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Mass Transfer Simulation of Liquid-Liquid Extraction Systems Using an Educational Software

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Abstract

In order to improve the learning process about the unit operation of Liquid Extraction, it is presented a GUI in Matlab® for designing extracting systems with different types of contact, where the stages reach the equilibrium between both liquid phases. The program called ExtractING is an application of theoretical studies and material balances presented in highly relevant documents and popular academic books, which has a general procedure that initiates by introducing feed and solvent quantities with their respective compositions, and a raffinate exit condition for multistage equipment. It is necessary to introduce the ternary system (solute, dissolvent, diluent) and an operating temperature to calculate equilibrium conditions with Van Laar activity model equations. Material balances, multiple iterative routines, and equilibrium diagrams were used to calculate raffinate and extract conditions in all the stages as well as the minimum number of stages needed for the required separation allowing the user to get the approximate size and cost of the equipment, making this software a powerful academic tool. With the program, it was compared the maximum separation for specified conditions between counter-current and crosscurrent equipment, the separation percentage behavior with an increasing feed quantity, and the separation behavior with variations of temperature.

Keywords: liquid-liquid extraction, graphical user interface, engineering education, Van Laar activity model

1. Introduction

Unit operation equipment has suffered important changes due to the advance in technology around the world creating a challenge to junior engineers in the computational area [1]. Generally, there are too many variables to manipulate in order to control some others [2]. It involves a refined training of engineers to assure in industrial processes high-quality products. In order to achieve this purpose, it is needed to prepare good professionals with specific training by introducing in their core curriculum laboratory practices, where the student can operate and study the behavior of the different variables involved in the unit operation being studied. One particular unit operation is the liquid-liquid extraction which is a complex operation due to the use of the equilateral triangular equilibrium diagram to graphically describe the concentrations in ternary systems [3]. It causes a complication at the time of running experiments in the laboratory because there are too many variables to manipulate to understand the complete process. In the academy, it is necessary to complement the knowledge obtained in experimental practices and in theoretical classes, with the implementation in the core program of a computer-based technology [4] that help the students to analyze the effect of more variables on the final product [5]. This technology could be the application of a user-friendly software [6] where the student can be able to understand and explain the phenomena happening inside a liquid-liquid extraction equipment using the most accepted equations and assumptions in this system when different operating conditions are changed. A new interactive graphical user interface made in Matlab to simulate liquid-liquid extraction systems is presented in this article, where the undergraduate students can manipulate different variables that let them understand the phenomena happening inside the operation. The students can see the effect of the temperature, number of stages, and feed to solvent ratio on the degree of solute separation. Th tool is an interactive software for studying liquid-liquid operations under a single stage, multistage crosscurrent, and multistage countercurrent using iterative routines and material balances, allowing the user to graphically visualize the operation.

2. Presentation of the Algorithm

The extraction problems, in general, can be solved by mass balances. It is used the Van Laar mathematical model for the calculation of solubility between liquids and the triangular diagram. The Van Laar activity model is implemented to describe the phase equilibrium in liquid mixtures, which is derived from the Van der Waals equation that assumes no volume change and zero entropy when mixing two pure liquids.

Equations 1, 2 and 3 are used to calculate the activity coefficient in a binary system.

$$Ln\gamma_i = A_{ij}\left(\frac{A_{ji}x_j}{A_{ij}x_i + A_{ji}x_j}\right)^2 \qquad (1)$$

$$Ln\gamma_j = A_{ji}\left(\frac{A_{ij}x_i}{A_{ji}x_j + A_{ij}x_i}\right)^2 \qquad (2)$$

$$A_{ji} = \frac{A_{ji}'}{RT} \qquad (3)$$

Where γ_i is the activity coefficient for component *i*, x_i is the composition for component *i*, A_{ji} is the binary interaction parameter between *i* and *j*. Three types of separation are used, the first one is the single stage extraction that consists of a simple contact calculation process. The second type of separation is the crosscurrent extraction, which is a succession of one-step extraction where the total amount of solvent is subdivided, and one part is mixed in each step. The refining of each step is brought into contact with a new solvent in the following, separating a new extract. This method is used in the industry, especially when the solute is highly miscible in the solvent, and the solvent recovery is unnecessary or very economical [7, 8]. The third type of separation is the countercurrent extraction with several stages. In this type, the feed and the solvent enter from opposite ends of the system, so that the fresh feed is contacted with a concentrated solvent and the fresh solvent is contacted with the less concentrated raffinate.

With the equations 1, 2 and3 and the types of separation mentioned, it was created the program ExtractING V1.0 designed for liquid-liquid extraction.

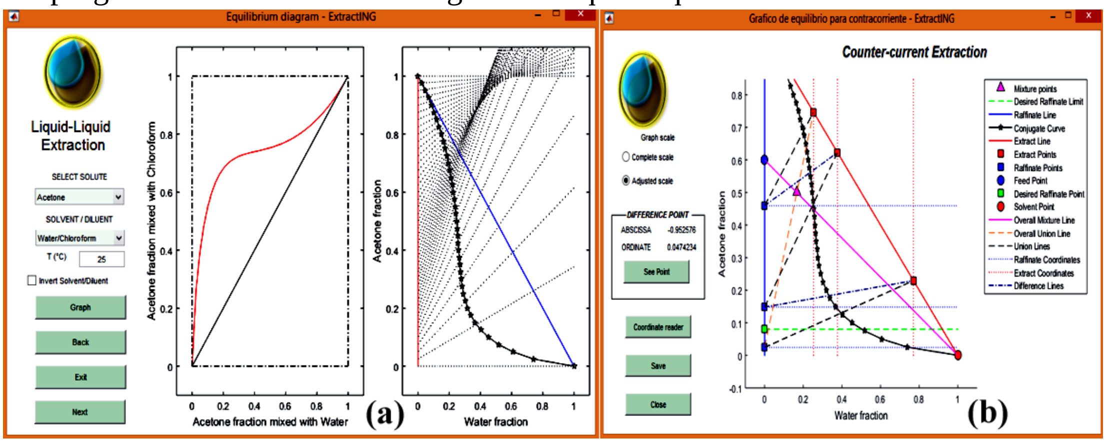

Figure 1. Output of the L-L extraction program (a) Equilibrium diagram for a system (b) Equilibrium diagram with a solved problem in countercurrent contact.

This program has an easy-to-use graphical interface, which is aimed at students, teachers, and professionals of chemical engineering as a design tool for liquid-liquid extraction. Figure 1a shows images for the equilibrium diagram calculation for a specified system (Acetone-Water-Chloroform) and figure 1b shows a countercurrent contact problem already solved with its respective equilibrium diagram representation.
The computer flowchart for countercurrent contact is shown in Figure 2. As it can be seen, material balances initiate with feed and solvent quantities and their respective solute, solvent and diluent compositions. To establish a limit on the equipment size, it is introduced an exit limit that is the maximum allowable solute fraction in raffinate.

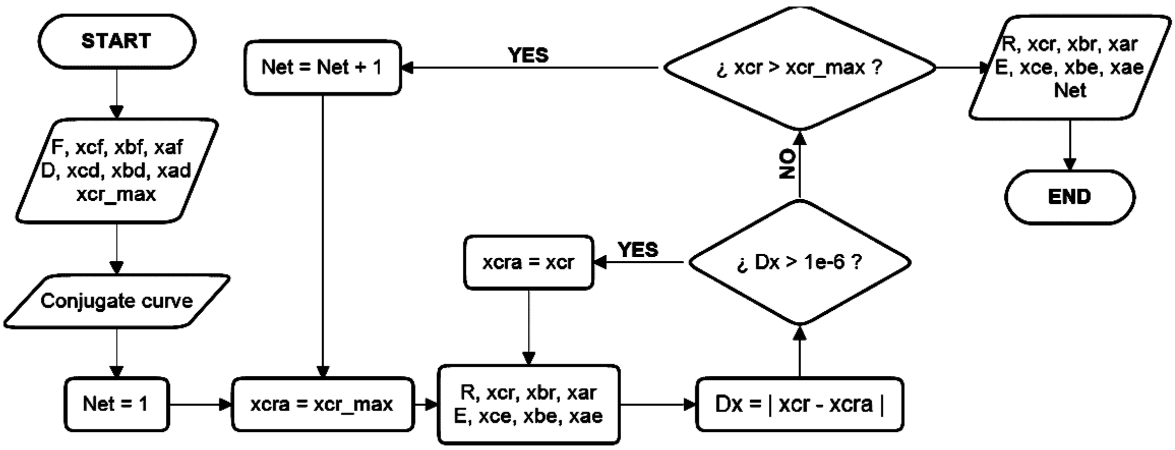

Figure 2. Flowchart for multistage countercurrent Liquid-Liquid extraction

3. Result and Discussion

Three case studies were analyzed with the help of the software ExtractING V1.0

Case study 1: Determination of the number of stages
In order to obtain an appropriate value of the number of stages and to obtain a specified separation percentage, it is necessary to introduce the feed and solvent flow with their respective compositions. It will be used the separation of an Acetone-Water-Chloroform system at 25°C, to separate the acetone diluted (solute) in a stream with chloroform (diluent) using water as a solvent. The following operating conditions were given: Feed (F): 300 kg with a composition of 60% Acetone and 40% chloroform. Solvent (D): 50 kg, 100% Water.

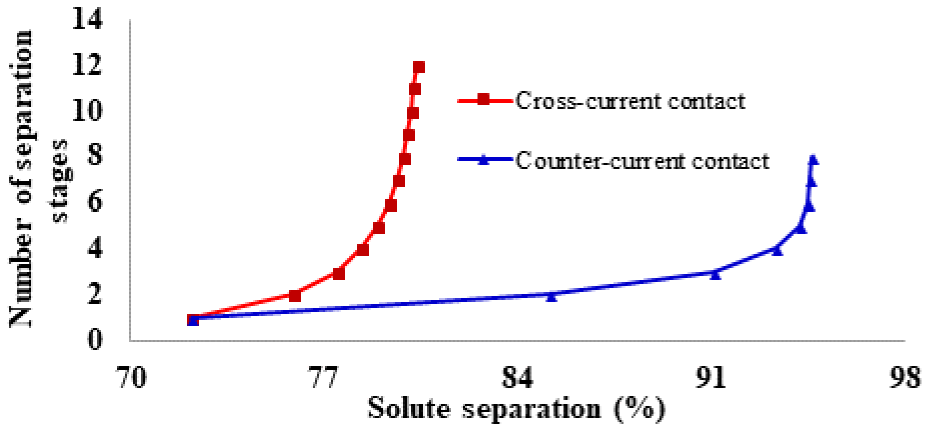

Figure 3. Behavior of the number of stages in the solute separation for cross and counter current contact.

As can be seen in Figure 3, the separation obtained with the multistage countercurrent contact using a small number of stages is higher than that the obtained with the cross-current contact, reaching a maximum separation percentage of approximately 96% while it was obtained 80% of separation for cross-current contact. A counter-current operation system would be more recommended instead of a cross current system. Both lines have an asymptotic behavior, which means that an increase in the number of separation steps does not have a considerable effect on solute removal.

Case study 2: Effect of feed to solvent ratio on the percentage of separation

In this case study, the behavior of the separation of different equipment will be evaluated when the load of the currents is varied. The amount of total solvent is maintained constant, and the feed amount is gradually increased to increase the feed to the solvent ratio (F / D). The mixture of Acetone-Water-Chloroform was treated with the aim to separate the acetone diluted (solute) in a stream with chloroform (diluent), using water as a solvent. The given operating conditions for the Feed (F) is variable but contains a composition of 60% Acetone and 40% chloroform. The amount of solvent (D) is 50 kg containing 100% Water.
Using the ExtractING program, data were obtained to analyze the effect of the load ratio in the percentage of separation obtained for each type of contact. The results are shown in Figures 4.

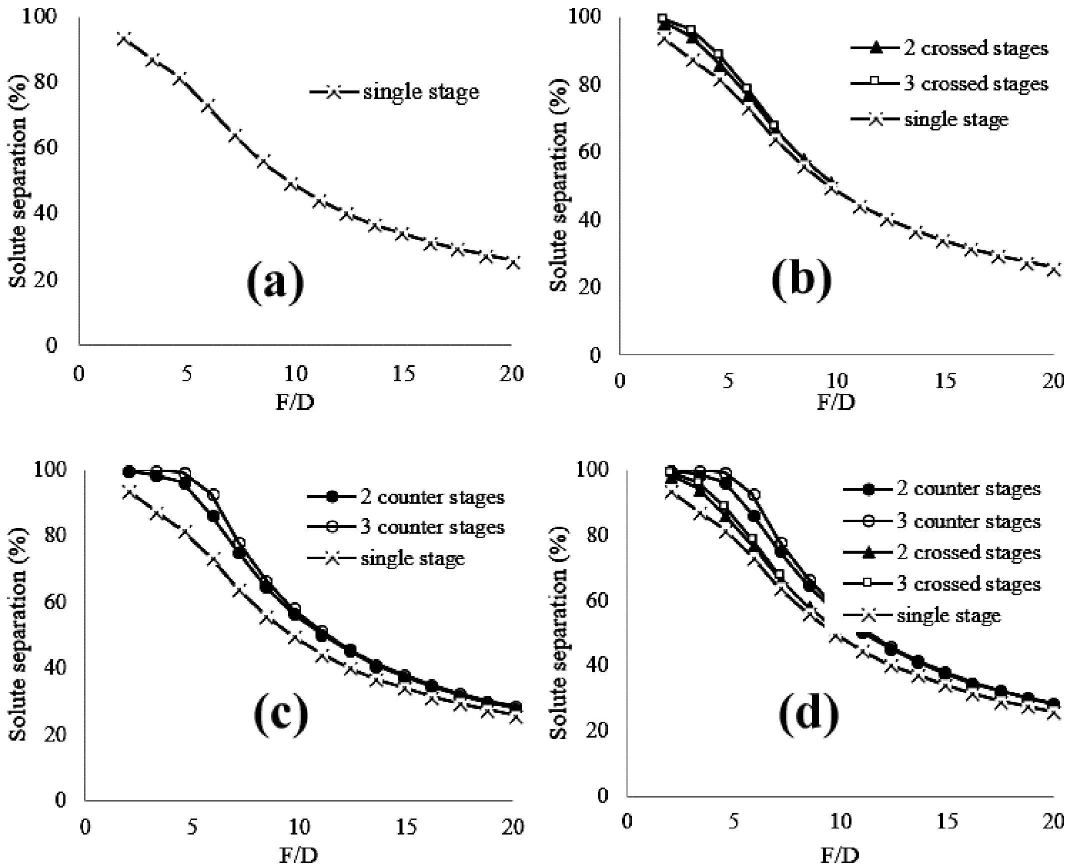

Figure 4. Behavior of the degree separation as a function of F/D a) Single stage, b) Crosscurrent, c) Countercurrent, d) Comparison crosscurrent - countercurrent

Figure 4a, b, c, and d show that an increase in the ratio feed/solvent causes a decrease in the percentage of solute separation, regardless of the type of contact.
When using a cross-current contact in the range of F/D from 2 to 10, the higher the number of stages, the higher the separation (see figure 4b). For ratios of F/D>10, the number of stages does not affect the degree of separation, so it is recommended to work with the lowest number of stages in this range. A similar behavior is obtained when using countercurrent contact (see figure 4c). However, with the use of countercurrent contact, higher degrees of separation are obtained when using the same number of stages (see figure 4 d). This pattern is maintained in the range of F/D from 2 to 20. For ratios of F/D>20, the separation tends to the same value, 20.

Case study 3: Effect of temperature on the percentage of separation

The effect of a temperature on the separation of fixed amounts of food and solvent was evaluated while maintaining constant the respective compositions of the mixture. The following operating conditions were given: 300 kg of Feed (F) with a composition of 60% Acetone and 40% chloroform. Solvent (D): 50 kg, 100% Water.

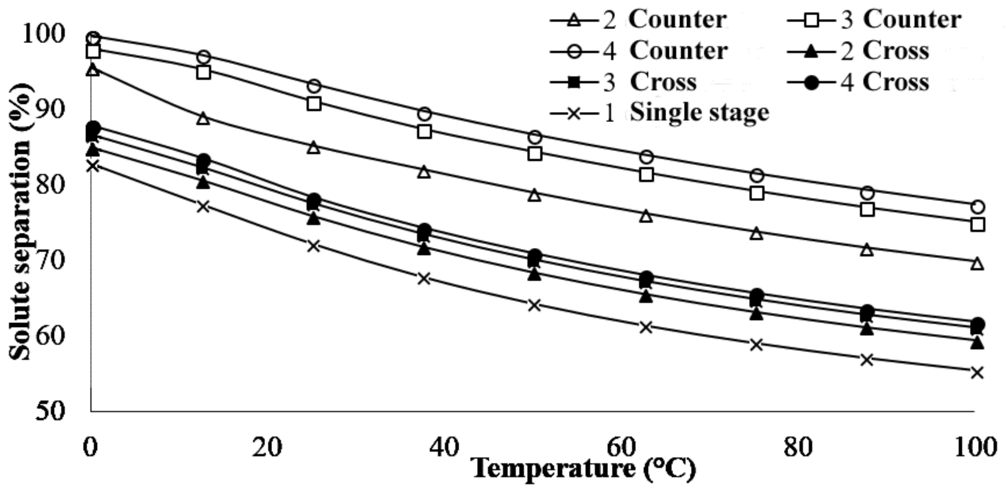

Figure 5. Behavior of the solute separation as a function of temperature.

Figure 5 shows that the higher the temperature, the lower the percentage of solute separation.

The separation increases at low temperatures, because the solubility in both components (solvent and diluent) decreases, causing that only the substances with more affinity get mixed in large proportions. It can be seen again that the operation in countercurrent contacts is more effective than the crosscurrent contacts no matter the temperature. The effect of the temperature is almost linear with slopes in the range from -0.27%/°C. to -0.20%/°C.

4. Conclusions

A mathematical tool for process and chemical engineers aimed at the design of liquid-liquid extraction has been presented with the application of three case studies. The program was designed easy to use where data of equilibrium can be selected from a database. However, the program lets to introduce new equilibrium data for components that are not in the database. This program can be used in simple laboratory experiments or in the industry when recovering specific solutes from liquids. Three case studies were presented to see the functionality of the software. The first case was the determination of the number of stages. It was found that the separation obtained with the multistage countercurrent contact using a small number of stages is higher than that the obtained with the cross-current contact, reaching a maximum separation percentage of approximately 96% while it was obtained 80% of separation for cross-current contact. For the second case, it was seen the effect of feed to solvent ratio on the percentage of separation. When using a cross-current contact in the range of F/D from 2 to 10, the higher the number of stages, the higher the solute separation. For ratios of F/D>10, the number of stages does not affect the degree of separation, so it is recommended to work with the lowest number of stages in this range. A similar pattern was obtained when using countercurrent contact. The third case study was the effect of temperature on the percentage of separation. The higher the temperature, the lower the percentage of solute separation. The effect of the temperature is almost linear with slopes in the range from -0.27%/ºC. to -0.20%/ºC.

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