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Model and Simulation of binary distillation column using data obtained from the UNIFAC method

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BACKGROUND
Distillation is a unit operation, it arises thousands years ago and continues to be widely used for separating mixtures, maintaining great importance in the chemical and oil industry, process started to be used in the form distillation columns of continuous operation, to be able to predict the operation of these equipment, it becomes necessary the study of the mathematical models.

OBJECTIVE
Modeling and simulation of a binary distillation column using as input data obtained from UNIFAC method.

RESULTS
The lower reflux reduces the concentration of the more volatile component in the distillate, being directly proportional. The range of linearity was estimated and had a value of 5,105.

CONCLUSION
By including the UNIFAC method allows to evaluate different types of substances and circumstances, so the scope of the general model of the column, which in this case is not limited to a single binary blend, is increased.

KEY WORDS
Binary Distillation, UNIFAC, VLE, Simulation, Model, MATLAB.

INTRODUCTION

Distillation is the most popular method of separation in the chemical and petrochemical industry, and one of the most studied in terms of control [1], [2]. This process consists of separating mixtures based on the difference in volatility of the components, through the application of heat flow, obtaining desired concentrations in the condensing and reboiler systems [3].

This process has a power supply located in the reboiler, where the highest temperature of the process is present and where the same energy is delivered. To close the cycle, the system has a sink located in the condenser, which removes the remaining surplus energy of the process[4].

Distillation units account for approximately 3% of global energy consumption [5]. Because of the cost, the need to minimize consumption, maximize results and avoid instability of the process. This instability can cause disruptions on the ground, low product quality and / or changes in the environment[4].

An effective way to optimize the distillation process is using precise mathematical models [6]. This helps to stimulate and control the processes of distillation and thus reduce energy consumption [7].

By simulating this process through a computer, it allows to make a controlled experiment, which is necessary in the engineering processes for decision making at critical points, planning and project design[8]. Likewise, it used to prevent certain behaviors of processes, without putting at risk the actual process and provide accurate information, even with minor differences between the actual operations and simulation [9].

Among works related to distillation, is the reference adaptive control of binary distillation column based on the Trieu Minh Vu and John Pumwa model [3], [10]. Likewise, the basic model and simulation of a binary distillation column, which made a representation to scale the team and focus on the dynamics of the concentration of material can be seen in [2].

In [11], a transfer model input / output binary distillation columns derived from differential equations is presented, where a linear representation and the simulation is obtained from unit cryogenic air separation data.

Based on the above, this paper presents the modeling and simulation of a binary distillation column using as input data obtained from UNIFAC method. The binary column is being modeled in continuous operation, with one input, two outputs and internal variables per number of stages. Being the main contribution, the development of this non-linear model involving the overall mass balance, mass by component, energy balance and corresponding thermodynamic relations, by implementing the UNIFAC method. In addition to the results of the behavior of the model regarding the mixture to be worked.

MATERIALS Y METHODS

Distillation is a physical process that allows separating a liquid mixture into its components [12]. When the mixture is vaporized, the vapor will have a different residual liquid composition. At the top of the column vapor is condensed, the product is distilled and the residual product is called bottom[13]. Figure 1 presents the basic scheme.

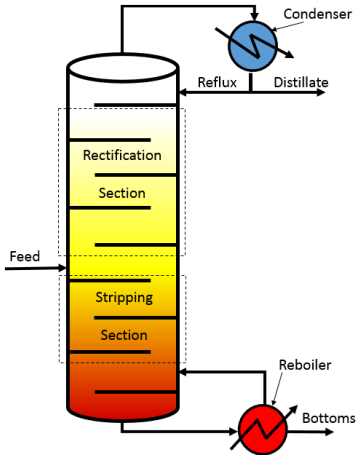

Fig. 1: Diagram of Binary Distillation Column

Given the complexity representing a complete modeling of the process, the following assumptions were established, considering that in each stage, mass transfer between the phases occurs instantaneously, all outflow from the column are liquid. A total condenser is modeled, with the assumption that the liquid coming out of it, is at a temperature below the boiling point and the pressure is constant in each stage, each one having 100% efficiency. The model is based on the scheme of the distillation column, shown in Figure 1.

The distillation column models are classified into three groups, fundamental model, empirical model and hybrid model [1],[2]. In this project, the fundamental model is used instead of the empirical model, due to the first allow to understand the dynamics of the distillation columns, and the latter not being optimal to predict the behavior of the system operating conditions[14].

To obtain the model, the equilibrium equations of general mass, by component and emerging balances are taking into accounts, depending on the mole fractions and the input variables [15]. According to the schematic design in Figure 1, the study is divided into four stage. These are the exhaustion or rectification stage, the feeding stage, reboiler and condenser stage.

Stage of rectification:

Figure 2 shows, the flows associated to the stage i. using the balance variables and initial considerations, in order to proceed to determine the system.

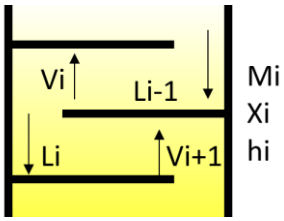

Fig. 2: Correction Stage Diagram

In Equation 1, the liquid and vapor into and out of the stage are taken into account, in order to obtain the mass balance.

$$\frac{d(Mi)}{dt} = L_{i-1} - L_i + V_{i+1} - V_i \quad (1)$$

Where L is the liquid flow, V is the flow of steam and M is the mass quantity. For the component mass balance, must take into account the concentration of the most volatile material in the liquid and the vapor flow of the element, resulting in total mass by composition. The total mass is represented in Equation 2.

$$\frac{d(MiXi)}{dt} = L_{i-1}X_{i-1} - L_iX_i + V_{i+1}Y_{i+1} - V_iY_i \quad (2)$$

Where X is the concentration of the more volatile liquid component and Y is the concentration of steam-volatile element. Additionally, the energy balance is formulated by using the same principle of the product of the liquid and vapor flow with enthalpy. The formula can be seen in equation 3.

$$\frac{d(Mihi)}{dt} = L_{i-1}h_{i-1} - L_ih_i + V_{i+1}H_{i+1} - V_iH_i - \beta_{Ai} \quad (3)$$

Where H is the enthalpy vapor, h is the enthalpy in liquid and β_{Ai} represents the adiabatic losses taken into the system.

Feed Stage:

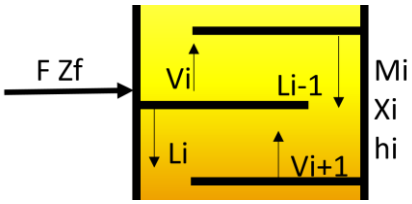

Fig. 3: Diagram of feed stage

This stage is characterized by an outer flow F, where Zf is the composition of the components, Tf is their temperature. These conditions are assumed to be known. The methodology is the same for the following stages shown in figure 3, represented by equations 4,5 and 6.

$$\frac{d(Mi)}{dt} = L_{i-1} - L_i + V_{i+1} - V_i + F \quad (4)$$

Where F is the feed flow entering the distillation column.

$$\frac{d(MiXi)}{dt} = L_{i-1}X_{i-1} - L_iX_i + V_{i+1}Y_{i+1} - V_iY_i + FZf \quad (5)$$

Where Zf is the composition of the liquid mixture feed flow.

$$\frac{d(Mihi)}{dt} = L_{i-1}h_{i-1} - L_ih_i + V_{i+1}H_{i+1} - V_iH_i + Fhf - \beta_{Ai} \quad (6)$$

Where hf is the enthalpy of the feed stream.

Reboiler:

As shown in Figure 4, in this heat exchanger, two flows are brought into countercurrent indirect contact, at different temperatures, in a period of time, resulting in loss during the heat exchange between the flows.

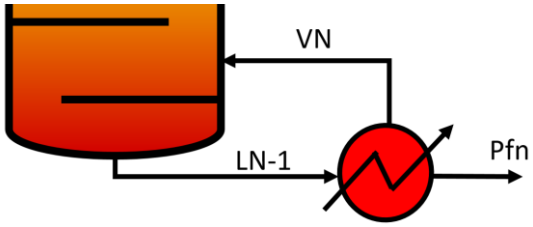

Fig. 4: Reboiler diagram

The liquid leaving the bottom of the column go to an exchanger and it is vaporized by the heat exchange that takes place inside. For the approximate balances, the same methodology in the rectification stage is used, through equations 7 and 8.

$$\frac{d(MN)}{dt} = L_{N-1} - V_N - Pf_N \quad (7)$$

Where Pf_N is the distillate product extracted from the stage N (Reboiler).

$$\frac{d(MNXN)}{dt} = L_{N-1}X_{N-1} - V_N Y_N - Pf_N X_N \quad (8)$$

Where X_N is the concentration of volatile component in the extracted product in stage N (reboiler). For the energy balance, the heat provided by the reboiler system and adiabatic losses are taken into account.

$$\frac{d(MNhN)}{dt} = L_{N-1}h_{N-1} - V_N H_N - Pf_N h_N - \beta_{AN} + QN \quad (9)$$

Where QN is the value added to the column through a reboiler, hn is the enthalpy of the distillate product (bottom), β_{AN} adiabatic losses in the reboiler

Condenser:

A total condenser is considered for this stage. This means that the steam that enters is completely transformed into liquid, independently of the flow of steam entering. The scheme of the condenser is shown in Figure 5.

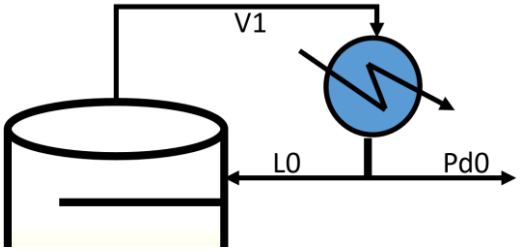

Fig. 5: Condenser Diagram

The following hypothesis is then formulated: the temperature of the liquid leaving the condenser is less than or equal to its boiling point. This difference is due to the fact that the liquid flowing in the cooling coil transfer a portion of its heat, before it exits definitively. It is considered as a supplementary parameter model. The methodology for which the balances are obtained is the same used in the course of rectification or exhaustion.

$$\frac{d(M0)}{dt} = V_1 - L_0 - Pd_0 \quad (10)$$

Where Pd_0 is the distillate product in the stage 0 (condenser).

$$\frac{d(M0X0)}{dt} = V_1 Y_1 - L_0 X_0 - Pd_0 X_0 \quad (11)$$

Where X_0 is the concentration of the most volatile product in the stage 0 (condenser).

$$\frac{d(M0h0)}{dt} = V_1 H_1 - L_0 h_0 - Pd_0 h_0 - \beta_{A0} + Q0 \quad (12)$$

Where Qo is the decreasing heat in the column through the condenser, ho is the enthalpy of the distillate (bottom) and β_{A0} adiabatic losses in the reboiler.

Summarizing the model, the system inputs are the feed flow *F*, the composition of the components of the feed mixture *ZF*, the adiabatic losses on each stage β_Ai, the temperature drop at the outflow of the condenser *T*,

the inlet temperature of the heating fluid entering the reboiler *TE*, the specific heat of the heating fluid *CP* and the construction coefficient of the reboiler *KConst*.

2.5 UNIFAC Method:

The UNIFAC method is a semi-empirical prediction system for activity coefficients of nonideal mixtures [16]. This uses the functional groups present in the molecules and through the interaction of each related coefficients [17]. The development of the algorithm is based on the mathematical model found in [18]. The related mathematical functions can be seen in equations 14, 15, 16.

The model has a combinatorial contribution to the activity coefficients and an essential residual energy for interactions, as can be seen in Equation 13.

$$\ln yi = lnyi^{C} + \ln yi^{R} \quad (13)$$

Where $lnyi^{C}$ is the combinatorial contribution and $lnyi^{R}$ is the residual contribution.

$$\ln yi^{C} = ln\left(\frac{\varphi_i}{\theta i}\right) + 1 - \frac{\varphi_i}{Xi} - \frac{Z}{2}\left[\ln\frac{\varphi_i}{Xi} + 1 - \frac{\varphi_i}{\theta i}\right] \quad (14)$$

Where φ_i is the molecular volume and θm is the area of the mole fraction.

$$\ln yi^{R} = \sum_k vk^{i}\,(\ln \tau k - \ln \tau k^{i}) \quad (15)$$

Where τk is the coefficient of residual activity

$$\ln \tau k = Qk[1 - \ln(\textstyle\sum_m \theta m Tmk) - \sum_n \theta n Tnm] \quad (16)$$

Where θm is the fraction of the area of the m group, Xm is the mole fraction of the m group and Tmk is the interaction parameter. The results are compared with experimental data taken from previous works [19]. The results can be seen in figure 6.

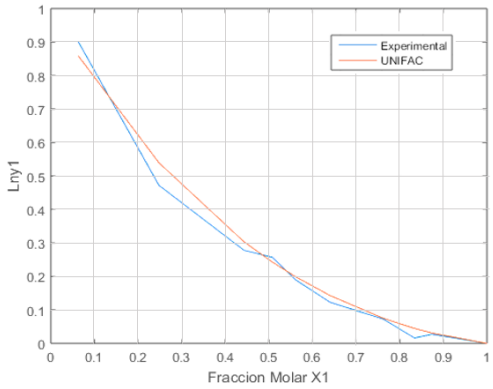

Fig. 6: Results UNIFAC VLE Di-ethyl Ketone(1) y n-Hexane(2) a 338.15 K

The theoretical value obtained by the resolution of the model corresponds to a good approximation to the real behavior of the mixture. Being the error of 1.01%.

$$Error = \sqrt{\frac{\sum_{i=1}^{n}(LnyExp - LnyUnifac)^2}{n}}$$

$$Error = 0.0101 = 1.01\%$$

The error proves that using the model as a data provider for the resolution of the distillation unit values is consistent with the actual behavior of the real counterpart. By integrating the UNIFAC method with the model of the column, the flow chart of Figure 7 is obtained.

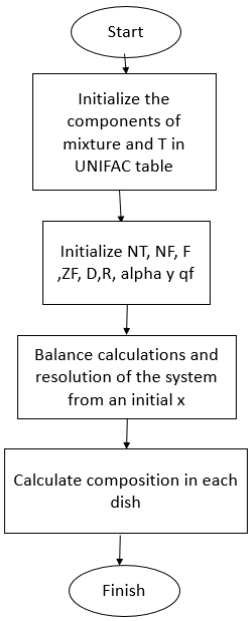

Fig. 7: Program Flow Chart

Through the program, the required data such as temperature are entered with the UNIFAC method. It then provides the behavior and the components of the mixture and the general model is complemented.

The UNIFAC method allows calculation of the activity coefficients, which correspond to the behavior of the mixture and allow adaptability model.

temperatura	325			UNO	DOS
grupo			subgrupo		
Alcano	1	1	CH3	1	1
		2	CH2	2	4
		3	CH		2
		4	C		
Alqueno	2	5	CH2=CH		
		6	CH=CH		
		7	CH2=C		
		8	CH=C		
		9	C=C		
Aromatico	3	10	ACH		
		11	AC		
	4	12	ACCH3		
		13	ACCH2		
		14	ACCH		
Alcohol	5	15	OH	1	
	6	16	CH3OH		
	7	17	H2O		
	8	18	ACOH		

x_1	0,34	y_1	2,14458
x_2	0,66	y_2	1,41552

Fig. 8: UNIFAC VLE

After entering the necessary data, the program proceeds to solve the system of equations and graphs, showing that correspond to the steady-state response of the distillation unit. To evaluate the results the estimated data are used to a distillation column referenced [14].

Given the mixture of ethanol and water, which flow (F) equal to 1 mol/min, composition(Z) value is 0.5 mol fraction and which state is a satured liquid represented by qf. The column has 41 stages (NT) and the feed stage (NF) is 21.

In figure 9, the behavior of concentration of the more volatile component in the fluid located in the distillation unit through the stages is shown. This value should approach “1” when it is on stage 0 (condenser) and “0” is observed in the stage 41 (reboiler).

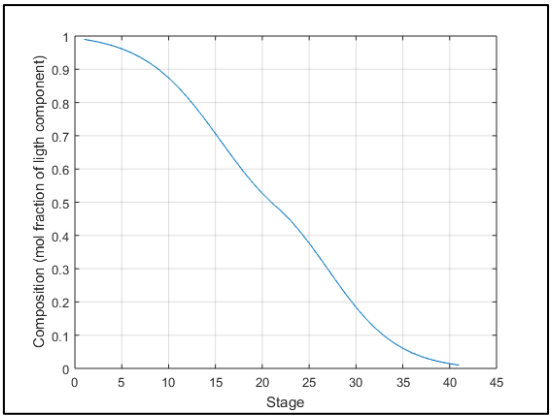

Fig. 9: Graph, concentration vs stages

To evaluate the model, a variation arises in the flow, which is decisive in the operation. The lower reflux reduces the concentration of the more volatile component in the distillate, being directly proportional. The range of linearity was estimated and had a value of 5.105, which can be seen in Figure 10.

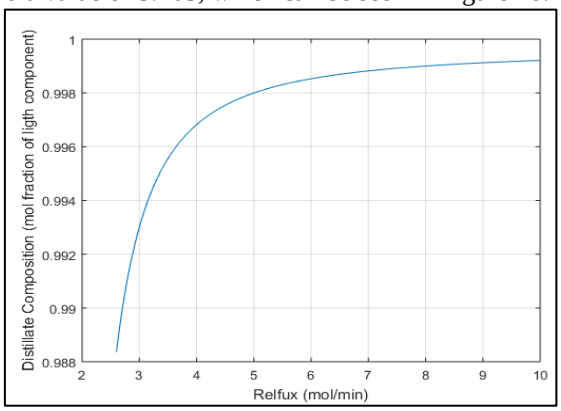

Fig. 10: Distillate concentration vs Reflux

In Figure 11, the concentration shown in the bottom based on the change of the reflux are shown. The concentration of the bottom is inversely proportional to the reflux, this is consistent with the estimate of the behavior shown in figure 10.

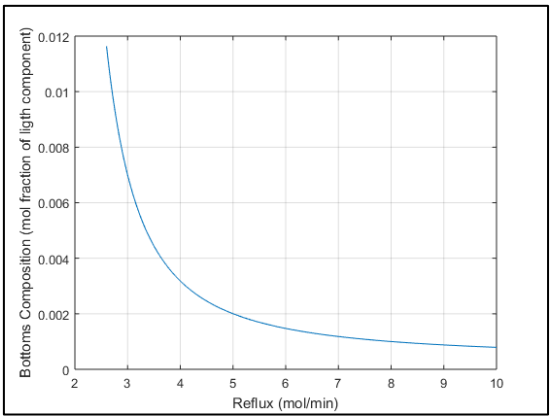

Fig. 11: Bottoms concentration - Reflux

Conclusions:

The model of the distillation column without thermodynamic implications has greater complexity, but results in behavior are very approximate, so the estimation of certain assumptions reduces the computation time used for the settlement.

By including the UNIFAC method allows to evaluate different types of substances and circumstances, so the scope of the general model of the column, which in this case is not limited to a single binary blend, is increased.

The input variables of the column and the number of stages and feed materials are directly related to the type of mixture, this should be estimated as best by some design method as McCabe-Thiele.

By changing the stationary model in relation to key variable in the operation of the column, the model must respond balancing of concentrations, making the obtained model similar to its real counterpart.

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REFERENCES

[1] Abdullah, Z., N. Aziz and Z. Ahmad, 2007. "Nonlinear Modelling Application in Distillation Column," *Chem. Prod. Process Model.*, 2: 3.

[2] Truong, H.S., I. Ismail and R. Razali, 2010. "Fundamental modeling and simulation of a binary continuous distillation column," *Intell. Adv. Syst. (ICIAS), Int. Conf.*, pp: 1-5

[3] George, A., P. Riya and M. Francis, 2015. "Model Reference Adaptive Control of Binary Distillation Column Composition using MIT Adaptive Mechanism," 4(06): 555-558.

[4] Ambrocio, A.L.P., C.A.M. Rebaza, W.C. Martinez and D.M. Sanchez, 2015. "DISEÑO E IMPLEMENTACION DE UN SISTEMA DE CONTROL DIFUSO A UNA COLUMNA DE DESTILACION," *Rev. Científica Ing.*, 2: 1.

[5] Rahimi, R., M.H. Soodmand, M. Zivdar, A. Alborzi and M. Rahmanian, 2015. "Modeling and Simulation of a Divided Wall Column for 1 , 3 Butadiene Purification," 12(1): 60-67.

[6] 2014. "Modeling and optimization of simultaneous photocatalysis of three dyes on ceramic-coated TiO2 nanoparticles using chemometrics methods: phytotoxicological," *Res. Chem*.

[7] Gil, I., J. Gómez and G. Rodríguez, 2012. "Control of an extractive distillation process to dehydrate ethanol using glycerol as entrainer," *Comput. Chem. Eng*.

[8] Ruiz, G.J., S.B. Kim, J. Moon, L. Zhang and A.A. Linninger, 2010. "Design and optimization of energy efficient complex separation networks," *Comput. Chem. Eng.*, 34(9): 1556-1563.

[9] Lee, S., D. Posarac and N. Ellis, 2011. "Process simulation and economic analysis of biodiesel production processes using fresh and waste vegetable oil and supercritical methanol," *Chem. Eng. Res. Des.*, 89(12): 2626-2642.

[10] Minh, V.T. and J. Pumwa, 2012. "Modeling and Adaptive Control Simulation for a Distillation Column," in *2012 UKSim 14th International Conference on Computer Modelling and Simulation*, pp: 61-65.

[11] Ammouri, F. and P. Rouchon, 2013. "Input / output transfer models of binary distillation columns derived from convection-diffusion partial differential equations," pp: 6136-6142.

[12] Luis, P., J. Degrève and B. Van der Bruggen, 2013. "Separation of methanol–n-butyl acetate mixtures by pervaporation: Potential of 10 commercial membranes," *J. Memb. Sci.*

[13] Sun, J., F. Wang, T. Ma, H. Gao, P. Wu and L. Liu, 2012. "Energy and exergy analysis of a five-column methanol distillation scheme," *Energy.*

[14] Skogestad, S., 2001. "Modelling and Dynamic Simulation for Process Control: Issues in dynamic modelling using distillation as an example," in *Modelling and Optimization of Chemical Processes.*

[15] Engineering, I., 2014. "Modeling and Control of Binary Distillation," pp: 105-111

[16] Pérez, O. and L. Zumalacárregui, 2010. "Simplificaciones en el Cálculo de Columnas de Destilación Alcohólica," 21(6): 103-112.

[17] Dong, L., D. Zheng, J. Li, N. Nie and X. Wu, 2013. "Suitability prediction and affinity regularity assessment of H2O+imidazolium ionic liquid working pairs of absorption cycle by excess property criteria and UNIFAC model," *Fluid Phase Equilib.*, 348: 1-8.

[18] Seader, J.D., W.D. Seider, D.R. Lewin, L. Boulle and A. Rycrof, 2006. *Separation Process Principles, 3rd Edition.*

[19] Smith, J.M., H.C. Van Ness and M.M. Abbott, 2005. *Introduction to chemical engineering thermodynamics*. McGraw-Hill.