2016 ASEE ANNUAL CONFERENCE & EXPOSITION

JAZZED about Engineering Education

Plotting McCabe-Thiele Diagrams in Microsoft Excel for Nonideal Systems

John L. Gossage
Dan F. Smith Department of Chemical Engineering
Lamar University, Beaumont, Texas

ASEE
AMERICAN SOCIETY FOR ENGINEERING EDUCATION

Outline

1. Typical Binary Distillation Problem
2. Drawing the McCabe-Thiele Diagram
3. Cubic B-Splines to Fit Equilibrium Data
4. Solving Cubic Equation
5. Using Excel to Draw the Diagram

Typical Distillation Problem

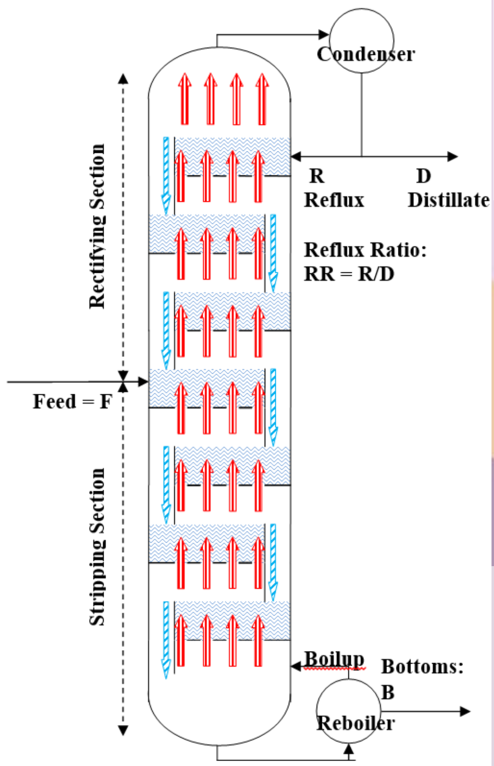
EtOH-Water Equil. Data @ 1 atm

Orjuela *et al.*, *Fluid Phase Equil.*, Vol 290, pages 63-67, 2010

#	x-EtOH	y-EtOH
1	0.0010	0.0047
2	0.0061	0.0721
3	0.0145	0.1539
4	0.0237	0.2301
5	0.0310	0.2851
6	0.0490	0.3559
7	0.0652	0.4181
8	0.0968	0.4534
9	0.1394	0.5314
10	0.3261	0.6047
11	0.4635	0.6518
12	0.5413	0.6751
13	0.6856	0.7451
14	0.7760	0.8005
15	0.8403	0.8457
16	0.9037	0.9010
17	0.9725	0.9721
18	0.9804	0.9774

FEED:
10 mol% EtOH
90 mol% Water
1 atm
80 mole% liquid

AZEOTROPE:
Note that for the last few points, x > y



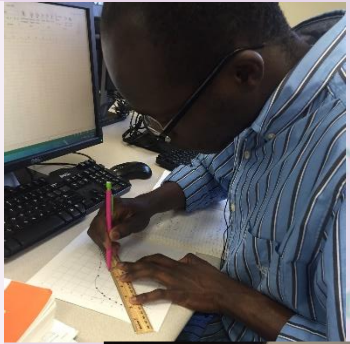
DISTILLATE:
85 mol% EtOH
15 mol% Water
RR = 3, 1 atm

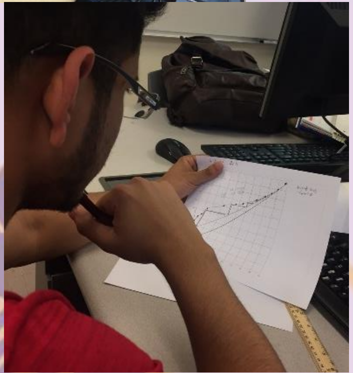
FIND:
1. Required Equilibrium Stages
2. Optimum Feed Stage
3. Azeotrope

BOTTOMS:
1 mol% EtOH
99 mol% Water
1 atm

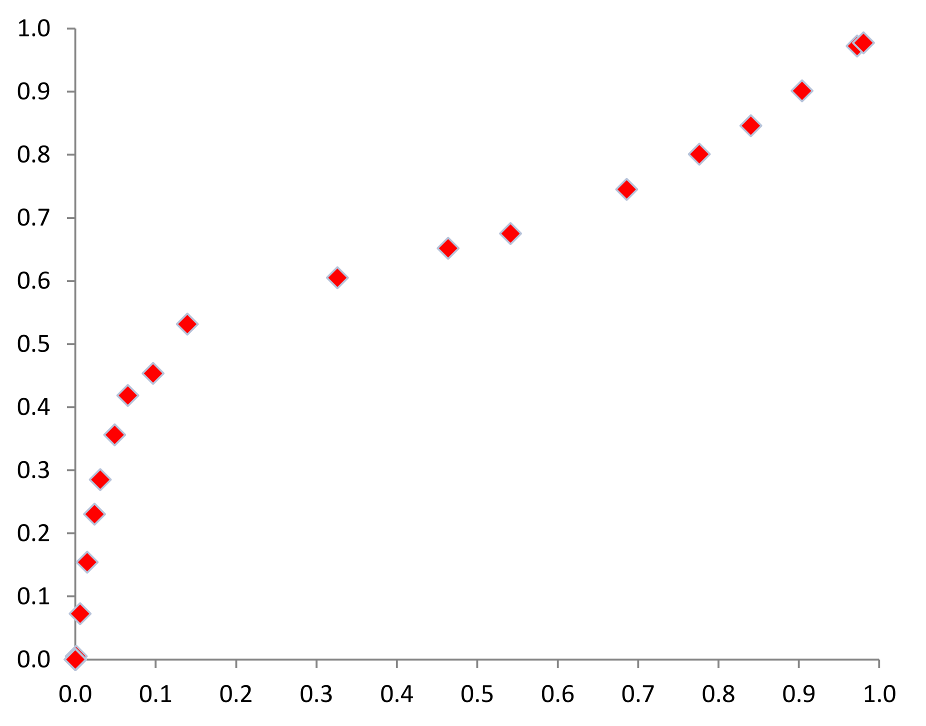
Drawing McCabe-Thiele Diagram

1. Plot Equilibrium Data Points
2. Draw 45° Line
3. Draw Feed Line
4. Draw Rectifying Operating Line
5. Draw Stripping Operating Line
6. Draw Equilibrium Curve
7. Draw Equilibrium Stages
8. Find Azeotrope

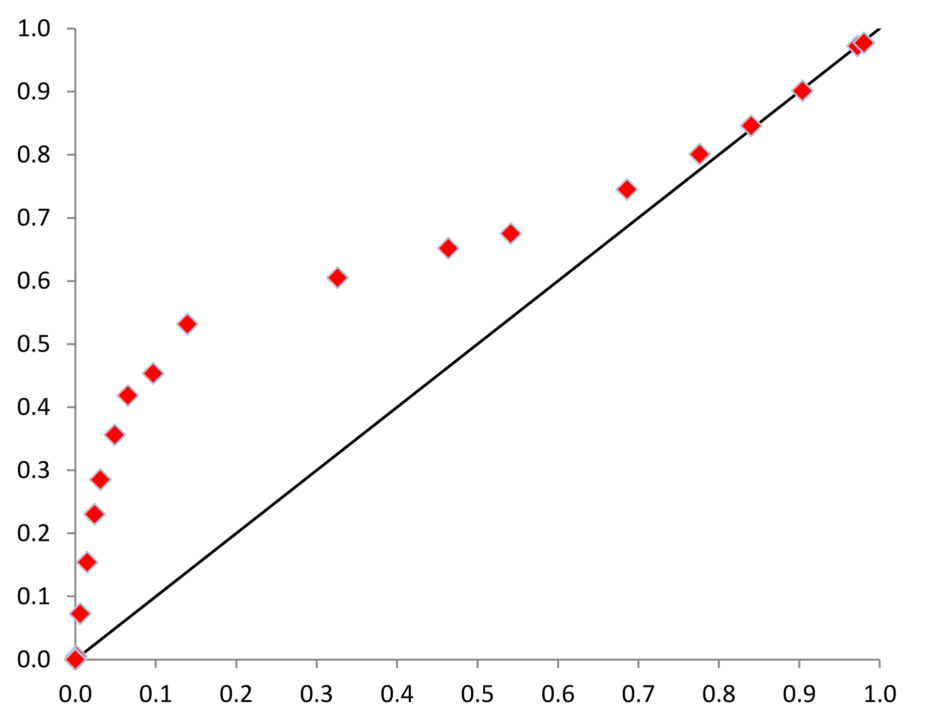




1. Plot Equilibrium Data Points :



2. Draw 45° Line:

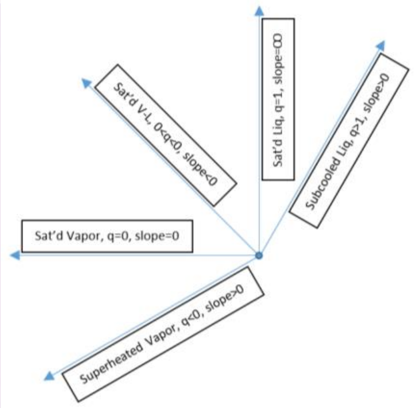


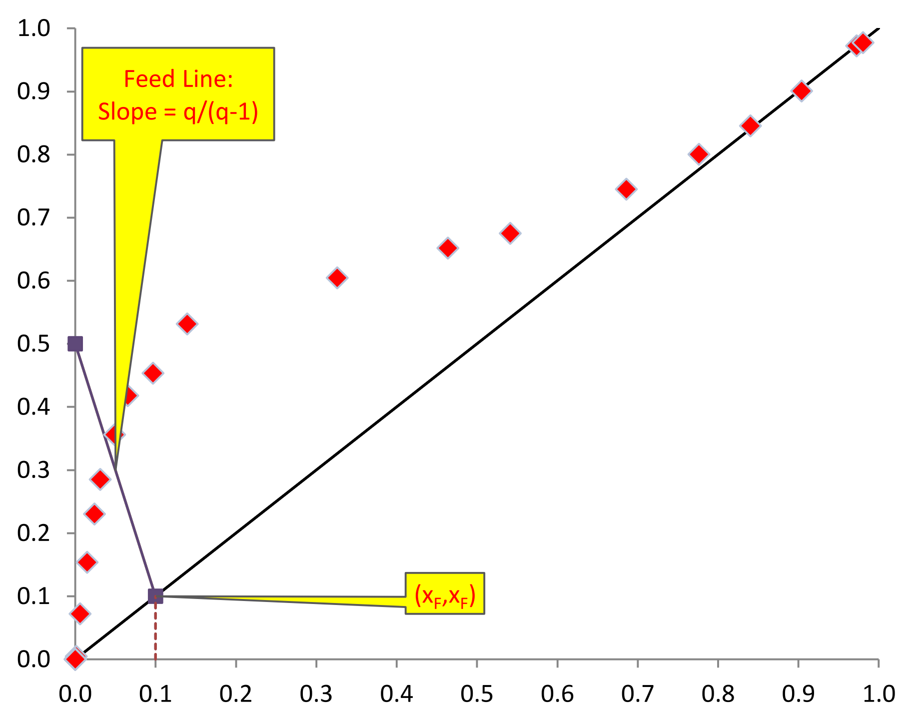
3. Draw Feed Line:

$$q = \frac{\left(\text{heat needed to vaporize 1 mole of feed at entering conditions}\right)}{\left(\text{molar latent heat of vaporization of feed}\right)}$$

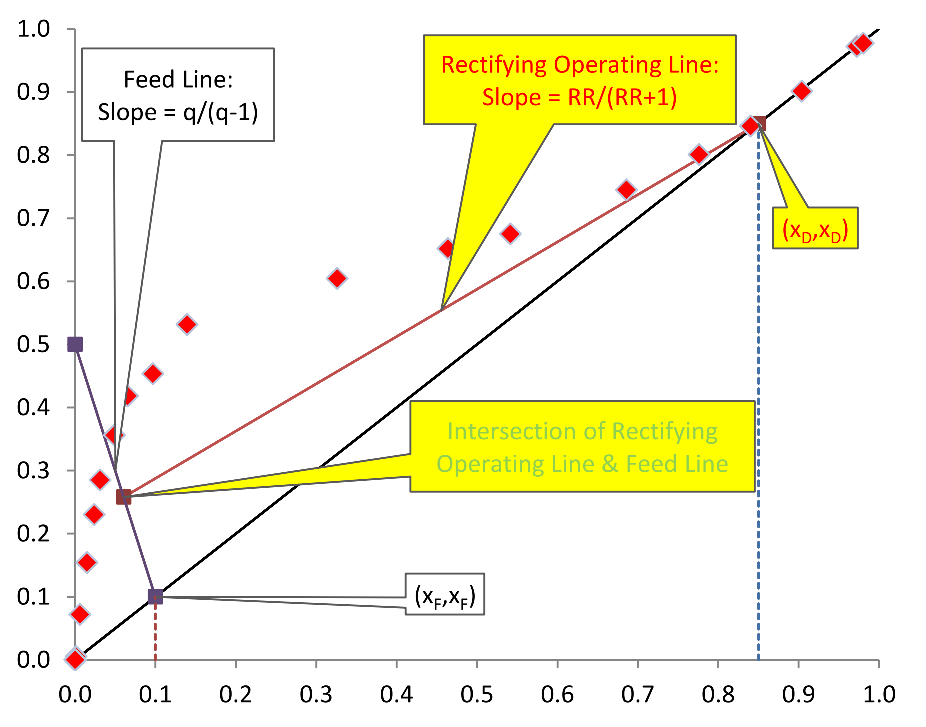
So, for a saturated feed:
q = liquid fraction

Feed Line Orientation:

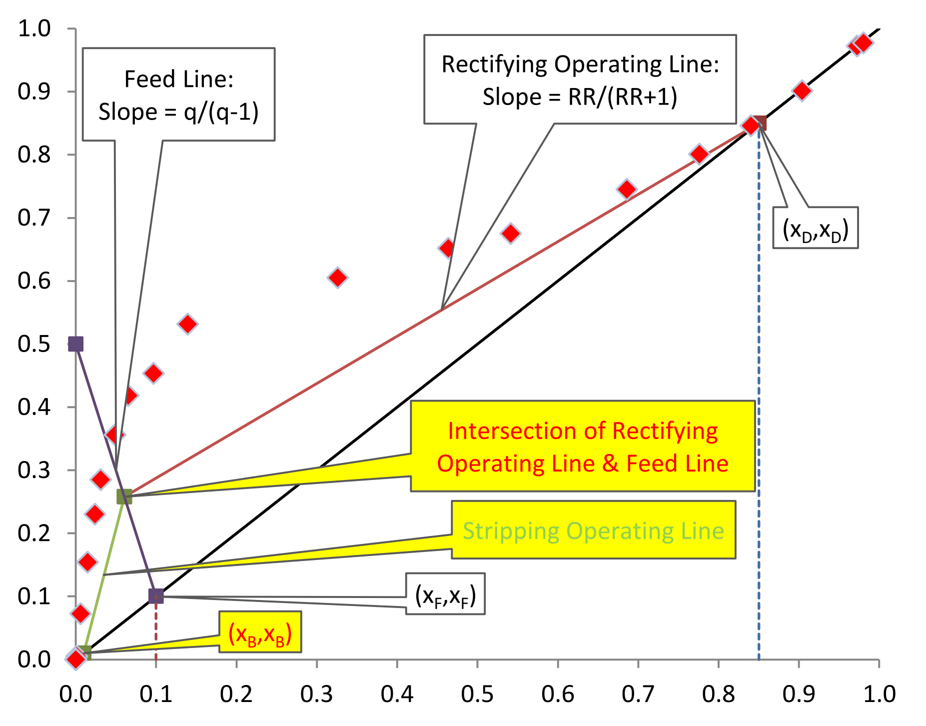




4. Draw Rectifying Operating Line:

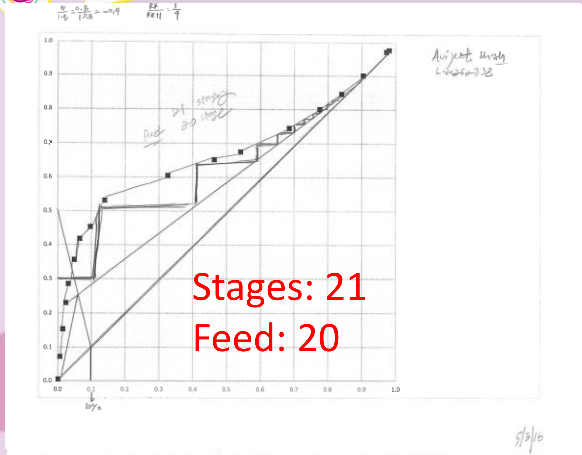


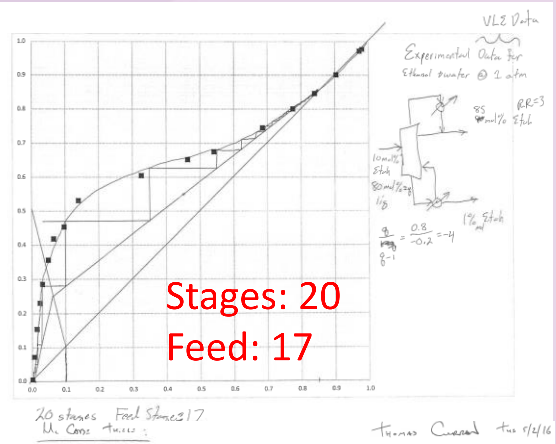
5. Draw Stripping Operating Line:

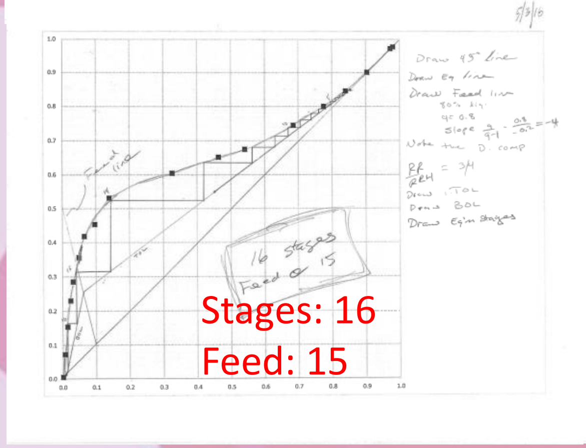


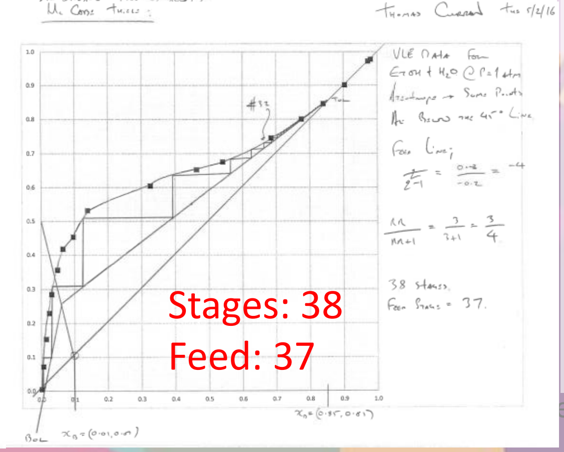
6. Draw Equilibrium Curve:

This is where the problem becomes tricky, as shown here:









Examples of student efforts to hand-draw this McCabe-Thiele diagram given a graph with pre-plotted data points.

Note how equilibrium curves vary, so Number of Stages and Feed Stage also vary.

Over the whole class, the Number of Stages ranged from 9 to 38, and the Feed Stage ranged from 8 to 37.

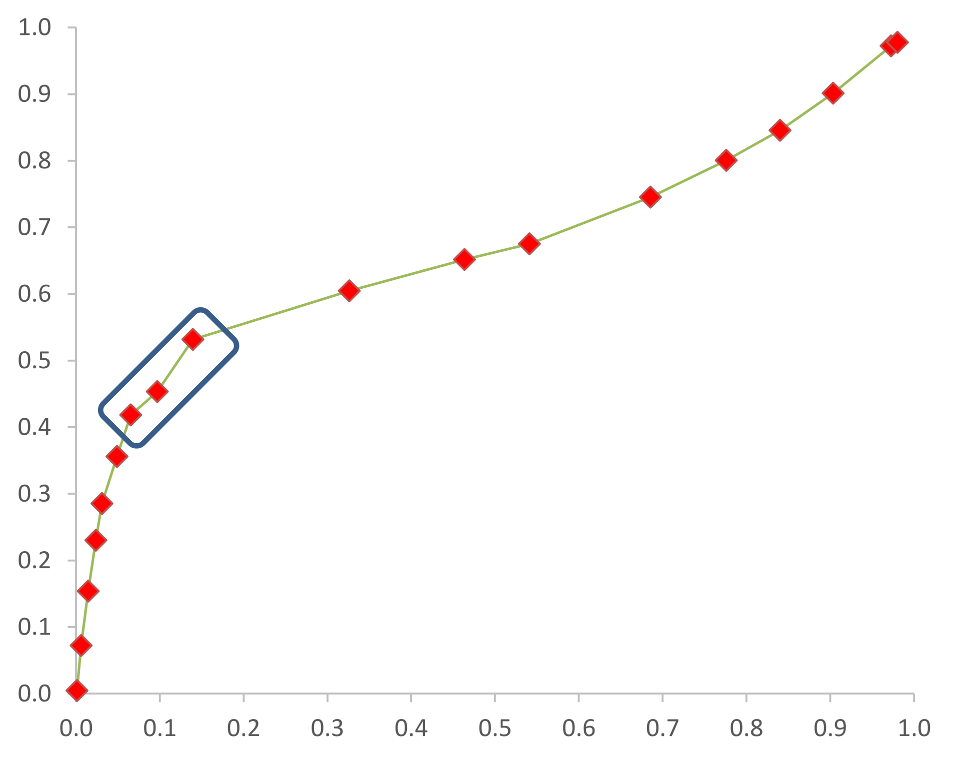
Time to draw ≈15 minutes.

Alternatives to Hand-Drawing Equilibrium Curve: Linear Interpolation

1. Play "connect-the-dots": *i.e.* use linear interpolation

This approach was used previously in the literature (1. Burns and Sung, *Chemical Engineering Education*, Winter 1996 & 2. Mathias, *Chemical Engineering Progress*, December 2009)

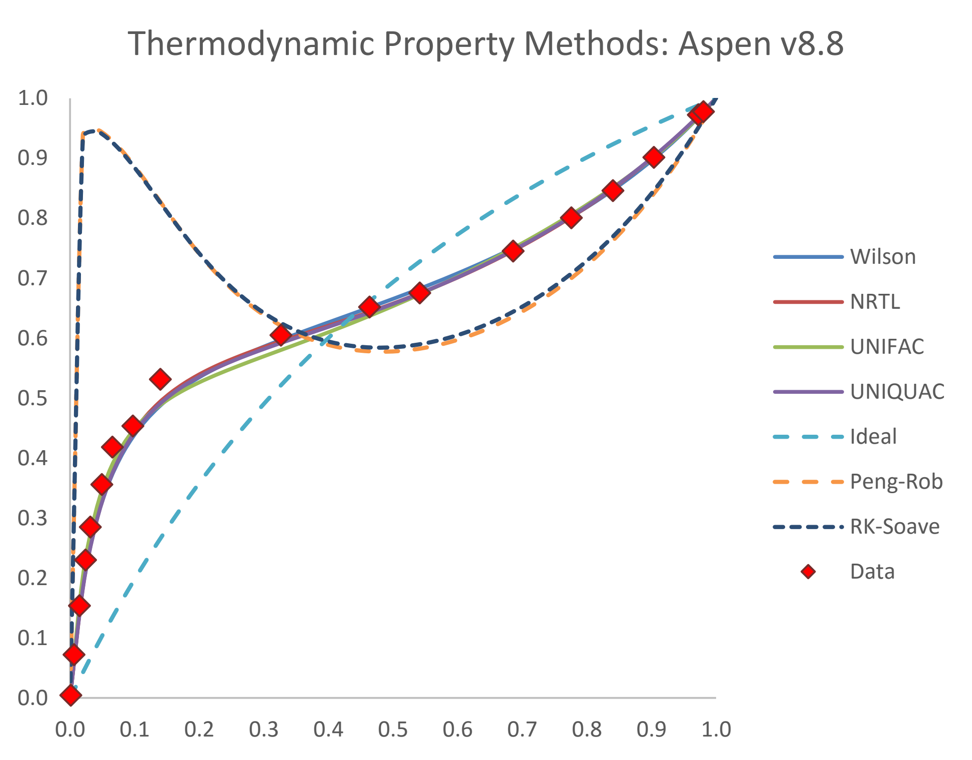
For closely-spaced data with minimal experimental error, this approach would be acceptable, but in the present case (and in general), it gives odd results, particularly near x = 0.1.

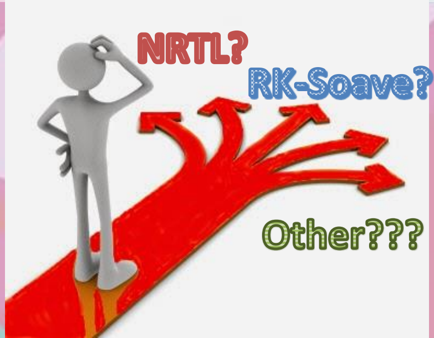


Alternatives to Hand-Drawing Equilibrium Curve: Thermodynamics

2. Use a Thermodynamic Property Method

- No thermodynamic property method works for every case
- Here, the gamma models (solid lines) work reasonably well (but don't compensate for data error)
- Here, EOS models (dashed lines) are very poor choices (due to nonideality of EtOH-Water mixture)





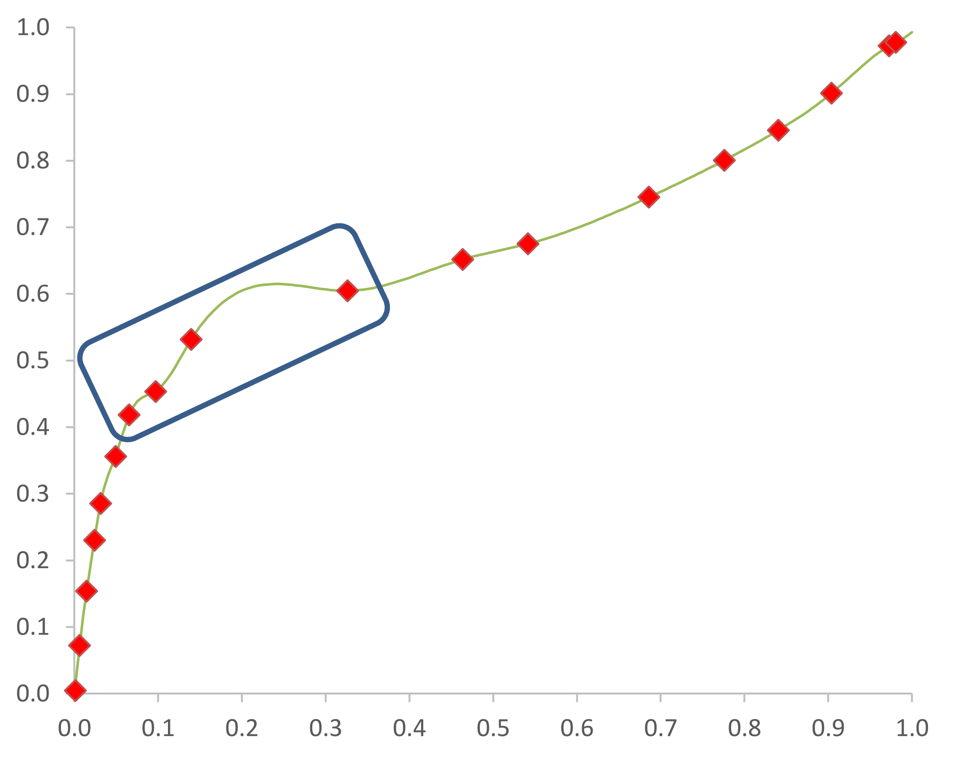
Alternatives to Hand-Drawing Equilibrium Curve: NCS

3. Use “normal” Cubic Splines (NCS)

This approach is problematic: the requirement that NCS’s pass smoothly through every data point magnifies data error: here it gives physically-unrealizable results near x = 0.2.

Other, more subtle, problems with NCS:

- Requires simultaneous solution of N linear equations
- Thus errors in data affect ALL results
- Must select an “end case”: what happens at x = 0 & x = 1?



Alternatives to Hand-Drawing Equilibrium Curve: CBS

4. Use Cubic B-Splines (CBS) to "connect" the equilibrium data points smoothly

CBS's don't pass through the actual data points ($\boldsymbol{x_j}$,$\boldsymbol{y_j}$) but instead they pass through "knots" ($\boldsymbol{XK_j}$,$\boldsymbol{YK_j}$) that are NEAR, but not necessarily ON, the data points. The knots are defined as follows:

$$\boldsymbol{XK_j} = (\boldsymbol{x_{j-1}} + 4 \cdot \boldsymbol{x_j} + \boldsymbol{x_{j+1}})/6$$
$$\boldsymbol{YK_j} = (\boldsymbol{y_{j-1}} + 4 \cdot \boldsymbol{y_j} + \boldsymbol{y_{j+1}})/6$$

Between the knots, the CBS is defined parametrically in terms of u (where $0 \le u \le 1$):

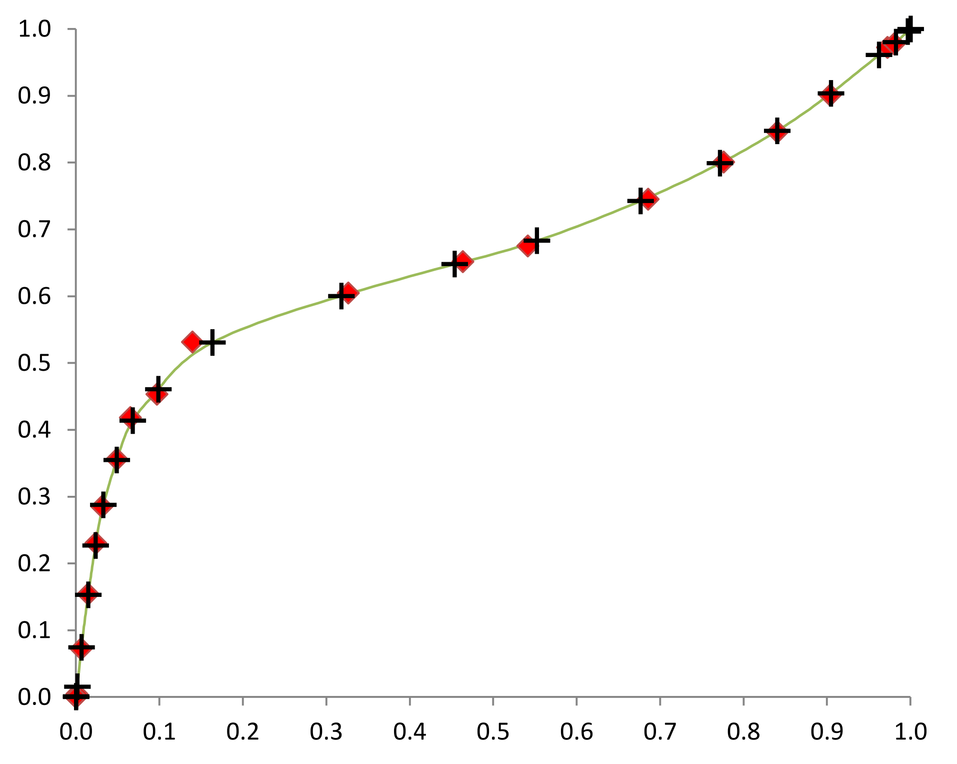
$$x_j(u) = \frac{(1-u)^3 \cdot \boldsymbol{x_{j-1}}}{6} + \frac{(3 \cdot u^3 - 6 \cdot u^2 + 4) \cdot \boldsymbol{x_j}}{6} + \frac{(-3 \cdot u^3 + 3 \cdot u^2 + 3 \cdot u + 1) \cdot \boldsymbol{x_{j+1}}}{6} + \frac{u^3 \cdot \boldsymbol{x_{j+2}}}{6}$$
$$y_j(u) = \frac{(1-u)^3 \cdot \boldsymbol{y_{j-1}}}{6} + \frac{(3 \cdot u^3 - 6 \cdot u^2 + 4) \cdot \boldsymbol{y_j}}{6} + \frac{(-3 \cdot u^3 + 3 \cdot u^2 + 3 \cdot u + 1) \cdot \boldsymbol{y_{j+1}}}{6} + \frac{u^3 \cdot \boldsymbol{y_{j+2}}}{6}$$

Thus $x_j(0) = \boldsymbol{XK_j}$, $x_j(1) = \boldsymbol{XK_{j+1}}$, $y_j(0) = \boldsymbol{YK_j}$, and $y_j(1) = \boldsymbol{YK_{j+1}}$, ensuring a smooth, continuous curve.

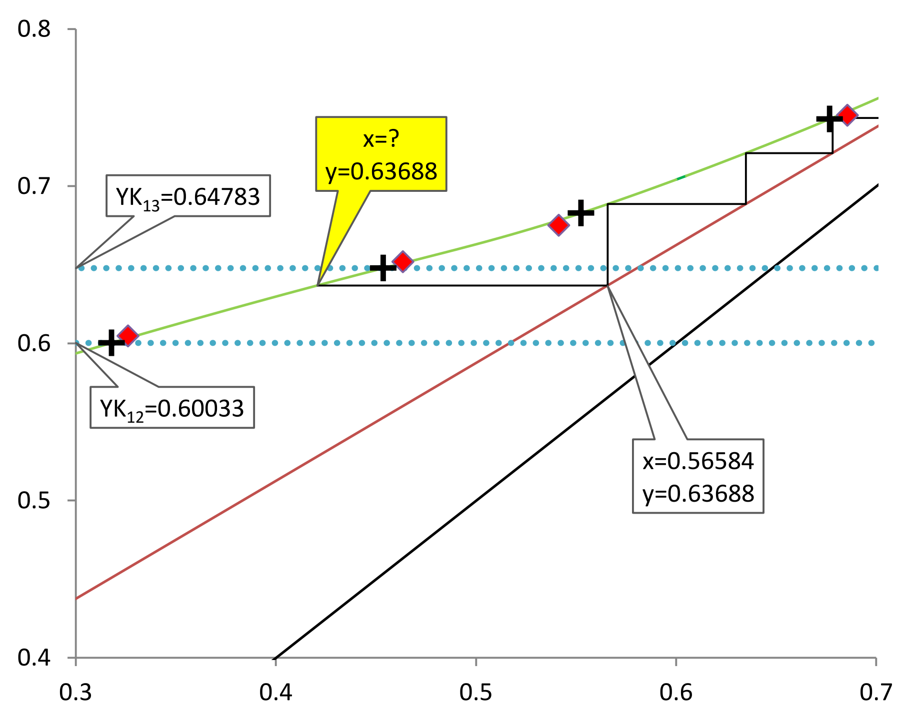
Alternatives to Hand-Drawing Equilibrium Curve: CBS (cont'd)

Augmenting equilibrium data points with three (0,0) points at beginning and three (1,1) points at end ensures curve will pass precisely through (0,0) and (1,1).

red diamonds: equilibrium data
black crosses: knots
green line: proposed equilibrium curve



7. Drawing Equilibrium Stages using CBS



Blow-up during construction of stage #19

Here, from the preceding stage, y = 0.63688

Need to determine the value of x (on the green equilibrium curve) in equilibrium with this y value

Get this x value by using two Visual Basic for Applications (VBA) user-defined functions: FXBS and FXCubic.

7. Drawing Equilibrium Stages using CBS: Step 2

Parametric equation definition of $y_j(u)$: the y-value of the CBS:

$$y_j(u) = \frac{(1-u)^3 \cdot \boldsymbol{y_{j-1}}}{6} + \frac{(3 \cdot u^3 - 6 \cdot u^2 + 4) \cdot \boldsymbol{y_j}}{6} + \frac{(-3 \cdot u^3 + 3 \cdot u^2 + 3 \cdot u + 1) \cdot \boldsymbol{y_{j+1}}}{6} + \frac{u^3 \cdot \boldsymbol{y_{j+2}}}{6}$$

Now if we know $y_j(u)$ is a given value, v, we can rearrange this to produce this cubic equation in u:

$$a_y \cdot u^3 + b_y \cdot u^2 + c_y \cdot u + d_y = 0$$

where

$$a_y = -\boldsymbol{y_{j-1}} + 3 \cdot \boldsymbol{y_j} - 3 \cdot \boldsymbol{y_{j+1}} + \boldsymbol{y_{j+2}}$$
$$b_y = 3 \cdot \boldsymbol{y_{j-1}} - 6 \cdot \boldsymbol{y_j} + 3 \cdot \boldsymbol{y_{j+1}}$$
$$c_y = -3 \cdot \boldsymbol{y_{j-1}} + 3 \cdot \boldsymbol{y_{j+1}}$$
$$d_y = \boldsymbol{y_{j-1}} + 4 \cdot \boldsymbol{y_j} + \boldsymbol{y_{j+1}} - 6 \cdot \boldsymbol{v}$$

Note that a corresponding cubic equation exists when $x_j(u)$ is known.

User-Defined Functions: FXBS and FXCubic

FXBS(DVrange As Range, IVrange As Range, IVvalue As Double) As Double

Applies the Cubic B-Spline method to smooth and fit equilibrium data to an equilibrium curve. Uses FXCubic.

Inputs:

1. DVrange: Equilibrium Data's Dependent Variable range (Location on Spreadsheet)
2. IVrange: Equilibrium Data's Independent Variable range (Location on Spreadsheet)
3. IVvalue: Independent Variable value

Output: Value of the Dependent Variable when the Independent Variable's value is IVvalue. ***If IVvalue < 0, then FXBS returns the Azeotrope.***

Example: FXBS(xdata,ydata,0.636879)= 0.420678, where "xdata" and "ydata" are locations of x & y data points

FXCubic(a As Double, b As Double, c As Double, d As Double, xlow As Double, xhigh As Double) As Double

Finds a real root of a cubic equation defined by

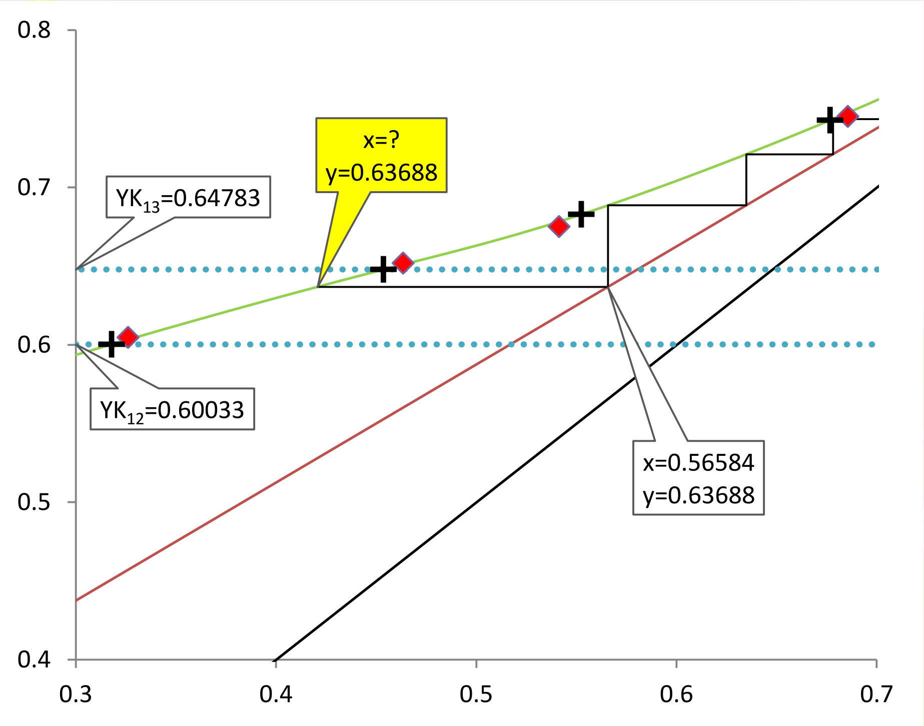
$$a \cdot x^3 + b \cdot x^2 + c \cdot x + d = 0$$

Inputs: Coefficients of the Cubic Equation and desired output range (between "xlow" and "xhigh")

Output: Real Root of the Cubic Equation, if possible between "xlow" and "xhigh"

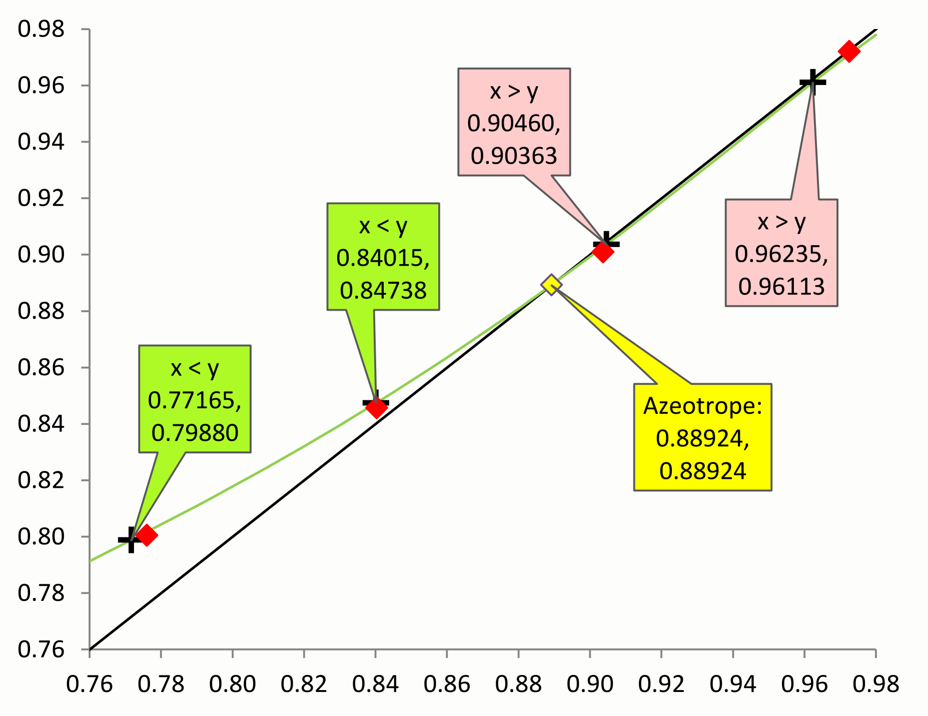
Method: uses Tschirnhaus transformation to form depressed cubic, then solves using the trigonometric method of François Viète via implementation of a method from http://www.1728.org/cubic2.htm.

7. Drawing Equilibrium Stages using CBS: Step 3



1. Given y = 0.636879 in the FXBS function
2. Find "j": the CBS section containing this y: here, j = 12, since $YK_{13} > y > YK_{12}$
3. Look up the values y_{j-1} = 0.5314, y_j = 0.6047, y_{j+1} = 0.6518, and y_{j+2} = 0.6751
4. Calculate the cubic equation coefficients: a_y=0.002400, b_y=-0.078600, c_y=0.361200, d_y=-0.219274
5. Use the FXCubic function to find the appropriate root: u= 0.716274
6. Look up the values x_{j-1} = 0.1394, x_j = 0.3261, x_{j+1} = 0.4635, and x_{j+2} = 0.5413
7. Calculate the value x = 0.420678
8. Drop vertically to the red operating line using x = 0.420678 to get the next y

8. Find Azeotrope



Expansion at High EtOH Concentrations

Green Callouts: Knots with x < y
Pink Callouts: Knots with x > y
Azeotrope Occurs where x = y (so the equilibrium curve crosses the 45° line)

Find Azeotrope by Solving This Cubic for u:

$$\left(a_y - a_x\right) \cdot u^3 + \left(b_y - b_x\right) \cdot u^2 + \left(c_y - c_x\right) \cdot u + \left(d_y - d_x\right) = 0$$

and then Azeotrope = $x_j(u) = y_j(u)$

Putting it all together in Excel:

#	x	45° line	Rect line	Strip line	Feed line	Eq line	Stages	Distillate	Feed	Bottoms	Orig Data	Azeotrope
	0.85000							0.00000				
	0.85000							0.85000				
	0.10000								0.00000			
	0.10000								0.10000			
	0.01000									0.00000		
	0.01000									0.01000		
	0.00000	0.00000										
	1.00000	1.00000										
	0.85000		0.85000									
	0.06053		0.25789									
	0.06053			0.25789								
	0.01000			0.01000								
	0.10000				0.10000							
	0.00000				0.50000							
	0.00000					0.00000						
	0.00074					0.00500						
	0.00123					0.01000						
	↕					↕						
	0.99129					0.99000						
	0.99566					0.99500						
	1.00000					1.00000						
0	0.85000						0.85000					
	0.84346						0.85000					
1	0.84346						0.84509					
	0.83722						0.84509					
2	0.83722						0.84042					
	0.83116						0.84042					
	↕						↕					
21	0.04302						0.17202					
	0.01680						0.17202					
22	0.01680						0.04334					
	0.00398						0.04334					
23	0.00398						0.00398					
	0.00398						0.00398					
	0.00000						0.00000					
	↕						↕					
	0.00100										0.00470	
	0.00610										0.07210	
	0.01450										0.15390	
	0.02370										0.23010	
	0.03100										0.28510	
	0.04900										0.35590	
	0.06520										0.41810	
	0.09680										0.45340	
	0.13940										0.53140	
	0.32610										0.60470	
	0.46350										0.65180	
	0.54130										0.67510	
	0.68560										0.74510	
	0.77600										0.80050	
	0.84030										0.84570	
	0.90370										0.90100	
	0.97250										0.97210	
	0.98040										0.97740	
	0.00000										0.00000	
	↕										↕	
	0.88924											0.88924

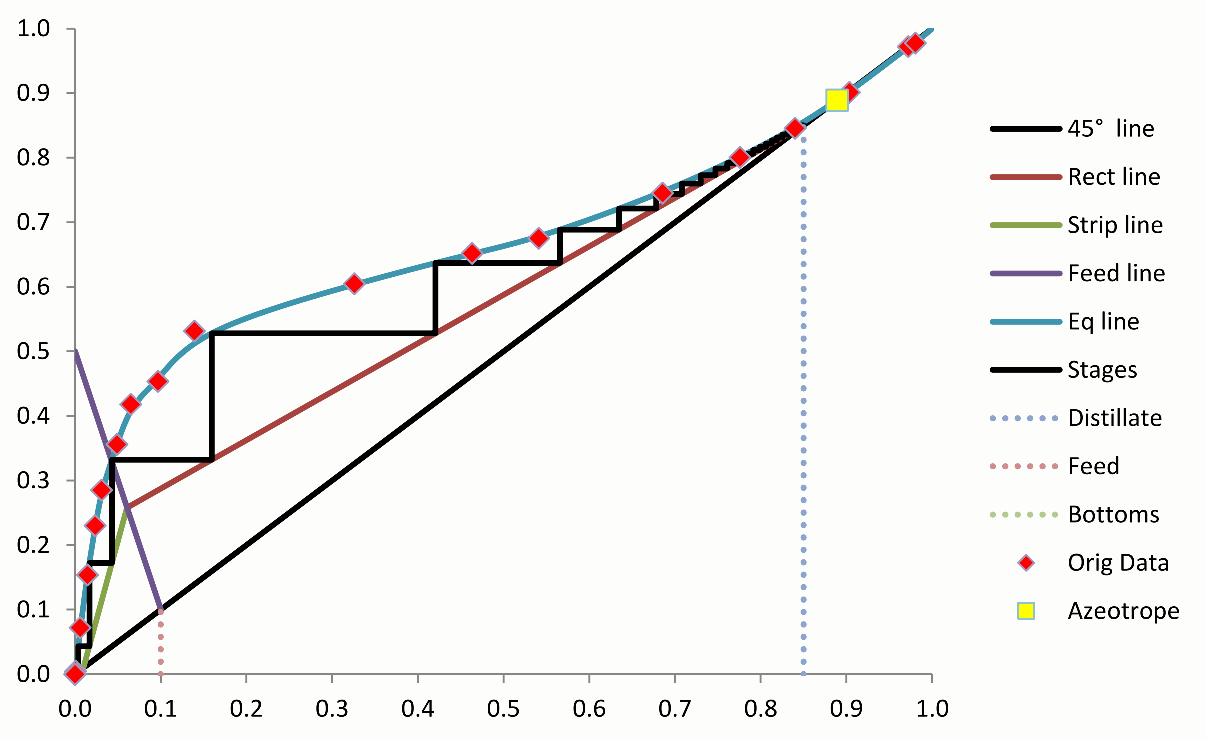
Easy Method to Draw Excel Plots:

1. Label adjacent columns, one for each plot line
2. Put all “x” values in a single column
3. Align column values with corresponding “x” values, leaving other “x” values blank
4. Select all the data, then Insert/Chart
5. Format the Chart as Desired

Putting it all together in Excel:

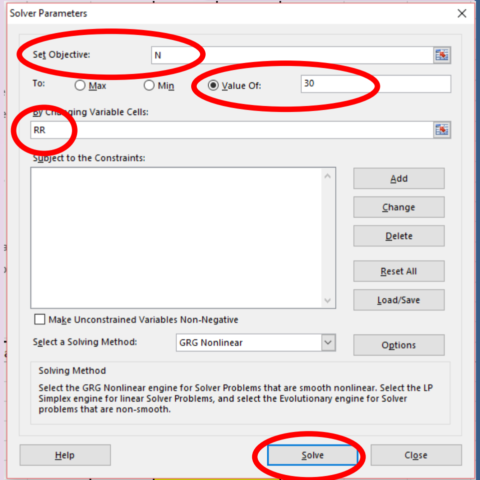
Inputs		Range
zf	0.1	xb < zf < xd
q	0.8	> -RR
xd	0.85	zf < xd < 1
xb	0.01	0 < xb < zf
RR	3	
η	1	0 < η ≤ 1

Outputs		
Azeo.	0.88924	if present, else 0
xf	0.06053	Intersection of feed
yf	0.25789	line with op lines
Stages	22.53015	N ≤ 50
Nf	21	Feed Stage



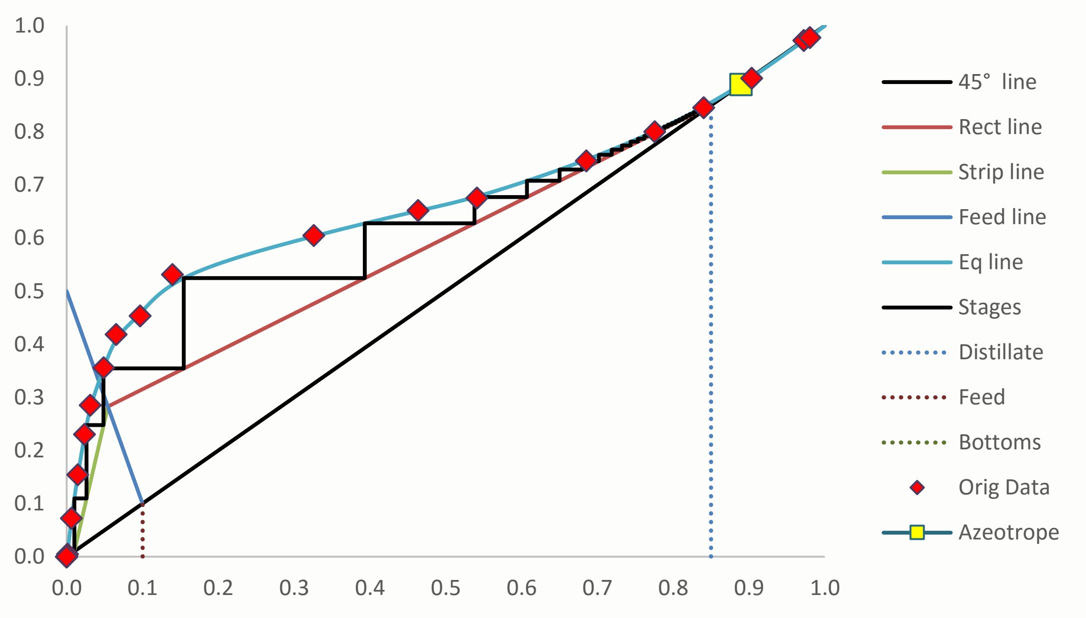
“What if?” Analysis in Excel: What RR is needed for N=30 stages?

1. Use “Solver”
2. Set “N” to Value of 30
3. Change “RR”



Inputs	
zf	0.1
q	0.8
xd	0.85
xb	0.01
RR	2.482797
η	1

Outputs	
Azeo.	0.88924
xf	0.05431
yf	0.28277
Stages	29.99997
Nf	28



Imagine how long drawing this by hand would take!

Conclusions:

Microsoft Excel with Visual Basic for Applications can calculate and display the McCabe-Thiele diagram for a nonideal binary distillation, given:

1. equilibrium *x*-*y* data
2. feed conditions
3. desired tops and bottoms purities
4. reflux ratio

Using the cubic B-spline method, the algorithm presented:

1. automatically smooths and fits the equilibrium data to an equilibrium curve
2. finds an azeotrope, if present

Outcome: quick and easy method to produce McCabe-Thiele diagrams for nonideal binary distillation

Acknowledgments: Colleagues **Peyton Richmond** (suggesting the CBS method) and **Daniel Knight** (thermodynamic help).