

The object of this column is to enhance our readers' collections of interesting and novel problems in chemical engineering. Problems of the type that can be used to motivate the student by presenting a particular principle in class, or in a new light, or that can be assigned as a novel home problem, are requested, as well as those that are more traditional in nature and that elucidate difficult concepts. Manuscripts should not exceed 14 double-spaced pages and should be accompanied by the originals of any figures or photographs. Please submit them to Professor James O. Wilkes (e-mail: wilkes@umich.edu), Chemical Engineering Department, University of Michigan, Ann Arbor, MI 48109-2136.

## EQUILIBRIUM-STAGED SEPARATIONS USING MATLAB AND MATHEMATICA

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Unit operations are ubiquitous in any chemical process. One of their main purposes is to achieve separation in order to recycle unconverted reactants or reach product purity specifications. If two phases are brought into intimate contact, a few components migrate from one phase to the other in every stage of the unit. Then, the two phases are separated. When we consider equilibrium-staged separations, we assume that both phases leaving each stage are in equilibrium and one is richer in one or more components. The most common unit operation is distillation. It is used, for instance, to separate crude petroleum into its various fractions such as kerosene and gasoline. In the pharmaceutical industry, liquid-liquid extraction is often employed. For example, antibiotics in aqueous fermentation are recovered using organic solvents. Finally, absorption and stripping are often involved in gas treatment plants—such as units used to remove acid gases ( $\text{CO}_2$  and  $\text{H}_2\text{S}$ ) from natural gas. In the present paper, we solve two problems while showing how graphical methods can be used to design the unit operations.

The first problem treats liquid-liquid extraction while the second problem deals with binary distillation.

### EXTRACTION OF ACETIC ACID FROM WATER USING ISOPROPYL ETHER

#### **Problem Statement**

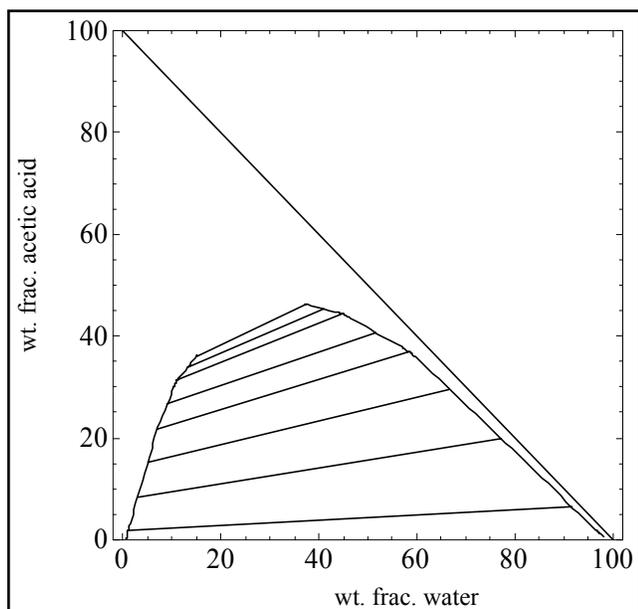
We want to separate<sup>(1)</sup> acetic acid from water using isopropyl ether in a single-feed countercurrent extractor. Use the



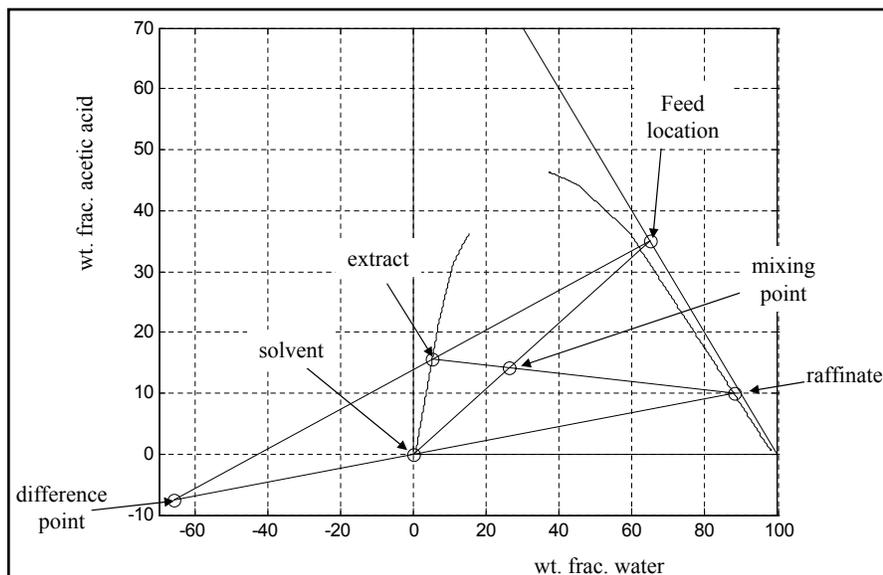
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***The author brings to the reader's attention that a program to determine the number of equilibrium stages using the Graphical User Interface (GUI) of Matlab is available.<sup>[8]</sup> This GUI program, written by Claudio Gelmi, was inspired by the earlier code of Dr. Housam Binous.***

Hunter and Nash<sup>[2]</sup> Graphical approach to compute the number of equilibrium stages required. Assume equilibrium data, at 1 atm and 25 °C, given by Wankat.<sup>[1]</sup> Solvent and feed flow rates are equal to 1000 kg/hr and 1475 kg/hr, respectively. Feed, a binary mixture of water and acetic acid, contains 35 wt % acetic acid. We wish to obtain a raffinate with only 10 wt % acetic acid.



**Figure 1.** Equilibrium diagram for the ternary system obtained using Mathematica.



## SEPARATION OF A MIXTURE OF BENZENE AND TOLUENE

### Problem Statement

Consider a binary mixture composed of benzene and toluene. Assume a constant relative volatility equal to 2.45. Use

◀ **Figure 2.** Mixing and operating points obtained using Matlab.

### Solution

To study the separation<sup>[1]</sup> of acetic acid from water using isopropyl ether for a single-feed countercurrent extractor, we will use the graphical method derived by Hunter and Nash<sup>[2]</sup> and later by Kinney<sup>[3]</sup> to obtain the number of equilibrium stages required to achieve a particular raffinate specification. This separation is usually difficult to realize with distillation due to the presence of a severe tangent pinch at high compositions of water, which prevent the distillate from being acid-free. A graphical solution performed by hand calculation has been presented by Wankat.<sup>[1]</sup> We will show how one can use Mathematica and Matlab to solve this problem more easily and accurately using the graphical approach of Hunter and Nash.<sup>[2]</sup> Equilibrium data, at 1 atm and 25 °C, are given by Wankat<sup>[1]</sup> and can be used to plot **Figure 1** — where the tie lines have been drawn (obtained using Mathematica). The same figure was obtained by the author using Matlab. Note that the conjugate line can be easily constructed using the equilibrium points. The feed is 1,000 kg/hr of a solution composed of 35 wt % acetic acid and 65 wt % water. The solvent used to perform the extraction is pure isopropyl ether with a flow rate equal to 1,475 kg/hr. We require that the raffinate composition in acid not exceed 10 wt %. First, we locate the mixing point and the difference point (see **Figure 2** obtained using Matlab). Then, we step off stages using alternatively the tie lines and the operating lines until we reach a raffinate composition lower than 10 wt %. This method is illustrated in **Figure 3**, obtained using Matlab. A similar figure was obtained by the author using Mathematica. We find that 5.35 equilibrium stages are required to achieve 10 wt % of acid in the raffinate. The Mathematica notebooks and Matlab programs are available from the author upon request or from the Mathematica Information Center<sup>[4]</sup> and Matlab File Exchange Center.<sup>[5]</sup>

the McCabe and Thiele graphical approach to compute the number of equilibrium stages required. Assume feed, bottom, and distillate mole fractions are equal to 0.5, 0.1, and 0.9 mole % benzene, respectively. Take a reflux ratio 1.5 times greater than the minimum reflux ratio.

**Solution**

We want to separate a binary ideal mixture formed of benzene and toluene. The relative volatility in this ideal case is the ratio of the vapor pressures of benzene and toluene. A straightforward calculation shows that this mixture's relative volatility varies only between 2.35 and 2.6 for a benzene mole fraction ranging from 0 to 1. Thus, as a simplifying assumption, we take an average value of 2.45. The feed is a two-phase mixture with a feed quality equal to 0.85. The distillate, feed, and bottom mole fractions are 0.9, 0.5, and 0.1, respectively. The reflux ratio is taken to be 1.514, which is approximately 1.5 times larger than the minimum reflux ratio. To obtain the minimum reflux ratio, we require that the two operating lines, the feed line, and the equilibrium curve intersect, as shown in Figure 4 – which was obtained using Mathematica. Then, we draw the McCabe and Thiele Diagram (see Figure 5 (next page), obtained using Matlab). A similar figure was obtained by the author using Mathematica. We conclude

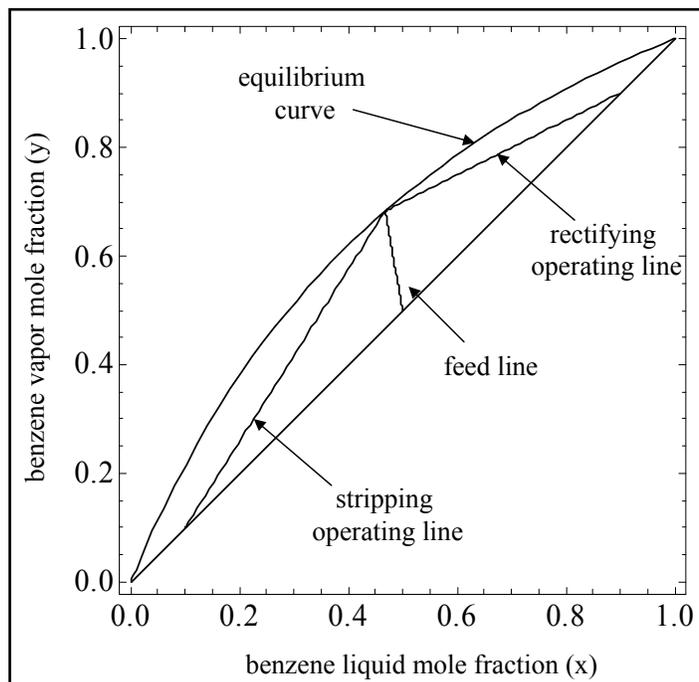


Figure 4. Finding the minimum reflux ratio using Mathematica.

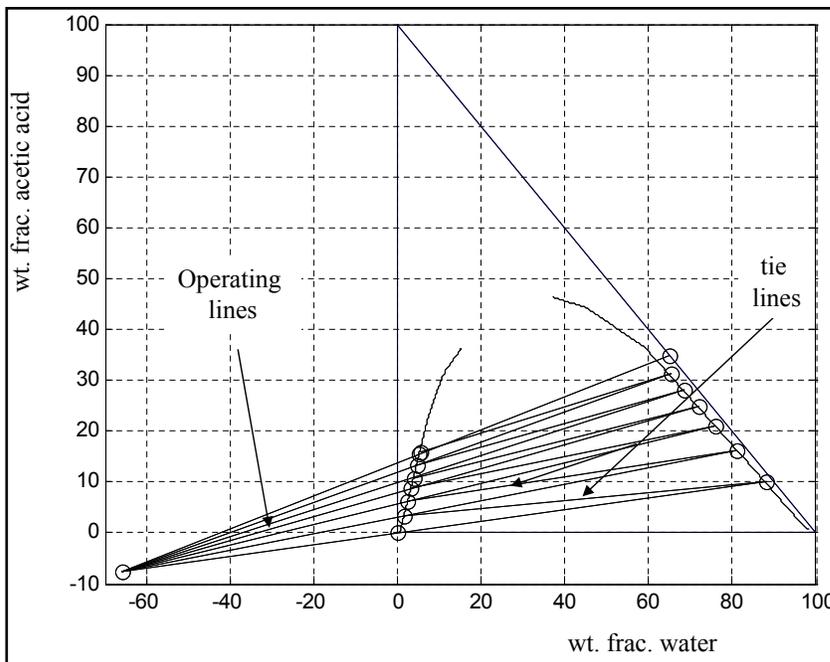


Figure 3. Hunter and Nash diagram obtained using Matlab.

that the required number of theoretical plates, to achieve product and bottom specifications, equals nine. The Mathematica notebooks and Matlab programs are available from the author upon request or at the Mathematica Information Center<sup>[6]</sup> and the Matlab File Exchange Center.<sup>[7]</sup> The author brings to the reader's attention that a program to determine the number of equilibrium stages using the Graphical User Interface (GUI) of Matlab is available.<sup>[8]</sup> This GUI program, written by Claudio Gelmi, was inspired by the earlier code of Housam Binous.

**THE MANIPULATE COMMAND OF MATHEMATICA 6.0**

**Problem Statement**

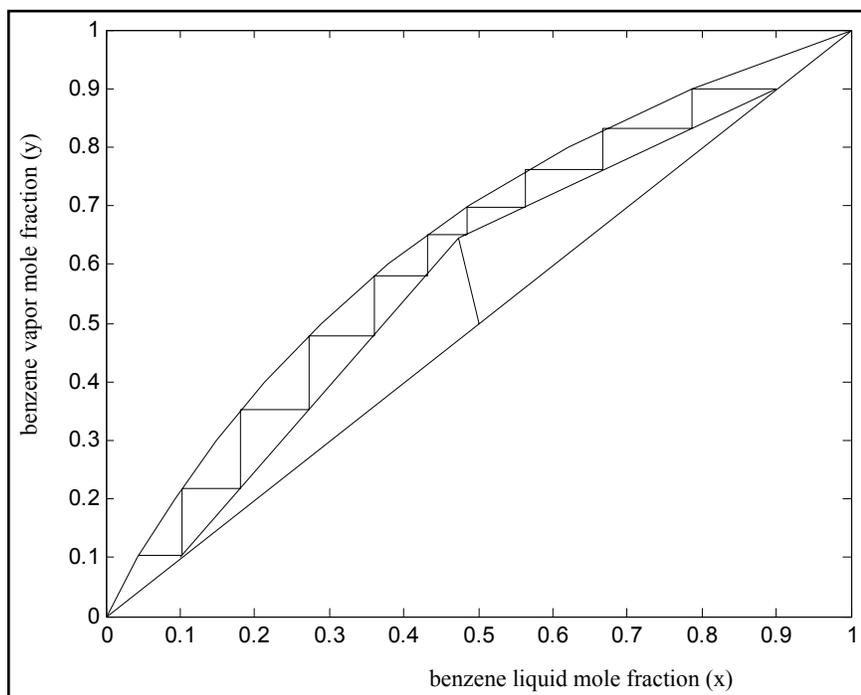
Use the new dynamic capabilities of Mathematica to prepare a demonstration where parameters such as relative volatility, feed composition, and solvent and feed flow rates . . . can be manipulated by sliders in order to study their impact on the number of equilibrium stages.

**Solution:**

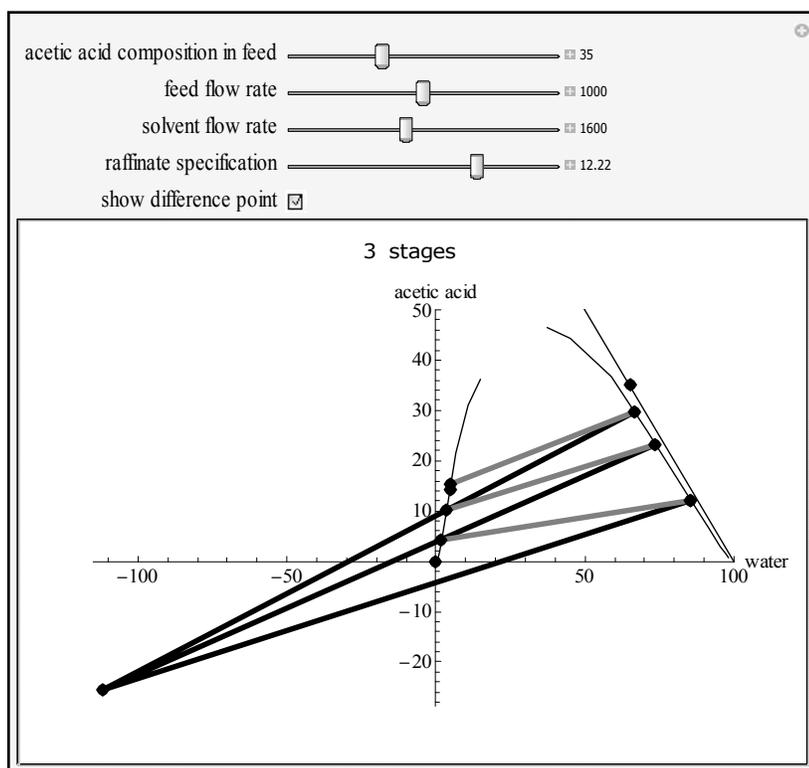
The output of Manipulate, a new function available in the new version of Mathematica (version 6.0), is an interactive object containing sliders. The output is not just a static result, it is an interactive program that allows the user to specify several selected simulation parameters using the sliders. The program then performs the computation and displays the result, usually in the form of a plot or a table. The slider is a control object, which can be dragged by the user in order to set a specified value of one parameter. The

author has modified his previous program using Mathematica (version 5.2) to take advantage of this new feature. **Figure 6** shows how the liquid-liquid extraction static simulation has been modified into an interactive program where one

can change the solvent and feed flow rates, the raffinate specification, and the acetic acid composition in the feed. **Figure 7** presents the simulation where sliders have been set up for feed quality, feed composition, distillate and bottom specifications, and relative volatility. These programs are available, among hundreds of demonstrations made with Manipulate, at the Wolfram Demonstration Project.<sup>[9,10,11]</sup> In both cases the program displays the number of equilibrium stages.



**Figure 5.** McCabe and Thiele Diagram obtained using Matlab.



**Figure 6.** Liquid-Liquid extraction using the Manipulate command.

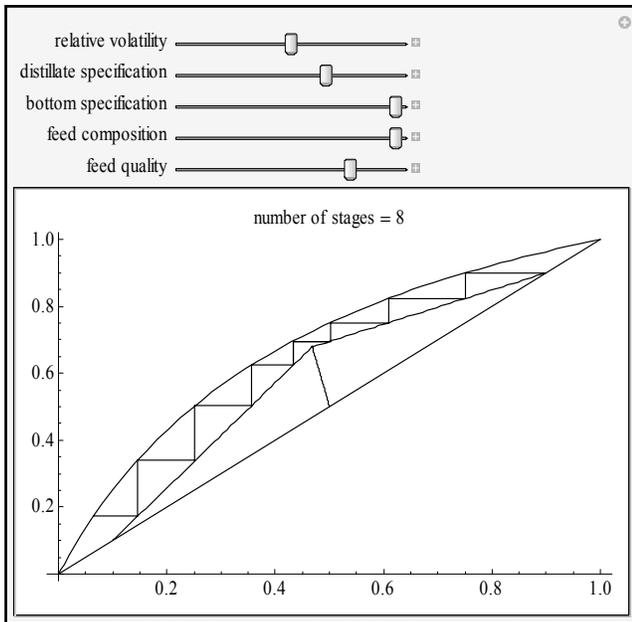
## MATHEMATICA AND MATLAB: TOOLS FOR TEACHING UNIT OPERATIONS

Teaching unit operations requires presenting to undergraduate students graphical methods such as the McCabe and Thiele or the Hunter and Nash model. These methods allow for the determination of the number of equilibrium stages for liquid-liquid extraction, distillation and absorption, and stripping problems. With powerful computer software such as Mathematica and Matlab, chemical engineering faculties can show readily how to compute the number of equilibrium stages for these classic junior or senior level problems. The author uses this opportunity not only to introduce students

to separation science but also to convince them that Mathematica and Matlab can be applied to many other interesting chemical engineering and applied mathematics problems.

## CONCLUSION

In this study, we show how Mathematica and Matlab can be used to solve problems that previously required tedious numerical and graphical techniques. First, we present the extraction of acetic acid from water using isopropyl ether. The graphical method, derived by Hunter and Nash, is used to obtain the number of equilibrium stages for a specific raffinate purity. Next, the McCabe-Thiele method is employed to give the number of equilibrium stages for a binary distillation problem. These classic problems are junior- and senior-level study material at the National Institute of Applied Sciences in Tunis. Students excel in these types of problems despite the fact that it is their first experience using Mathematica and Matlab.



**Figure 7.** Distillation using the Manipulate command.

## REFERENCES

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6. <<http://library.wolfram.com/infocenter/MathSource/5077/>>
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10. <<http://demonstrations.wolfram.com/ExtractionOfAceticAcidFromWaterUsingIsopropylEther/>>
11. <<http://demonstrations.wolfram.com>> □