Solving mass transfer problems on the computer using Mathcad

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The author has a longtime interest in the use of the computer in chemical engineering computation. In the past, many of these computations were very time consuming. In today's industrial and academic world, the computer can be used to rapidly and accurately make these computations.

Many of these problems were traditionally solved by hand using graphical means. The great advantage of the graphical techniques is that they provide a picture of the occurring phenomena. As a teaching tool this was indispensable. However, the graphical solutions were often very approximate and took a great deal of time and effort. The author has written several hundred routines in Chemical Engineering, with an emphasis on graphics and iterative computations. "Mathcad" was the software of choice because no writing of code was necessary and the graphics produced were superb. Often the programs written were capable of solving the problem completely. For example, the binary distillation program can be used to completely design the column. It could also provide graphics that could be supplied to students, so that they could generate their own graphical solutions to the engineering problem. For example, in binary distillation xy and txy diagrams are available for about 60 different binary systems, using Wilson or NRTL equations. These may be copied and distributed to students in order to teach the McCabe-Thiele procedure. The computer solution to the problem is capable of solving it completely. It can deal with details such as minimum (even if an enriching section pinch occurs) and total reflux. For a specified reflux ratio the program can obtain the number of ideal stages and the optimum feed location. Since the program is provided with a routine for obtaining the Murphree stage efficiency for each ideal stage, real stages can be (with appropriate graphical output) handled. It will also deal with the column diameter. The effect of compositions, reflux ratio and feed condition can be readily demonstrated to beginning students.

If the equilibrium information is provided as experimental txy data, programs are available, using Barker's method to find the Wilson or NRTL parameters. Systems that are pseudo-binary such as acetic acid and water can in many cases be treated. These programs will plot the experimental data points and the resulting smoothed curve on the same graph. This allows the user to see immediately the quality of the fit. One special program in continuous binary distillation solves the separation of n-butanol from water, which requires two columns and a decanting tank to separate the heterogeneous liquids.

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A few enthalpy-concentration diagrams have been generated which has made it possible to perform Ponchon-Savarit calculations. The graphical outputs have been printed on legal sized paper in order to have room for the delta points. Enthalpy-concentration diagrams without the distillation can be printed for distribution to students.

In addition to continuous binary distillation, programs have been written for binary batch distillation. These were written for constant reflux ratio with variable distillate composition and for constant distillate composition and variable reflux ratio. These are provided with animation to demonstrate the sequence of conditions with time with a specified number of ideal stages and a specified initial charge composition.

Continuous multi-component distillation is also represented. These use the K values presented in "Equilibrium Staged Separations" by Wankat[1] on page 26. Programs that will solve sharp or sloppy separations have been written. One demonstration program solves a system with four hydrocarbon components, with a sharp separation using both the Wang and Henke technique (without energy balances) and the Fenske-Underwood-Gilliland technique. The results compare very favorably.

Recently azeotropic distillation has been programmed. Two systems have been examined. These are water, ethanol using benzene as the entraining agent and water, ethanol using toluene as the entraining agent. The ternary Wilson equation was used was used for the constant pressure vapor-liquid equilibrium. Curve fitting was used to obtain the liquid-liquid equilibrium. Although these programs work, this is still a work in progress. Alternate methods for expressing the equilibria are being examined.

The use of packed towers in gas absorption has been examined. The old procedures involved graphical plotting to find the equilibrium mole or mass fractions. Data was prepared in tabular form so that a graphical integration could be performed in order to obtain the packing height. This procedure was a slow, time consuming operation. The computer alternate involves punching in equilibrium data, and using the available computer regression fit for the data. An equation for the equilibrium values of y as a function of x can be obtained. This is not difficult because the data is often nearly linear. The equation for the height of the packing may be solved by integration between limits on the computer.

Countercurrent liquid extraction was examined. Some of the results were presented in August of 2004 in Prague in the Czech Republic at Karlovy University[2]. Six different systems were shown (still more are on the machine). Four of the systems were of the type where two binary pairs are completely miscible and only one binary pair has immiscibility. Such a system will have a plait point. The programs for these systems simulated countercurrent extraction. Two other systems, each having but one binary pair of components completely miscible were also used. These systems do not have a plait point. For these systems counter-current extraction with reflux was used. Known example problems from the literature were chosen for these, in order to show that the procedures worked correctly and give correct results. These were the extraction of styrene from ethyl benzene using ethylene glycol and the other was the extraction of oleic acid from cottonseed oil using liquid propane at 98.5 C and 625 psia. Both of these programs involved the use of a solvent free basis. In all of the extraction problems an xy diagram was computer generated showing the equilibrium curve, a curved operating line and the ideal stages.

More recently a keynote lecture was presented in August of 2006 at Karlovy University in Prague, dealing with binary batch distillation[3]. These have been generated for systems not having any azeotropes. Batch distillation is time dependant. The programs for both constant reflux ratio distillation and constant distillate composition were animated.

The use of the McCabe[4]-Thiele method and the Ponchon[5]-Savarit[6] for solving binary distillation problems in Chemical Engineering have a long history going back to the early 1920 ‘s. For those unfamiliar with the techniques, they are highly graphical in nature. In ages before the advent of modern digital computation these were the methods used to design distillation equipment. The McCabe-Thiele method although somewhat approximate due to the assumption of constant molal overflow was usually the preferred method over the more rigorous Ponchon-Savarit procedure. This was due to the necessity of providing large enthalpy-concentration diagrams upon which to solve the problem. These were not always widely available for all systems and were cumbersome to generate. Today these methods are still in use but they are difficult to teach to beginning Chemical Engineers. The drafting techniques taught to beginning engineering students was no longer being taught (with good reason). It is often very difficult for beginning students to draw the necessary graphics with the necessary care and skill to obtain a reasonably usable design. In recent years commercial computer software has become available and is widely used in industry. However, the licensing of this software is quite expensive and in some cases the results may be unsatisfactory. For some years now, the authors have been supplying computer generated constant pressure phase diagrams (in color) for use in the Chemical Engineering laboratory. The system distilled is methanol and water at 1 atmosphere total pressure. The students are supplied with an x-y diagram, a t-x-y diagram and a large format (11 x 14) enthalpy-concentration diagram upon which graphical design work may be done. (Examples of the t-x-y and x-y diagrams appear in the appendix.) Considerable space has been left on the enthalpy-concentration diagram above the dew point curve and below the bubble point curve to allow space for delta point construction. The chart has some 40 tie lines computer generated upon it and an auxiliary curve to generate tie lines tie lines not appearing on the chart. The authors do have complete computer generated Ponchon-Savarit solutions for the systems ethanol-water and methanol-water.

Such charts do not have to be confined to use in the laboratory. Workshops can be run in order to teach the design techniques. The students can be equipped with the necessary graphs and the solutions can be projected using the computer projector. They can follow the projected solution, drawing the operating lines and the ideal stages since these are programmed. The program is not confined to methanol and water. Twenty-six different binary systems are in the program, none of them with azeotropes. The systems available are:

System =

	0
0	"1-propanol & 1-butanol"
1	"2-butanone & 2-butanol"
2	"Acetaldehyde & ethanol"
3	"Acetone & 2-propanol"
4	"Acetone & ethanol"
5	"Acetone & water"
6	"Ammonia & water"
7	"Benzene & chlorobenzene"
8	"Benzene & toluene"
9	"Carbon disulfide & tetrachloromethane"
10	"Carbon tetrachloride & benzene"
11	"Dichloromethane & tetrachloromethane"
12	"Dimethoxymethane & tert-butanol"
13	"Ethanol & 1-butanol"
14	"Ethanol & acetic acid"
15	"Methanol & 2-propanol"
16	"Methanol & ethylenediamine"
17	"Methanol & water"
18	Methyl isocyanate & tetrachloromethane"
19	"Nitrogen & Oxygen"
20	"Nitrogen & Oxygen"
21	"n-hexane & n-octane"
22	"n-propylamine & water"
23	"Tert-butanol & 2-methyl-1-propanol"
24	"Tetrachloromethane & chlorobenzene"
25	"Water & acetic acid"
26	"Water & acrylic acid"

P =

	0
0	760
1	760
2	760
3	760
4	760
5	760
6	760
7	760
8	760
9	760
10	760
11	760
12	760
13	760
14	760
15	760
16	760
17	760
18	760
19	760
20	380
21	760
22	760
23	760
24	760
25	760
26	760

It should be noted that additional systems might at any time be added to the list. A database is provided such that the program is capable of providing most of the information necessary to design the column. The output is both numerical and graphical. The graphical output will consist of the following:

a. Number of ideal stages at total reflux
b. Minimum reflux ratio
c. Number of ideal stages and optimum feed location for a given reflux
d. The same for real plates or stages

Numerical values are provided for each of the above on the graphs. Additional numerical output is the tower diameter, the weir length, the required tray spacing and the product of the tray spacing and the number of real stages.

The input required must be the distillate mole fraction, the feed mole fraction and the bottoms mole fraction all given for the more volatile component. In addition the value of q (See Treybal[4] pages 341-343) must be stated in order establish the state of the feed. The actual reflux ratio or the ratio of the reflux ratio to the minimum value must be supplied. The program is equipped in all cases with default values that will run. These may be overridden. A feed rate will also be necessary. The appendix will also show the real stage graphic.

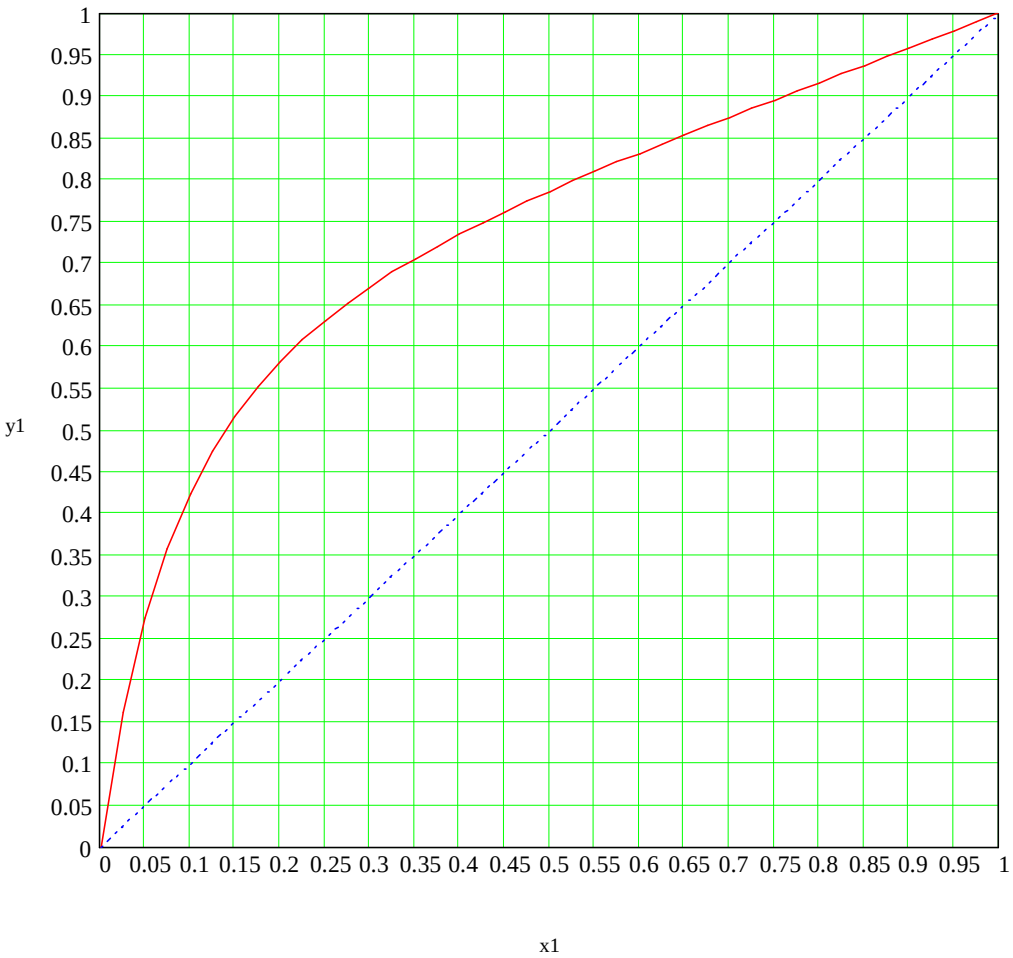
APPENDIX

P = 760

x1, y1 phase diagram

Pressures are in mm Hg.

System = "Methanol & water"



P = 760

t, x1, y1 phase diagram

Pressures are in mm Hg.
Temperatures are in degrees C.

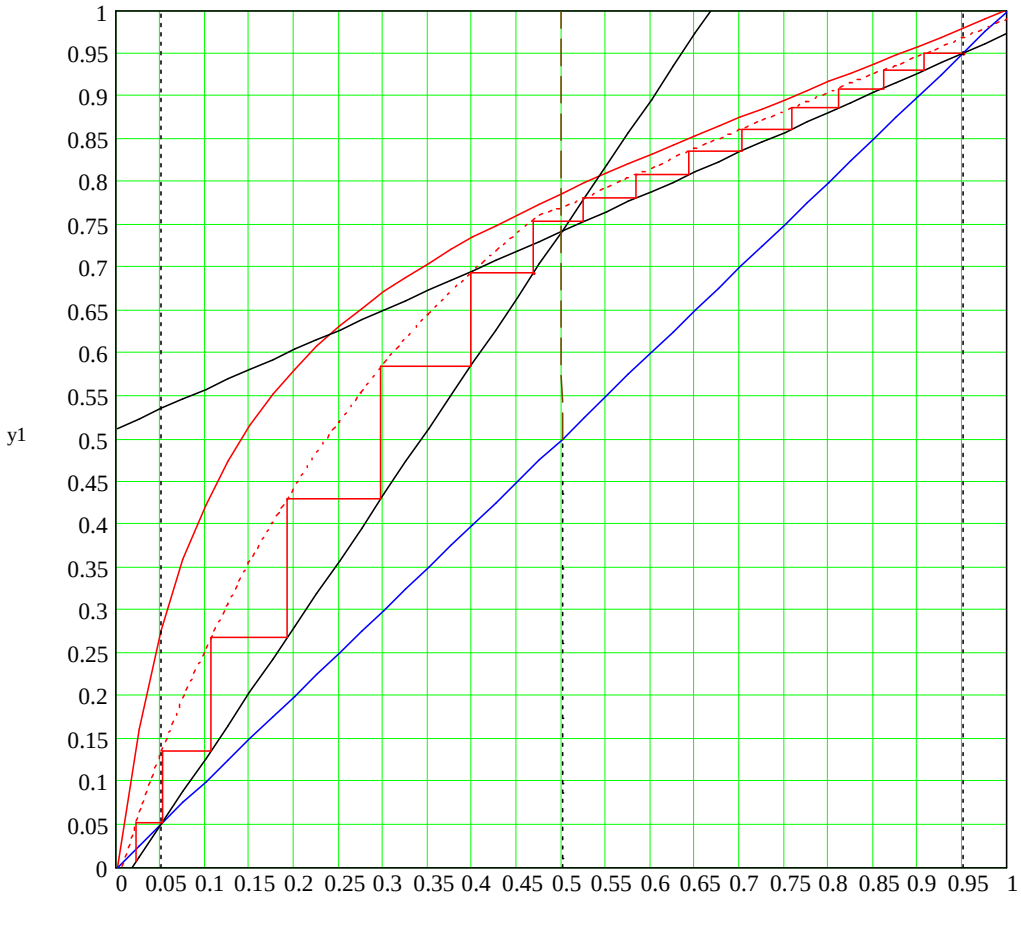
System = "Methanol & water"

P = 760

Pressures are in mm Hg.

Real stages at the reflux ratio, R

System = "Methanol & water"



Nstages = 14.028

Nfreal = 9

Nideal = 8.516

Nf = 6

q = 1

xd = 0.95

zf = 0.5

xw = 0.05

R = 0.857

Rmin = 0.572

xaz = "no azeo"

Overalleff = 0.607

$\frac{R}{Rmin} = 1.5$

Nstages should be rounded off to the next largest integer.

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BIOGRAPHICAL INFORMATION

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He has been on the faculty of NJIT for 38 years where he has taught Chemical Engineering, Chemistry and Mathematics. His B. Ch. E. was received in 1957, his M. Ch. E. was received in 1960 and his Ph. D. in Chemical Engineering was received in 1971, all from New York University, School of Engineering.

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