y = 0.880535	T(°C) = 203.913
10	x = 0.570653	y = 0.862105	T(°C) = 205.543
11	x = 0.542976	y = 0.84822	T(°C) = 206.744

$$xF = 0.542976 \quad xF = 0.542979 \quad (\text{error} = 0.0028807 \%)$$

$$r/d2 = 0.580683$$

1	xr = 0.986363	y = 0.997069	T(°C) = 194.193
2	x = 0.968515	y = 0.993136	T(°C) = 194.422
3	x = 0.939862	y = 0.986579	T(°C) = 194.839
4	x = 0.896536	y = 0.976053	T(°C) = 195.582
5	x = 0.836616	y = 0.960137	T(°C) = 196.834
6	x = 0.763216	y = 0.938125	T(°C) = 198.724
7	x = 0.685575	y = 0.911161	T(°C) = 201.149
8	x = 0.615214	y = 0.882638	T(°C) = 203.725
9	x = 0.559839	y = 0.85679	T(°C) = 206.006
10	x = 0.520902	y = 0.836447	T(°C) = 207.743
11	x = 0.495641	y = 0.822143	T(°C) = 208.929

$$xR = 0.495641 \quad xR = 0.495644 \quad (\text{error} = 0.00440457 \%)$$

$$\text{int1} = \frac{1}{(xF - xD)^2 \left(1 - \frac{rd1}{rd1+1}\right)} = 7.45042$$

$$\text{int2} = \frac{1}{(xR - xD)^2 \left(1 - \frac{rd2}{rd2+1}\right)} = 6.28684$$

$$V' = 0.899015 \text{ mol}$$

$$\text{energetic demand} = 0.0152333 \text{ kWh}$$

$$\text{time} = \frac{V \lambda}{Q} = 0.0304666 \text{ h}$$

$$r/d1 = 0.580683$$

1	xr = 0.986363	y = 0.997069	T(°C) = 194.193
2	x = 0.968515	y = 0.993136	T(°C) = 194.422
3	x = 0.939862	y = 0.986579	T(°C) = 194.839
4	x = 0.896536	y = 0.976053	T(°C) = 195.582
5	x = 0.836616	y = 0.960137	T(°C) = 196.834
6	x = 0.763216	y = 0.938125	T(°C) = 198.724
7	x = 0.685575	y = 0.911161	T(°C) = 201.149
8	x = 0.615214	y = 0.882638	T(°C) = 203.725
9	x = 0.559839	y = 0.85679	T(°C) = 206.006
10	x = 0.520902	y = 0.836447	T(°C) = 207.743
11	x = 0.495641	y = 0.822143	T(°C) = 208.929

$$xF = 0.495641 \quad xF = 0.495644 \quad (\text{error} = 0.00440457 \%)$$

$$r/d2 = 0.63693$$

1	xr = 0.986363	y = 0.997069	T(°C) = 194.193
2	x = 0.967474	y = 0.992904	T(°C) = 194.436
3	x = 0.9355	y = 0.985554	T(°C) = 194.907
4	x = 0.884981	y = 0.973113	T(°C) = 195.803
5	x = 0.813257	y = 0.953456	T(°C) = 197.393
6	x = 0.725489	y = 0.925548	T(°C) = 199.847
7	x = 0.635694	y = 0.891397	T(°C) = 202.938
8	x = 0.559172	y = 0.856458	T(°C) = 206.034
9	x = 0.503482	y = 0.826683	T(°C) = 208.556
10	x = 0.467436	y = 0.805014	T(°C) = 210.308
11	x = 0.445844	y = 0.790989	T(°C) = 211.402

$$xR = 0.445844 \quad xR = 0.445846 \quad (\text{error} = 0.00408098 \%)$$

$$\text{int1} = \frac{1}{(xF - xD)^2 \left(1 - \frac{rd1}{rd1+1}\right)} = 6.28684$$

$$\text{int2} = \frac{1}{(xR - xD)^2 \left(1 - \frac{rd2}{rd2+1}\right)} = 5.38736$$

$$V' = 0.865596 \text{ mol}$$

$$\text{energetic demand} = 0.014667 \text{ kWh}$$

$$\text{time} = \frac{V \lambda}{Q} = 0.0293341 \text{ h}$$



```

r/d1 = 0.63693
1  xr = 0.986363  y = 0.997069  T(°C) = 194.193
2  x = 0.967474  y = 0.992904  T(°C) = 194.436
3  x = 0.9355  y = 0.985554  T(°C) = 194.907
4  x = 0.884981  y = 0.973113  T(°C) = 195.803
5  x = 0.813257  y = 0.953456  T(°C) = 197.393
6  x = 0.725489  y = 0.925548  T(°C) = 199.847
7  x = 0.635694  y = 0.891397  T(°C) = 202.938
8  x = 0.559172  y = 0.856458  T(°C) = 206.034
9  x = 0.503482  y = 0.826683  T(°C) = 208.556
10 x = 0.467436  y = 0.805014  T(°C) = 210.308
11 x = 0.445844  y = 0.790989  T(°C) = 211.402
xF = 0.445844  xF = 0.445846  (error = 0.00408098 %)
r/d2 = 0.711729
1  xr = 0.986363  y = 0.997069  T(°C) = 194.193
2  x = 0.966199  y = 0.992618  T(°C) = 194.454
3  x = 0.92993  y = 0.984234  T(°C) = 194.997
4  x = 0.86978  y = 0.969153  T(°C) = 196.109
5  x = 0.782298  y = 0.944143  T(°C) = 198.195
6  x = 0.676627  y = 0.907769  T(°C) = 201.456
7  x = 0.574224  y = 0.863831  T(°C) = 205.392
8  x = 0.494121  y = 0.821252  T(°C) = 209.001
9  x = 0.441325  y = 0.787946  T(°C) = 211.636
10 x = 0.410342  y = 0.765993  T(°C) = 213.276
11 x = 0.393386  y = 0.753111  T(°C) = 214.203
xF = 0.393386  xF = 0.393387  (error = 0.0023263 %)
r/d1 = 0.711729
1  xr = 0.986363  y = 0.997069  T(°C) = 194.193
2  x = 0.966199  y = 0.992618  T(°C) = 194.454
3  x = 0.92993  y = 0.984234  T(°C) = 194.997
4  x = 0.86978  y = 0.969153  T(°C) = 196.109
5  x = 0.782298  y = 0.944143  T(°C) = 198.195
6  x = 0.676627  y = 0.907769  T(°C) = 201.456
7  x = 0.574224  y = 0.863831  T(°C) = 205.392
8  x = 0.494121  y = 0.821252  T(°C) = 209.001
9  x = 0.441325  y = 0.787946  T(°C) = 211.636
10 x = 0.410342  y = 0.765993  T(°C) = 213.276
11 x = 0.393386  y = 0.753111  T(°C) = 214.203
xF = 0.393386  xF = 0.393387  (error = 0.0023263 %)
r/d2 = 0.817158
1  xr = 0.986363  y = 0.997069  T(°C) = 194.193
2  x = 0.964584  y = 0.992255  T(°C) = 194.476
3  x = 0.922532  y = 0.982461  T(°C) = 195.119
4  x = 0.848943  y = 0.963551  T(°C) = 196.555
5  x = 0.739886  y = 0.930458  T(°C) = 199.406
6  x = 0.612431  y = 0.881417  T(°C) = 203.834
7  x = 0.499003  y = 0.824101  T(°C) = 208.768
8  x = 0.420064  y = 0.773094  T(°C) = 212.754
9  x = 0.374054  y = 0.737596  T(°C) = 215.286
10 x = 0.349961  y = 0.716906  T(°C) = 216.673
11 x = 0.33805  y = 0.706071  T(°C) = 217.374
xF = 0.33805  xF = 0.338048  (error = -0.00940195 %)

int1 =  $\frac{1}{(xF - xD)^2 \left(1 - \frac{rd1}{rd1+1}\right)}$  = 5.38736
int2 =  $\frac{1}{(xR - xD)^2 \left(1 - \frac{rd2}{rd2+1}\right)}$  = 4.69698
V' = 0.843935 mol
energetic demand = 0.0143 kWh
time =  $\frac{V \lambda}{Q}$  = 0.0286 h

int1 =  $\frac{1}{(xF - xD)^2 \left(1 - \frac{rd1}{rd1+1}\right)}$  = 4.69698
int2 =  $\frac{1}{(xR - xD)^2 \left(1 - \frac{rd2}{rd2+1}\right)}$  = 4.18401
V' = 0.836309 mol
energetic demand = 0.0141708 kWh
time =  $\frac{V \lambda}{Q}$  = 0.0283416 h

```

$r/d1 = 0.817158$

1	$xr = 0.986363$	$y = 0.997069$	$T(^{\circ}C) = 194.193$
2	$x = 0.964584$	$y = 0.992255$	$T(^{\circ}C) = 194.476$
3	$x = 0.922532$	$y = 0.982461$	$T(^{\circ}C) = 195.119$
4	$x = 0.848943$	$y = 0.963551$	$T(^{\circ}C) = 196.555$
5	$x = 0.739886$	$y = 0.930458$	$T(^{\circ}C) = 199.406$
6	$x = 0.612431$	$y = 0.881417$	$T(^{\circ}C) = 203.834$
7	$x = 0.499003$	$y = 0.824101$	$T(^{\circ}C) = 208.768$
8	$x = 0.420064$	$y = 0.773094$	$T(^{\circ}C) = 212.754$
9	$x = 0.374054$	$y = 0.737596$	$T(^{\circ}C) = 215.286$
10	$x = 0.349961$	$y = 0.716906$	$T(^{\circ}C) = 216.673$
11	$x = 0.33805$	$y = 0.706071$	$T(^{\circ}C) = 217.374$

$x_F = 0.33805$     $x_R = 0.338048$    (error =  $-0.00940195$  ‰)

$r/d2 = 0.976955$

1	$xr = 0.986363$	$y = 0.997069$	$T(^{\circ}C) = 194.193$
2	$x = 0.962471$	$y = 0.991779$	$T(^{\circ}C) = 194.505$
3	$x = 0.912297$	$y = 0.979972$	$T(^{\circ}C) = 195.296$
4	$x = 0.81918$	$y = 0.955177$	$T(^{\circ}C) = 197.247$
5	$x = 0.680282$	$y = 0.909162$	$T(^{\circ}C) = 201.33$
6	$x = 0.528405$	$y = 0.840522$	$T(^{\circ}C) = 207.399$
7	$x = 0.409635$	$y = 0.765469$	$T(^{\circ}C) = 213.314$
8	$x = 0.338811$	$y = 0.706776$	$T(^{\circ}C) = 217.329$
9	$x = 0.303192$	$y = 0.671777$	$T(^{\circ}C) = 219.486$
10	$x = 0.286809$	$y = 0.654175$	$T(^{\circ}C) = 220.51$
11	$x = 0.279584$	$y = 0.646079$	$T(^{\circ}C) = 220.967$

$r/d1 = 0.976955$

1	$xr = 0.986363$	$y = 0.997069$	$T(^{\circ}C) = 194.193$
2	$x = 0.962471$	$y = 0.991779$	$T(^{\circ}C) = 194.505$
3	$x = 0.912297$	$y = 0.979972$	$T(^{\circ}C) = 195.296$
4	$x = 0.81918$	$y = 0.955177$	$T(^{\circ}C) = 197.247$
5	$x = 0.680282$	$y = 0.909162$	$T(^{\circ}C) = 201.33$
6	$x = 0.528405$	$y = 0.840522$	$T(^{\circ}C) = 207.399$
7	$x = 0.409635$	$y = 0.765469$	$T(^{\circ}C) = 213.314$
8	$x = 0.338811$	$y = 0.706776$	$T(^{\circ}C) = 217.329$
9	$x = 0.303192$	$y = 0.671777$	$T(^{\circ}C) = 219.486$
10	$x = 0.286809$	$y = 0.654175$	$T(^{\circ}C) = 220.51$
11	$x = 0.279584$	$y = 0.646079$	$T(^{\circ}C) = 220.967$

$x_F = 0.279584$     $x_R = 0.279584$    (error =  $-0.00262337$  ‰)

$r/d2 = 1.24458$

1	$xr = 0.986363$	$y = 0.997069$	$T(^{\circ}C) = 194.193$
2	$x = 0.959617$	$y = 0.991133$	$T(^{\circ}C) = 194.545$
3	$x = 0.897526$	$y = 0.976303$	$T(^{\circ}C) = 195.563$
4	$x = 0.775023$	$y = 0.941875$	$T(^{\circ}C) = 198.393$
5	$x = 0.595792$	$y = 0.873949$	$T(^{\circ}C) = 204.499$
6	$x = 0.422118$	$y = 0.774568$	$T(^{\circ}C) = 212.644$
7	$x = 0.309482$	$y = 0.678269$	$T(^{\circ}C) = 219.099$
8	$x = 0.254159$	$y = 0.615815$	$T(^{\circ}C) = 222.607$
9	$x = 0.230681$	$y = 0.585139$	$T(^{\circ}C) = 224.163$
10	$x = 0.221342$	$y = 0.572121$	$T(^{\circ}C) = 224.793$
11	$x = 0.217723$	$y = 0.566943$	$T(^{\circ}C) = 225.039$

$x_R = 0.279584$     $x_R = 0.279584$    (error =  $-0.00262337$  ‰)

$$\text{int1} = \frac{1}{(x_F - x_D)^2 \left(1 - \frac{rd1}{rd1+1}\right)} = 4.18401$$

$$\text{int2} = \frac{1}{(x_R - x_D)^2 \left(1 - \frac{rd2}{rd2+1}\right)} = 3.84035$$

$V' = 0.848197 \text{ mol}$

energetic demand =  $0.0143722 \text{ kWh}$

$$\text{time} = \frac{V \lambda}{Q} = 0.0287445 \text{ h}$$

$x_R = 0.217723$     $x_R = 0.217723$    (error =  $-0.000370382$  ‰)

$$\text{int1} = \frac{1}{(x_F - x_D)^2 \left(1 - \frac{rd1}{rd1+1}\right)} = 3.84035$$

$$\text{int2} = \frac{1}{(x_R - x_D)^2 \left(1 - \frac{rd2}{rd2+1}\right)} = 3.6955$$

$V' = 0.892418 \text{ mol}$

energetic demand =  $0.0151215 \text{ kWh}$

$$\text{time} = \frac{V \lambda}{Q} = 0.0302431 \text{ h}$$

$r/d1 = 1.24458$

1	$xr = 0.986363$	$y = 0.997069$	$T(^{\circ}C) = 194.193$
2	$x = 0.959617$	$y = 0.991133$	$T(^{\circ}C) = 194.545$
3	$x = 0.897526$	$y = 0.976303$	$T(^{\circ}C) = 195.563$
4	$x = 0.775023$	$y = 0.941875$	$T(^{\circ}C) = 198.393$
5	$x = 0.595792$	$y = 0.873949$	$T(^{\circ}C) = 204.499$
6	$x = 0.422118$	$y = 0.774568$	$T(^{\circ}C) = 212.644$
7	$x = 0.309482$	$y = 0.678269$	$T(^{\circ}C) = 219.099$
8	$x = 0.254159$	$y = 0.615815$	$T(^{\circ}C) = 222.607$
9	$x = 0.230681$	$y = 0.585139$	$T(^{\circ}C) = 224.163$
10	$x = 0.221342$	$y = 0.572121$	$T(^{\circ}C) = 224.793$
11	$x = 0.217723$	$y = 0.566943$	$T(^{\circ}C) = 225.039$

$xR = 0.217723$     $xF = 0.217723$    (error = -0.000370382 %)

$r/d2 = 1.77298$

1	$xr = 0.986363$	$y = 0.997069$	$T(^{\circ}C) = 194.193$
2	$x = 0.955622$	$y = 0.990224$	$T(^{\circ}C) = 194.602$
3	$x = 0.875169$	$y = 0.970569$	$T(^{\circ}C) = 195.998$
4	$x = 0.707278$	$y = 0.919129$	$T(^{\circ}C) = 200.427$
5	$x = 0.478331$	$y = 0.811784$	$T(^{\circ}C) = 209.768$
6	$x = 0.297147$	$y = 0.6654$	$T(^{\circ}C) = 219.862$
7	$x = 0.205952$	$y = 0.549555$	$T(^{\circ}C) = 225.845$
8	$x = 0.170316$	$y = 0.491247$	$T(^{\circ}C) = 228.347$
9	$x = 0.1578$	$y = 0.468463$	$T(^{\circ}C) = 229.248$
10	$x = 0.153571$	$y = 0.46046$	$T(^{\circ}C) = 229.555$
11	$x = 0.152161$	$y = 0.457756$	$T(^{\circ}C) = 229.658$

$xR = 0.152161$     $xR = 0.152161$    (error = 0.00283012 %)

$$\text{int1} = \frac{1}{(xF - xD)^2 \left(1 - \frac{rd1}{rd1+1}\right)} = 3.6955$$

$$\text{int2} = \frac{1}{(xR - xD)^2 \left(1 - \frac{rd2}{rd2+1}\right)} = 3.88443$$

$V' = 1.0042$  mol

energetic demand = 0.0170157 kWh

$$\text{time} = \frac{V \lambda}{Q} = 0.0340313 \text{ h}$$

$r/d1 = 1.77298$

1	$xr = 0.986363$	$y = 0.997069$	$T(^{\circ}C) = 194.193$
2	$x = 0.955622$	$y = 0.990224$	$T(^{\circ}C) = 194.602$
3	$x = 0.875169$	$y = 0.970569$	$T(^{\circ}C) = 195.998$
4	$x = 0.707278$	$y = 0.919129$	$T(^{\circ}C) = 200.427$
5	$x = 0.478331$	$y = 0.811784$	$T(^{\circ}C) = 209.768$
6	$x = 0.297147$	$y = 0.6654$	$T(^{\circ}C) = 219.862$
7	$x = 0.205952$	$y = 0.549555$	$T(^{\circ}C) = 225.845$
8	$x = 0.170316$	$y = 0.491247$	$T(^{\circ}C) = 228.347$
9	$x = 0.1578$	$y = 0.468463$	$T(^{\circ}C) = 229.248$
10	$x = 0.153571$	$y = 0.46046$	$T(^{\circ}C) = 229.555$
11	$x = 0.152161$	$y = 0.457756$	$T(^{\circ}C) = 229.658$

$xR = 0.152161$     $xR = 0.152161$    (error = 0.00283012 %)

$r/d2 = 3.26275$

1	$xr = 0.986363$	$y = 0.997069$	$T(^{\circ}C) = 194.193$
2	$x = 0.949739$	$y = 0.988875$	$T(^{\circ}C) = 194.688$
3	$x = 0.83914$	$y = 0.960842$	$T(^{\circ}C) = 196.776$
4	$x = 0.600716$	$y = 0.876189$	$T(^{\circ}C) = 204.3$
5	$x = 0.324994$	$y = 0.693697$	$T(^{\circ}C) = 218.155$
6	$x = 0.165512$	$y = 0.482657$	$T(^{\circ}C) = 228.692$
7	$x = 0.107054$	$y = 0.360588$	$T(^{\circ}C) = 233.017$
8	$x = 0.0893731$	$y = 0.315844$	$T(^{\circ}C) = 234.374$
9	$x = 0.0843472$	$y = 0.30231$	$T(^{\circ}C) = 234.764$
10	$x = 0.0829442$	$y = 0.298463$	$T(^{\circ}C) = 234.873$
11	$x = 0.0825545$	$y = 0.297389$	$T(^{\circ}C) = 234.904$

$xR = 0.0825545$     $xR = 0.0825545$    (error = 0.0000873998 %)

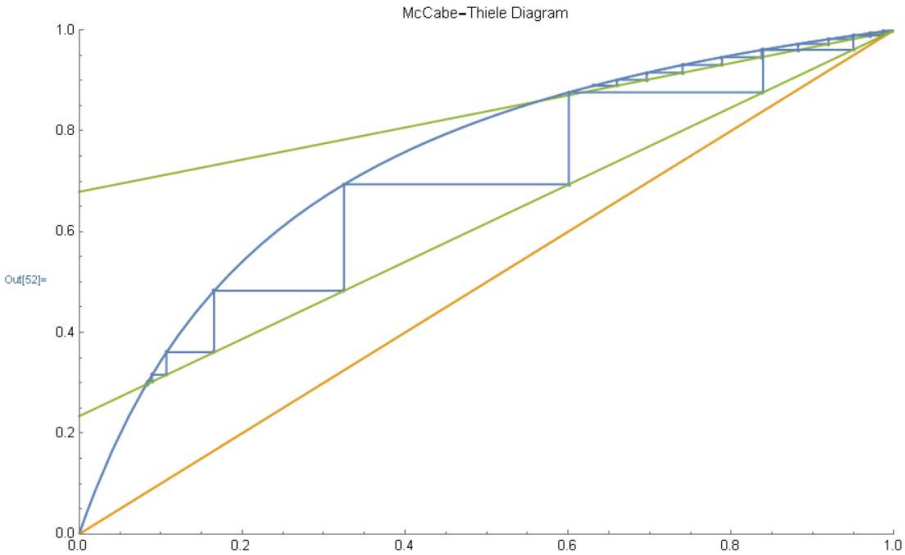
$$\text{int1} = \frac{1}{(xF - xD)^2 \left(1 - \frac{rd1}{rd1+1}\right)} = 3.88443$$

$$\text{int2} = \frac{1}{(xR - xD)^2 \left(1 - \frac{rd2}{rd2+1}\right)} = 5.09692$$

$V' = 1.32975$  mol

energetic demand = 0.0225318 kWh

$$\text{time} = \frac{V \lambda}{Q} = 0.0450636 \text{ h}$$



(\*Generation of a matrix which contains all the different reflux ratios along with the amount of vapour generated, the energy needed and the time required in those lapses\*)

```
In[53]= list = Drop[list, 3]; listz = Drop[listz, 5];
          |elimina          |elimina
results = Prepend[Partition[listz, 5], {"rd1", "rd2", "V", "energy", "time"}];
          |añade al- |particiona
MatrixForm[Transpose[results]]
          |forma de matriz |transposición
Out[54]/MatrixForm=
{rd1  0.468463  0.499689  0.536266  0.580683  0.63693  0.711729  0.817158  0.976955  1.24458  1.77298
 rd2  0.499694  0.536266  0.580683  0.63693  0.711729  0.817158  0.976955  1.24458  1.77298  3.26275
 V    1.00025  0.943668  0.899015  0.865596  0.843935  0.836309  0.848197  0.892418  1.0042  1.32975
 energy 0.0169488 0.0159899 0.0152333 0.014667 0.0143 0.0141708 0.0143722 0.0151215 0.0170157 0.0225318
 time  0.0338975 0.0319799 0.0304666 0.0293341 0.0286 0.0283416 0.0287445 0.0302431 0.0340313 0.0450636}
```

(\*Addition to show the total vapour generated, energy demand and time\*)

```
In[55]= Total[Drop[Transpose[results][[3]], 1]];
          |total |elim- |transposición
Print["Total vapour generated = ", Total[Drop[Transpose[results][[3]], 1]], " mol"];
          |escribe          |total |elim- |transposición
Total[Drop[Transpose[results][[4]], 1]];
          |total |elim- |transposición
Print["Total energy demand = ", Total[Drop[Transpose[results][[4]], 1]], " kWh"];
          |escribe          |total |elim- |transposición
Total[Drop[Transpose[results][[5]], 1]];
          |total |elim- |transposición
Print["Total time = ", Total[Drop[Transpose[results][[5]], 1]], " hours"];
          |escribe          |total |elim- |transposición
```

Total vapour generated = 9.46334 mol

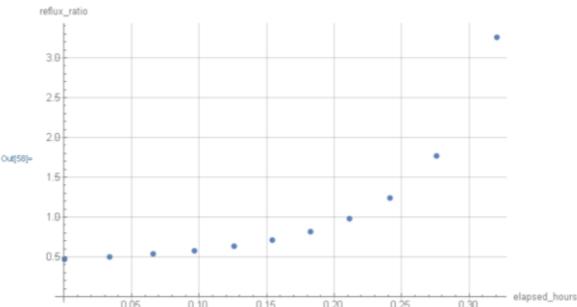
Total energy demand = 0.160351 kWh

Total time = 0.320702 hours

```

IN57)- (*Creation of a graph that plots the reflux ratio variation over time*)
reflux = Drop[Append[Transpose[results][[1]], Transpose[results][[2, INT + 1]], 1];
acctime = Accumulate[Prepend[Drop[Transpose[results][[5]], 1], 0]];
ListPlot[Table[{acctime[[i]], reflux[[i]], {i, 1, INT + 1}], AxesLabel -> {elapsed_hours, reflux_ratio}, GridLines -> Automatic]

```



(\*Construction of a matrix that shows how the upper plate remains constant along time to provide a uniform distillate while the bottom one is getting poorer in the volatile compound and increasing its temperature\*)

```

IN58)- MatrixForm[Partition[Join[Prepend[Partition[Join[Table[Partition[list, 33][[1]][[4]], {i, 1, 3}],
forma de mat- |particiona |junta |añade a-- |particiona |junta |tabla |particiona
Table[Partition[list, 33][[1]][[4]], {i, 1, 3}], Prepend[Partition[Join[Table[Partition[list, 33][[1]][[4]], {i, 1, 3}],
|tabla |particiona |añade a-- |particiona |junta |tabla |particiona
Table[Partition[list, 33][[2]][[4]], {i, 31, 33}], 3], {x, y, T}], Prepend[Partition[Join[Table[Partition[list, 33][[1]][[4]], {i, 1, 3}],
|tabla |particiona |añade a-- |particiona |junta |tabla |particiona
Table[Partition[list, 33][[4]][[4]], {i, 31, 33}], 3], {x, y, T}], Prepend[Partition[Join[Table[Partition[list, 33][[1]][[4]], {i, 1, 3}],
|tabla |particiona |añade a-- |particiona |junta |tabla |particiona
Table[Partition[list, 33][[6]][[4]], {i, 31, 33}], 3], {x, y, T}], Prepend[Partition[Join[Table[Partition[list, 33][[1]][[4]], {i, 1, 3}],
|tabla |particiona |añade a-- |particiona |junta |tabla |particiona
Table[Partition[list, 33][[8]][[4]], {i, 31, 33}], 3], {x, y, T}], Prepend[Partition[Join[Table[Partition[list, 33][[1]][[4]], {i, 1, 3}],
|tabla |particiona |añade a-- |particiona |junta |tabla |particiona
Table[Partition[list, 33][[10]][[4]], {i, 31, 33}], 3], {x, y, T}], Prepend[Partition[Join[Table[Partition[list, 33][[1]][[4]], {i, 1, 3}],
|tabla |particiona |añade a-- |particiona |junta |tabla |particiona
Table[Partition[list, 33][[12]][[4]], {i, 31, 33}], 3], {x, y, T}], Prepend[Partition[Join[Table[Partition[list, 33][[1]][[4]], {i, 1, 3}],
|tabla |particiona |añade a-- |particiona |junta |tabla |particiona
Table[Partition[list, 33][[14]][[4]], {i, 31, 33}], 3], {x, y, T}], Prepend[Partition[Join[Table[Partition[list, 33][[1]][[4]], {i, 1, 3}],
|tabla |particiona |añade a-- |particiona |junta |tabla |particiona
Table[Partition[list, 33][[16]][[4]], {i, 31, 33}], 3], {x, y, T}], Prepend[Partition[Join[Table[Partition[list, 33][[1]][[4]], {i, 1, 3}],
|tabla |particiona |añade a-- |particiona |junta |tabla |particiona
Table[Partition[list, 33][[18]][[4]], {i, 31, 33}], 3], {x, y, T}], Prepend[Partition[Join[Table[Partition[list, 33][[1]][[4]], {i, 1, 3}],
|tabla |particiona |añade a-- |particiona |junta |tabla |particiona
Table[Partition[list, 33][[20]][[4]], {i, 31, 33}], 3], {x, y, T}], 3]]

```

---

( x )	( 0.986363 )	( 0.630951 )
( y )	( 0.997069 )	( 0.889405 )
( T )	( 194.193 )	( 203.117 )
( x )	( 0.986363 )	( 0.588027 )
( y )	( 0.997069 )	( 0.870365 )
( T )	( 194.193 )	( 204.817 )
( x )	( 0.986363 )	( 0.542976 )
( y )	( 0.997069 )	( 0.84822 )
( T )	( 194.193 )	( 206.744 )
( x )	( 0.986363 )	( 0.495641 )
( y )	( 0.997069 )	( 0.822143 )
( T )	( 194.193 )	( 208.929 )
( x )	( 0.986363 )	( 0.445844 )
( y )	( 0.997069 )	( 0.790989 )
( T )	( 194.193 )	( 211.402 )
( x )	( 0.986363 )	( 0.393386 )
( y )	( 0.997069 )	( 0.753111 )
( T )	( 194.193 )	( 214.203 )
( x )	( 0.986363 )	( 0.33805 )
( y )	( 0.997069 )	( 0.706071 )
( T )	( 194.193 )	( 217.374 )
( x )	( 0.986363 )	( 0.279584 )
( y )	( 0.997069 )	( 0.646079 )
( T )	( 194.193 )	( 220.967 )
( x )	( 0.986363 )	( 0.217723 )
( y )	( 0.997069 )	( 0.566943 )
( T )	( 194.193 )	( 225.039 )
( x )	( 0.986363 )	( 0.152161 )
( y )	( 0.997069 )	( 0.457756 )
( T )	( 194.193 )	( 229.658 )
( x )	( 0.986363 )	( 0.0825545 )
( y )	( 0.997069 )	( 0.297389 )
( T )	( 194.193 )	( 234.904 )

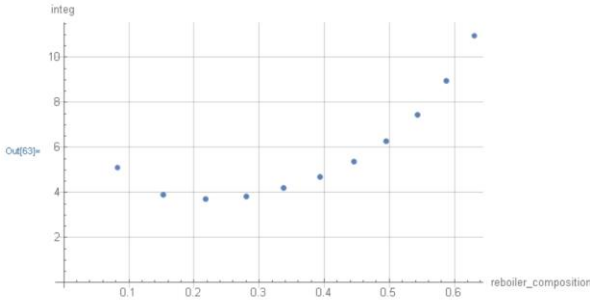
---

(\*Generation of a graph that shows how the integral draws a parabola thus justifying the resolution of this problem using small intervals to improve the accuracy of results\*)

```

In[60]:= listv = Drop[listv, 2]; listw = Drop[listw, 2]; integral = Join[listv, listw];
           |elimina          |elimina          |junta
           |-----|-----|-----
integral = Prepend[Partition[integral, 2], {"xx", "int"}]; MatrixForm[Transpose[integral]];
           |añade a...|particiona          |forma de mat...|transposición
           |-----|-----|-----
x = Drop[Transpose[integral][[1]], 1]; int = Drop[Transpose[integral][[2]], 1];
           |elim...|transposición          |elim...|transposición
           |-----|-----|-----
ListPlot[Table[{x[[i]], int[[i]]}, {i, 1, INT * 2}], AxesLabel -> {reboiler_composition, integ}, GridLines -> Automatic]
           |represen...|tabla          |etiqueta de ejes          |parrilla de li...|automático

```



## APPENDIX 2: REAL DISTILLATION COLUMN

```

h[-] Quit[]
system('clear')

h[0] (*
(* Input values *)
(* p = pressure [Pa]; Fm = kg of feed (F); Fp = % of MEG in the feed; Dp = Constant = % of MEG in the distillate (D);
Rp = % of MEG in the reboiler(R); λ = molar latent heat [J/mol]; Q = power of the reboiler [W]; MWMEG = molar mass of MEG;
MWDEG = molar mass of DEG; c = % of MEG in the last stage*)
p = 100000;
Fm = 2.09; Fp = 13; c = 96.8; f = 0.365;
MWMEG = 0.062; MWDEG = 0.106;
(*Introduce the previously calculated relative volatility equation highlighted in grey and replace x by p*)
α = 4.625282642123176 + 1.405129451139797 * 10^-6 p - 6.198082280842811 * 10^-12 p^3;
(*Introduce the previously calculated equilibrium temperature equation highlighted in red*)
temp[x, y, _1] := 442.6688229674054 + 0.0011896095099302557 x - 4.704782397480638 * 10^-9 x^2 - 73.09209593852118 y - 0.00010804948392970379 x y + 36.34886672394359
x1[y, _1] :=  $\frac{y}{y + \alpha - y\alpha}$ 
y1[x, _1] :=  $\frac{\alpha x}{1 + (\alpha - 1)x}$ 
x2[y, _1] :=  $\frac{y}{y + f\alpha - yf\alpha}$ 
y2[x, _1] :=  $\frac{f\alpha x}{1 + (f\alpha - 1)x}$ 

Dp =  $\frac{100 \text{ MWMEG } y1\left[\frac{c}{c} \frac{\text{MWMEG}}{(100-c)}\right]}{\text{MWDEG} \left(1 - y1\left[\frac{c}{c} \frac{\text{MWMEG}}{(100-c)}\right]\right) + \text{MWMEG } y1\left[\frac{c}{c} \frac{\text{MWMEG}}{(100-c)}\right]}$ ;

xF =  $\frac{\frac{Fp}{\text{MWMEG}}}{\frac{Fp}{\text{MWMEG}} + \frac{(100-Fp)}{\text{MWDEG}}}$ ; F =  $\frac{Fm}{xF \text{ MWMEG} + (1 - xF) \text{ MWDEG}}$ ; xD =  $\frac{\frac{Dp}{\text{MWMEG}}}{\frac{Dp}{\text{MWMEG}} + \frac{(100-Dp)}{\text{MWDEG}}}$ ;

Dp =  $\frac{100 \text{ MWMEG } y1\left[\frac{c}{c} \frac{\text{MWMEG}}{(100-c)}\right]}{\text{MWDEG} \left(1 - y1\left[\frac{c}{c} \frac{\text{MWMEG}}{(100-c)}\right]\right) + \text{MWMEG } y1\left[\frac{c}{c} \frac{\text{MWMEG}}{(100-c)}\right]}$ ;

xF =  $\frac{\frac{Fp}{\text{MWMEG}}}{\frac{Fp}{\text{MWMEG}} + \frac{(100-Fp)}{\text{MWDEG}}}$ ; F =  $\frac{Fm}{xF \text{ MWMEG} + (1 - xF) \text{ MWDEG}}$ ; xD =  $\frac{\frac{Dp}{\text{MWMEG}}}{\frac{Dp}{\text{MWMEG}} + \frac{(100-Dp)}{\text{MWDEG}}}$ ;

Print["Pressure = ", p, " Pa", " α = ", α]
|describe
Print["Fm = ", Fm, " kg of F", " F = ", F, " mol"]
|describe
Print["Fp = ", Fp, "% of MEG in F", " xF = ", xF]
|describe
Print["Dp = ", Dp, "% of MEG in D", " xD = ", xD]
|describe

```

Pressure = 100000 Pa    α = 4.70381

Fm = 2.09 kg of F    F = 21.536 mol

Fp = 13% of MEG in F    xF = 0.203485

Dp = 99.3021% of MEG in D    xD = 0.995906



(\*Introduce the desired amount of plates (ne) considering two more will be added during the calculations since the column is operating batch-wise and the column includes a partial condenser\*)

```
w[0] = ne = 10; rD1 = 200;
Print["r/d1 = ", rD1];
Do[
  Begin[
    lista = {x0, xD};
    n = 0;
    yy = 
$$\frac{rd1}{rd1 + 1} xD + \frac{1}{rd1 + 1} x0$$
;
    xx = x1[yy];
    n = n + 1;
    Print["n = ", n, " x = ", xx, " y = ", yy, " T(°C) = ", temp[p, xx] - 273, " w/w% in liquid phase = ", 
$$\frac{100 \text{ PBREG } xx}{\text{PBDEG} - \text{PBDEG } xx + \text{PBREG } xx}$$
, " w/w% in vapour phase = ", 
$$\frac{100 \text{ PBREG } yy}{\text{PBDEG} - \text{PBDEG } yy + \text{PBREG } yy}$$
];
    lista = Append[lista, xx];
    lista = Append[lista, yy];
  ]
]
Do[
  {
    yy = 
$$\frac{rd1}{rd1 + 1} xx + \frac{1}{rd1 + 1} x0$$
;
    lista = Append[lista, xx];
    lista = Append[lista, yy];
    xx = x2[yy];
    lista = Append[lista, xx];
    lista = Append[lista, yy];
    n = n + 1;
  }
]
Print["n = ", n, " x = ", xx, " y = ", yy, " T(°C) = ", temp[p, xx] - 273, " w/w% in liquid phase = ", 
$$\frac{100 \text{ PBREG } xx}{\text{PBDEG} - \text{PBDEG } xx + \text{PBREG } xx}$$
, " w/w% in vapour phase = ", 
$$\frac{100 \text{ PBREG } yy}{\text{PBDEG} - \text{PBDEG } yy + \text{PBREG } yy}$$
], {ne}];

yy = 
$$\frac{rd1}{rd1 + 1} xx + \frac{1}{rd1 + 1} x0$$
;
lista = Append[lista, xx];
lista = Append[lista, yy];
xx = x1[yy];
lista = Append[lista, xx];
lista = Append[lista, yy];
n = n + 1;
Print["n = ", n, " x = ", xx, " y = ", yy, " T(°C) = ", temp[p, xx] - 273, " w/w% in liquid phase = ", 
$$\frac{100 \text{ PBREG } xx}{\text{PBDEG} - \text{PBDEG } xx + \text{PBREG } xx}$$
, " w/w% in vapour phase = ", 
$$\frac{100 \text{ PBREG } yy}{\text{PBDEG} - \text{PBDEG } yy + \text{PBREG } yy}$$
];
yy = 
$$\frac{rd1}{rd1 + 1} xx + \frac{1}{rd1 + 1} x0$$
;
lista = Append[lista, xx];
lista = Append[lista, yy];
xx = x2[yy];
lista = Append[lista, xx];
lista = Append[lista, yy];
n = n + 1;
Print["n = ", n, " x = ", xx, " y = ", yy, " T(°C) = ", temp[p, xx] - 273, " w/w% in liquid phase = ", 
$$\frac{100 \text{ PBREG } xx}{\text{PBDEG} - \text{PBDEG } xx + \text{PBREG } xx}$$
, " w/w% in vapour phase = ", 
$$\frac{100 \text{ PBREG } yy}{\text{PBDEG} - \text{PBDEG } yy + \text{PBREG } yy}$$
];
lista = Partition[lista, 2];
```

```
r/d1 = 200
1  xr = 0.981031  y = 0.995906  T(°C) = 195.625  w/w% in liquid phase = 96.8  w/w% in vapour phase = 99.3021
2  x = 0.967993  y = 0.981105  T(°C) = 196.719  w/w% in liquid phase = 94.6494  w/w% in vapour phase = 96.8123
3  x = 0.946508  y = 0.968132  T(°C) = 198.522  w/w% in liquid phase = 91.1891  w/w% in vapour phase = 94.6721
4  x = 0.911943  y = 0.946754  T(°C) = 201.421  w/w% in liquid phase = 85.8306  w/w% in vapour phase = 91.2281
5  x = 0.858428  y = 0.912361  T(°C) = 205.911  w/w% in liquid phase = 78.0055  w/w% in vapour phase = 85.8939
6  x = 0.7803  y = 0.859112  T(°C) = 212.466  w/w% in liquid phase = 67.5049  w/w% in vapour phase = 78.1021
7  x = 0.6755  y = 0.781373  T(°C) = 221.258  w/w% in liquid phase = 54.9057  w/w% in vapour phase = 67.6422
8  x = 0.549817  y = 0.677094  T(°C) = 231.803  w/w% in liquid phase = 41.6691  w/w% in vapour phase = 55.0859
9  x = 0.417848  y = 0.552037  T(°C) = 242.875  w/w% in liquid phase = 29.5688  w/w% in vapour phase = 41.8873
10 x = 0.297273  y = 0.420724  T(°C) = 252.99  w/w% in liquid phase = 19.8353  w/w% in vapour phase = 29.8153
11 x = 0.200327  y = 0.300749  T(°C) = 261.124  w/w% in liquid phase = 12.78  w/w% in vapour phase = 20.1003
12 x = 0.0517548  y = 0.204285  T(°C) = 273.589  w/w% in liquid phase = 3.09363  w/w% in vapour phase = 13.0559
```

in[39] = (\*This instruction plots the graph and shows a comparison between the theoretical value of the feed composition and the one obtained\*)

```
Print["xF = ", lista[[2 ne + 2]][[1]], " xF = ", xF]
```

escribe

```
graf = Plot[ $\left\{ \frac{\alpha x}{1 + (\alpha - 1)x}, \frac{f \alpha x}{1 + (f \alpha - 1)x}, x, \frac{rd1}{rd1 + 1} x + \frac{1 xD}{rd1 + 1} \right\}$ , {x, 0, 1}, Frame -> True,
```

```
GridLines -> Automatic, PlotRange -> {{0, 1}, {0, 1}}, GridLines -> Automatic, DisplayFunction -> Identity];
```

```
graf1 = ListPlot[lista, PlotStyle -> PointSize[.005], PlotRange -> {{0, 1}, {0, 1}}, DisplayFunction -> Identity];
```

```
graf2 = ListPlot[lista, PlotJoined -> True, PlotRange -> {{0, 1}, {0, 1}}, DisplayFunction -> Identity];
```

```
Show[graf, graf1, graf2, DisplayFunction -> $DisplayFunction]
```

$x_F = 0.200327$      $x_F = 0.203485$

