

SPREADSHEET-BASED SIMULATOR OF A FLASH DRUM:

Class Project Example for Material & Energy Balances and Phase Equilibria Courses

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We demonstrate a spreadsheet-based class project that can be continuously used from a Material & Energy Balances course to a Phase Equilibria (Chemical Engineering Thermodynamics II) course. In this project, students are asked to develop a process simulator for a flash drum using an Excel spreadsheet.

Indeed, Excel spreadsheets have been used as teaching aids in many chemical engineering problems and courses. As long as the formula organization in the spreadsheet is clearly designed, Excel provides clear visibility at each step, which makes it easy to repeat the same long multiple-step calculations with different parameters. Compared to the licensing fees of many commercial computational tools, Excel has a better chance of being available due to common use of Microsoft software products. Furthermore, based on the authors' industry experience, Excel spreadsheets are used commonly in workplaces, making it most advantageous for students to gain familiarity with using spreadsheets for engineering problems.^[1-11]

For this class project, we chose a flash drum to be simulated because a flash drum is a standard chemical engineering process unit, which is a basis both for vapor-liquid equilibrium (VLE) and for distillation processes. Therefore, it is beneficial for students to become familiar with this particular process as it will be very helpful in their separation class, unit operation labs, process design class, and out in industry. This project gives students the opportunity to develop a process simulator in which the graphic user interface looks similar to that of a commercial process simulator. Thus, students become familiar with applying Excel to fundamental and important chemical engineering calculations and gain an understanding that a simulator is a model solver with a graphic user interface.

The following learning outcomes are intended for this class project:

1. *Reduction in students' perception of a difference between calculations performed by hand and calculations*

performed by simulators. Students should understand that a commercial process simulator is a model equation solver with a graphic user interface to give numerical results.^[3,12]

2. *Students will gain experience using Excel to solve complex chemical engineering problems including VLE problems requiring iterative approaches and material and energy balance problems involving solutions of linear equations using matrix approaches.*
3. *Students will critically analyze a process using the simulator they develop.*

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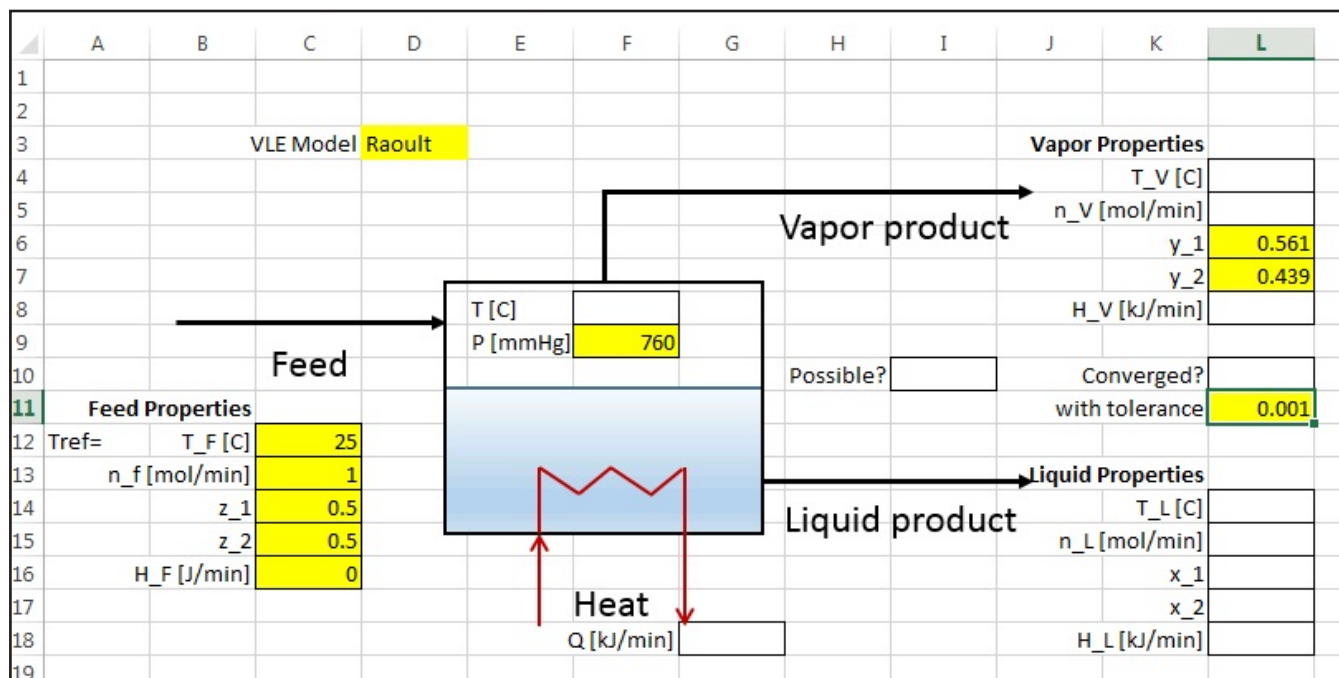


Figure 1. Screen capture of the assignment on an Excel worksheet. The worksheet called PFD contains the process flow diagram (PFD) for the flash drum with given process variables (shaded cells with borderlines) and unknown process variables (empty cells with borderlines).

In this paper a sample project—which was used in ChE 2100: Material and Energy Balances and ChE 3120: ChE Thermodynamics II at Missouri S&T—is demonstrated. The sample solution demonstrates each step of the calculation: the vapor-liquid equilibrium calculation, the mole balance calculation for liquid/vapor product rates, and the energy balance calculation for the required heat amount. Although the Rachford-Rice equation is a popular approach introduced in the classic thermodynamics textbook,^[13] the mole balance calculation is performed separately for the Material and Energy Balances students. It is also noted that the design of the spreadsheet formulation in this work can be simplified using the APEx add in.^[14] However, we choose a more fundamental approach considering students who are not familiar with Excel.

PROJECT FOR MATERIAL AND ENERGY BALANCES CLASS

An Excel spreadsheet template file with the image of the process flow diagram (Figure 1) and the problem statement is assigned to each student approximately after the midpoint of the semester. A sample statement is presented below:

Problem Statement

Develop a spreadsheet-based process simulator for a flash drum that separates a liquid mixture of binary mixture ($i=1$) *n*-hexane and ($i=2$) benzene into vapor and liquid products (i : index for components). Construct the formulas in the given spreadsheet to calculate the unknown process variables for the given conditions. You may perform the calculations

on a separate spreadsheet but be sure to have the solutions for the unknown process variables appear in the blank cells pictured in Figure 1 in order to model as closely as possible to a real process simulator. Answer the following questions (A, B, C and D).

- Solve for the operation temperature, T , of the flash drum and the liquid product stream mole fractions, x_1 and x_2 for the given operation pressure, $P=760$ mm Hg, and the given vapor product stream mole fraction, $y_1=0.561$. Assume that the mixture follows Raoult's law. Error tolerance for trial and error calculation is 0.1%. Whether or not T is converged within the given tolerance must be indicated on cell L10 in Figure 1.
- Solve for the flow rates of the vapor and liquid product streams (n_L and n_V) if the feed flow rate, n_F , is 1 mol/min and the feed mole fraction is $z_1=0.50$. Whether or not the flow rates of the streams are feasible should be indicated in cell I10 in Figure 1.
- Calculate the heat required for this process, Q . The feed stream temperature is $T=25^\circ\text{C}$, which is set as a reference temperature, T_{ref} . Ignore the pressure effect on the enthalpy change. Also, assume that mixture is ideal (no heat of mixing).
- Using the simulator you construct, calculate the process conditions to increase $y_1 > 0.561$ and discuss whether that condition is possible.

It is noteworthy that each student (or group) will be assigned different mixture compounds and a different set of given conditions. For example, instead of a given set of P and y_1 as

	A	B	C	D	E	F	G	H	I	J	K
1	Antoine Eqn	P _{vap,i} [mmHg]	A _i	B _i	C _i	Tmin	Tmax	T _{guess} [C]			
2	i=1: n-Hexane	901.528	6.88555	1175.817	224.867	13	69.5	74.280	→	answer	
3	i=2 Benzene	633.009	6.89272	1203.531	219.888	14.5	80.9	74.280			
4											
5											
6											
7											
8											
9	Dew T calc	y _i (given)	y _i /p _{vap}		P _{cal}	759.9996		x _i			
10	i=1: n-Hexane	0.561	0.000622		P(given)	760		0.4729	→	answer	
11	i=2 Benzene	0.439	0.000694		error	4.81E-07		0.5271			
12					tolerance (given)	0.001					
13											
14											
15											
16											
17											

Figure 2. Screen capture of worksheet QA: The Antoine equation and DEW-T calculation part for solving T and x_i. Change T_{guess} (cell H2) until the error, cell F11, becomes smaller than the given tolerance. Make sure that cell H3 = cell H2 so that T_{guess} is updated for both components together.

in this sample project, T and x_i can be given. Consequently, an instructor can assign each group a different project easily, which can prevent students from copying other students' work. All of the required thermodynamic properties such as Antoine equation parameters, critical properties, and heat capacity parameters, must be looked up either from appendices of the textbook used in this class,^[15] or elsewhere.^[16,17]

Sample Solution of Question A: Vapor-Liquid Equilibrium Calculation Using Raoult's law

Students can construct the formulas for solving the unknown variables anywhere, either in the same worksheet as the main problem or in another worksheet. In this sample solution, the question is solved on worksheet QA and the main worksheet PFD then references calculated values on QA.

First, Antoine equations must be set up to calculate the vapor pressures of each component p_{vap,i} (in the cell range of A1:H3 in Figure 2). Since T and x_i are unknown (this type of problem is classified as "DEW-T problem" in References 13 and 15), T can be found by trial and error. Therefore, as shown in Figure 2, Antoine equations for each component are set up to give vapor pressures at an initial guess of T, T_{guess} in cell H2. Note here that there are also BUBL-P, BUBL-T, and DEW-P problems.^[13,15] In this sample, we choose to demonstrate DEW-T problem.

The second step is to set up a formula for the calculation of x_i and P using T_{guess} and given y_i (in the cell range of A9:H11 in Figure 2). The given variables y_i, P, and the tolerance are set up so that they should be automatically assigned from the PFD worksheet. The formulas displayed in Figure 2 can be

derived from Raoult's law.^[13,15] The pressure in cell F9, P_{cal}, is calculated using the dew point pressure equation, shown in Figure 2. As long as T_{guess} is incorrect, this calculated pressure, P_{cal}, will be different than the given P in cell F10. A formula is used to calculate the relative error of P_{cal} with respect to P in cell F11.

For the third step, T must be found from trial and error. Two approaches are possible: (1) manual trial and error, or (2) using "Solver" provided in the spreadsheet. Depending on the curriculum of the department or students' level of understanding, it is the instructor's choice which approach should be chosen. If the manual trial and error approach is chosen, students have to understand whether the next T_{guess} must be increased or decreased depending on whether P_{cal} is smaller or larger than P. If P_{cal} > P, T_{guess} must be decreased. The trial and error continues until the error becomes smaller than the given tolerance. If the Solver approach is chosen, the Solver should be set up to adjust T_{guess} in cell H2 to minimize the error in cell F11. Once T is solved, x₁ and x₂ are calculated in cells H10 and H11.

Finally, set up the formulas so that the solved results x₁, x₂, and T should appear on the PFD worksheet as the operation temperature, T (cell F8), the liquid product temperature, T_L (cell L14), the vapor product temperature, T_V (cell L4), and the liquid product compositions, x₁ and x₂, cell L16 and L17, in Figure 1. The convergence indicator cell L10 is input as "=IF('QA'!F11<L11,"yes","no")." If the T is solved (relative error of P is within the tolerance), the cell shows "yes."

Sample Solution of Question B: Solve Mole Balance Equation for Product Flow Rates

Based on the solved and given compositions (x_i and y_i), n_L and n_V are solved based on the mole balances. This system of equations describing the total mole balance and the component 1 balance can be written in matrix form:

$$\begin{pmatrix} \mathbf{n}_F \\ z_1 \mathbf{n}_F \end{pmatrix} = \begin{bmatrix} 1 & 1 \\ x_1 & y_1 \end{bmatrix} \cdot \begin{pmatrix} \mathbf{n}_L \\ \mathbf{n}_V \end{pmatrix} \quad (1)$$

The unknowns, n_L and n_v , are solved in the following form:

$$\begin{pmatrix} \mathbf{n}_L \\ \mathbf{n}_V \end{pmatrix} = \begin{bmatrix} 1 & 1 \\ x_l & y_l \end{bmatrix}^{-1} \cdot \begin{pmatrix} \mathbf{n}_F \\ z, \mathbf{n}_V \end{pmatrix} \quad (2)$$

The matrix inversion in Eq. (2) is implemented as follows: (1) Select a cell area, which should have the same dimensions of the original matrix, cell range

of D9:E10 for the inverted matrix; (2) Type “=MINVERSE(D2:E3)”, then press “Ctrl+Shift+Enter.”

	A	B	C	D	E	F
1				Original matrix		
2				1	1	
3				0.4729	0.561	
4						
5						
6						
7						
8		vector(solution)		inverse matrix		vector
9	answer	0.6926		6.369967	-11.3547	1
10		0.3074		-5.36997	11.35467	0.5

Figure 3. Screen capture of the worksheet “QB.” The matrix equation is solved for n_i and n_v .

[illegible]

Figure 4. Screen capture of the worksheet “QC”: The enthalpy balance equation is solved for Q and H. Heat capacity parameters must be looked up and input in column G through J. Input the value of T_b in cell K6 and K13. The values of T_{guess} , n_I , n_V , and x_i were calculated in the previous questions.

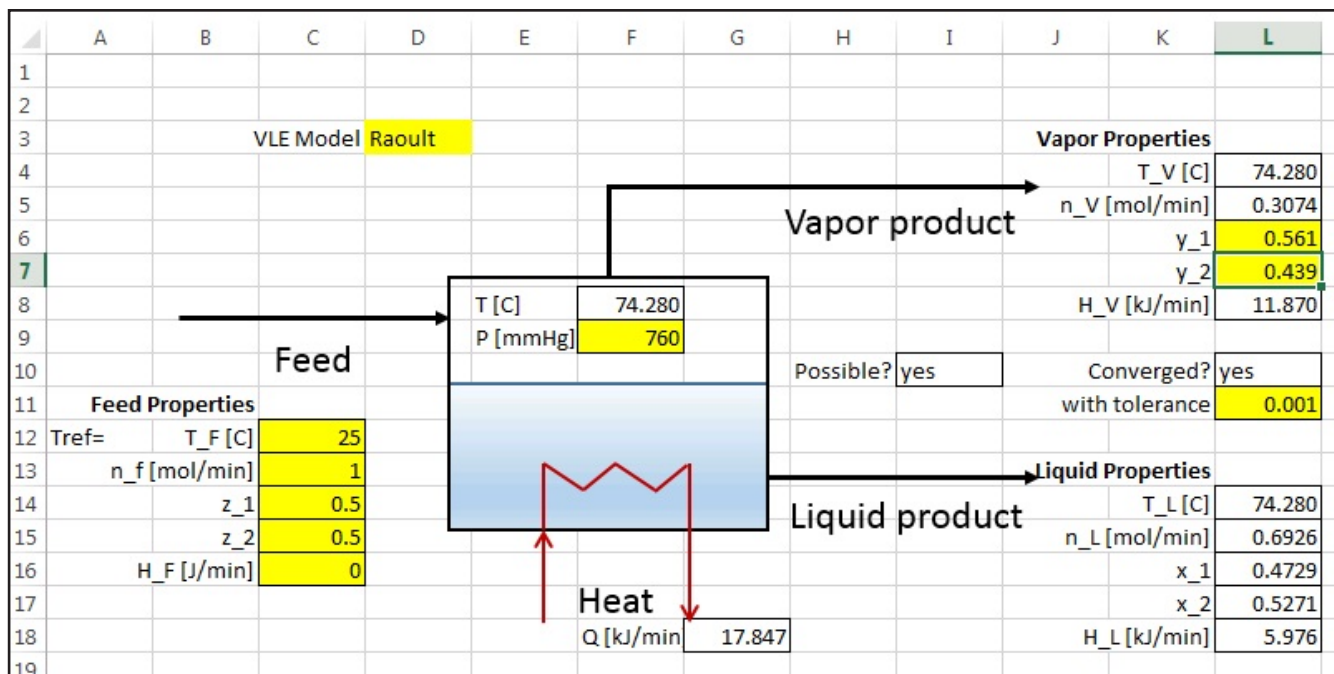


Figure 5. Screen capture of the worksheet PFD with the sample answers from questions A, B, and C.

The matrix multiplication in Eq. (2) follows the similar procedure by selecting the cell range of B9:B10 and typing “=MMULT(D9:E10,F9:F10).” It was found that demonstrating “Ctrl+Shift+Enter” in class was very helpful to students. Screen capture of this step is shown in Figure 3. It was also constructed on a different worksheet, “QB.” The given values, y_1 (cell E3), n_F (cell F9), and z_1 (cell F10), are also linked to the corresponding values in the PFD worksheet. Finally, make those solutions for n_L (cell L15) and n_V (cell L5) appear on the PDF worksheet in Figure 1. The feasibility indicator (cell I10) is input as “=IF (OR(L5<0,L5>C13),”No”,”Yes”)” to distinguish whether the solution of n_L and n_V is possible or not. If n_V is less than 0 or larger than n_F , the solution is physically not possible.

Sample Solution of Question C: Enthalpy Balance to Solve for Q

The calculation of Q is also implemented on another worksheet, “QC,” and demonstrated in Figure 4. Using the stream information obtained from Questions A and B, Q in cell A2 can be calculated from the enthalpy energy balance as shown in Figure 4. H is enthalpy and the sub index indicates each stream (L,V,F: liquid, vapor, feed, respectively). Since the temperature of the feed stream, T_F , was set as T_{ref} and the pressure effect on H is ignored, $H_F=0$. Assuming an ideal mixture (mixing enthalpy is ignored), H_L (cell B2) and H_V (cell C2) can be calculated from

the following:

$$H_L = n_L (x_1 \Delta \hat{H}_{L,1} + x_2 \Delta \hat{H}_{L,2}) \text{ and } H_V = n_V (y_1 \Delta \hat{H}_{V,1} + y_2 \Delta \hat{H}_{V,2}) \quad (3)$$

Here, $\Delta \hat{H}_{L,i}$ indicates molar enthalpy change of component i in liquid phase. For each component i, it can be calculated by integrating the molar liquid heat capacity of the component i, $C_{p,i}^L$, from T_{ref} to T. For the vapor phase, $\Delta \hat{H}_{V,i}$ must be calculated over three hypothetical processes: (Path A) the component i at T_{ref} is heated to its T_b (normal boiling point); (Path B) the saturated liquid is vaporized to the saturated vapor at T_b ; (Path C) the saturated vapor is heated to T. Implementation of each step is demonstrated in Figure 4. For each component in each phase, heat capacity parameters are input in columns G, H, I, and J. Integration of heat capacity was implemented by using analytically integrated forms in cells F5, F7, F12, F14, F24, and F28. For Path B, enthalpy change calculations, heat of vaporization, and normal boiling point temperatures are input in cell F6, F13, K6, and K13. The answers for Q (cell G18), H_L (cell L18), and H_V (cell L8) are also displayed in the PDF worksheet in Figure 1. Figure 5 shows the completed simulator with all the unknown variables solved.

Sample Solution of Question D: Discussion on Varying the Process Condition (“What If” Scenarios)

Students may choose any value of $y_1 > 0.561$. For example, $y_1 = 0.6$ is chosen for this sample solution of a “What if” scenario. In the PFD worksheet of the completed simulator in Figure 5, $y_1 = 0.561$ (cell L6), is replaced with $y_1 = 0.6$. The cell for the convergence indicator (cell L10), turns into “no” because the simulator is not yet solved for the new condition. To make the simulation results converge for the new condition of $y_1 = 0.6$, the DEW-T calculation worksheet QA, shown in

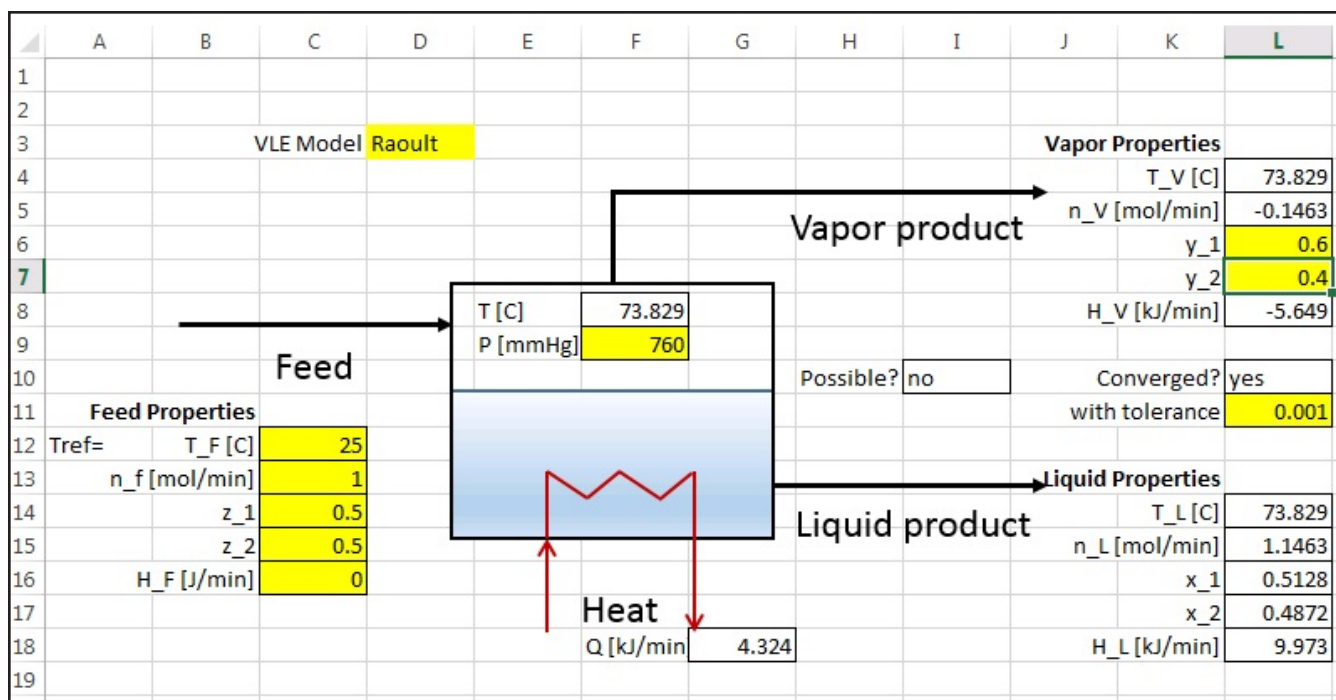


Figure 6. Screen capture of the worksheet PFD with the sample answers from question D: The new simulation results from the new condition of $y_1=0.6$. The resulting product stream flow rates are not possible ($n_L > n_F$ and $n_V < 0$).

Figure 2, must be solved again. Once the new DEW-T calculation is completed, n_L , n_V , and Q are automatically updated. The new calculation results are shown in Figure 6. The feasibility indicator, cell I10, is now “no” because the product flow rates are not possible. Since this project is given for the Material and Energy Balances class, students may discuss that the amount of component 1 in the feed is not enough to satisfy the desired vapor product concentration. After submission of the project, a “food for thought” question will be given: “What are the possible ranges for y_1 ?” This question will serve as a segue for students to begin considering topics covered in their Thermodynamics II course.

PROJECT FOR PHASE EQUILIBRIA COURSE

The sample project demonstrated can be used in the next-level course related to the phase equilibria (Chemical Engineering Thermodynamics II at Missouri S&T) with the following variation:

- Upgrade Question A using the two-parameter Margules equation instead of Raoult's law.
- Look up the experimental data to compare to the results from both approaches (Raoult's law and Margules equation).

This question can be changed with any activity coefficient model or any cubic equation of state.

Sample Solution: Upgrade the Simulator with the Two-Parameter Margules Equation

For this sample solution, we follow the iteration scheme suggested in Chapters 10 and 14 of the textbook.^[13] The worksheet QA is replicated to a new worksheet, QAMargules, which will be modified for this solution in Figure 7. The initial guess for x_1 and T , $x_{1,guess}$ (cell H10) and T_{guess} (cell H2), may be taken from the results of Raoult's law in Question A. Activity coefficients, γ_i (cells D10 and D11), can be calculated using the Margules equation with $x_{i,guess}$ in the following:

$$\ln \gamma_1 = x_{2,guess}^2 [A_{12} + 2(A_{21} - A_{12})x_{1,guess}] \quad (4)$$

$$\ln \gamma_2 = x_{1,guess}^2 [A_{21} + 2(A_{12} - A_{21})x_{1,guess}] \quad (5)$$

Students are asked to find the required Margules model parameters, A_{12} and A_{21} , from Reference 17 and input them in cells H6 and H7. Using those activity coefficients, the liquid compositions are calculated as $x_{i,cal}$ (cells E10 and E11):

$$x_{1,cal} = \frac{y_{1,P}}{\gamma_1 P_{vap,1}}, \text{ and } x_{2,cal} = \frac{y_{2,P}}{\gamma_2 P_{vap,2}} \quad (6)$$

Note that $x_{2,cal} \neq 1 - x_{1,cal}$ yet. Subsequently, those must be renormalized in cells F10 and F11:

$$x_{i,norm} = \frac{x_{i,cal}}{x_{1,cal} + x_{2,cal}} \quad (7)$$

	A	B	C	D	E	F	G	H	I	J
1	Antoine Eqn	P_vap,i [mmHg]	A_i	B_i	C_i	Tmin	Tmax	T_guess [C]		
2	i=1: n-Hexane	820.71	6.88555	1175.817	224.867	13	69.5	71.2071	→	answer
3	i=2 Benzene	573.09	6.89272	1203.531	219.888	14.5	80.9	71.2071	←	
4										
5		$p_{vap,i}[mmHg] = 10^{\left(A_i - \frac{B_i}{T_{guess}[^{\circ}C] + C_i}\right)}$					P(given)	760		
6							A12	0.4714	Margules	
7							A21	0.3706	Parameters	
8										
9	Dew T calc	y_i (given)		r_i	x_i_cal	x_i_norm		x_i_guess		
10	i=1: n-Hexane	0.561		1.087176	0.477845	0.4778		0.4778	→	answer
11	i=2 Benzene	0.439		1.11476	0.522241	0.5222		0.5222	←	
12										
13										
14										
15		$\ln \gamma_1 = x_{2,guess}^2 [A_{12} + 2(A_{21} - A_{12})x_{1,guess}]$			$x_{1,cal} = \frac{y_1 P}{\gamma_1 p_{vap,1}}$		$x_{i,norm} = \frac{x_{i,cal}}{x_{1,cal} + x_{2,cal}}$			
16		$\ln \gamma_2 = x_{1,guess}^2 [A_{21} + 2(A_{12} - A_{21})x_{2,guess}]$			$x_{2,cal} = \frac{y_2 P}{\gamma_2 p_{vap,2}}$					
17										
18										
19								error x1	8.21E-06	
20								error T	3.92E-05	
21								T-iteration loop		
22		p_vap_1_new	820.7802		Tnew	71.20989				
23										
24		$p_{vap,1,new} = P \left(\frac{y_1}{\gamma_1} + \frac{y_2 p_{vap,1}}{\gamma_2 p_{vap,2}} \right)$			$T_{new} = \frac{B_1}{A_1 - \log_{10} p_{vap,1,new}} - C_1$					
25										
26										

Figure 7. Screen capture of the worksheet QAMargules: DEW-T calculation using the Margules equation.

This Eq. (7) makes $x_{2,norm} = 1 - x_{1,norm}$. An iterative method is then used to solve for $x_{1,guess}$ to be matched with $x_{1,norm}$ from Eq. (7). As in the sample solution of Question A, two approaches are also possible: (1) manual iteration, or (2) using Solver. For the manual iteration, if $x_{1,guess}$ and $x_{1,norm}$ are different, the recalculated and renormalized $x_{1,norm}$ (cell F10) is copied and pasted into the cell H10 as a new $x_{1,guess}$ for the next iteration step from Eq. (4) to Eq. (7). This “x-iteration loop” (cell range D9:H11) is continued until converged (the relative error between $x_{1,guess}$ and $x_{1,norm}$ becomes small enough in cell I19). If the Solver method is chosen, the Solver should be set up to adjust $x_{1,guess}$ in cell H10 (set up cell H11 as $x_{2,guess} = 1 - x_{1,guess}$) to minimize the error in cell I19. Note here that cell I19 must be $|x_{1,guess} - x_{1,norm}|$ not the relative error $|x_{1,guess} - x_{1,norm}|/x_{1,guess}$, which the Solver cannot minimize.

Once the x-iteration loop is converged, T must be solved with the “T-iteration loop.” For the next iteration of T, the new value of T_{guess} , T_{new} (cell F22), is estimated with the following:

$$p_{vap,1,new} = P \left(\frac{y_1}{\gamma_1} + \frac{y_2 p_{vap,1}}{\gamma_2 p_{vap,2}} \right) \quad (8)$$

$$T_{new} = \frac{B_1}{A_1 - \log_{10} p_{vap,1,new}} - C_1 \quad (9)$$

This is used again for T_{guess} . The x-iteration loop and subsequently the T-iteration loop must be repeated. The answers of T (cell H2) and x_1 (cell H10), must be updated on the subsequent pages so that the PFD worksheet shows the modified results using the Margules equation. The relative error of T in cell I20 can be used in the convergence indicator (cell L11) of the PFD worksheet. If an automated approach is preferred to teaching iterative approaches, Solver may be used by setting $x_{1,guess} = x_{1,norm}$ as a constraint while varying $x_{1,guess}$ and T to minimize the relative error of T.

Experimental values from Reference 17 are $x_1 = 0.4840$, $y_1 = 0.5610$, and $T = 71^\circ\text{C}$ at $P = 760$ mm Hg. Using Raoult’s law, $x_1 = 0.4729$ and $T = 74.3^\circ\text{C}$ are obtained from this simulator at those experimental y_1 and P values. Using the Margules equation, $x_1 = 0.4778$ and $T = 71.2^\circ\text{C}$ are obtained. For this sample system, the results from Margules model are found to be closer to the experimental data.

STUDENT FEEDBACK AND EVALUATION

The expected learning outcomes (1) and (3) were achieved: The evaluation based on a student's final grade on this project indicated that more than 90% of students acquired the skill to use an Excel spreadsheet to solve the vapor-liquid phase equilibrium problem and the simple mass and enthalpy balance problems. Some students showed an improved utilization of Excel spreadsheets: they created a cell that indicates whether the next T_{guess} should be increased or decreased for Question A. Some students also proposed different "what if" scenarios for Question D, such as the feasible ranges of z_1 . It was also observed that some students used an Excel spreadsheet for other homework problems without being asked to, which indicates that students found Excel to be a useful tool when solving similar problems.

Learning outcome (2) also seems to be achieved: Students who took the course related to distillation process (Staged Mass Transfer course), commented that they could understand the importance of the model selection in simulation of distillation column, and considered the feasibility of simulation results.

CONCLUSION

We demonstrated an Excel spreadsheet-based class project sample where students are asked to develop a simulator for a flash drum. This project can bridge a Material & Energy Balances class and a Phase Equilibrium class to improve student understanding of separation processes later in the curriculum. It was found that students extended the utilization of Excel in other chemical engineering problems. Students commented that they can better understand the connectivity of the material in chemical engineering courses and that this project helped their simulation homework in a separations class.

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17. Gmehling J, Onken U, Arlt W, Grenzheuer P, Weidlich U, Kolbe B, & Rarey J (2014) *Vapor-Liquid Equilibrium Data Collection, Chemistry Data Series Volume I 1981-2014* (DECHEMA, Frankfurt, Germany). □

The Class and Home Problems section is intended to present novel and innovative scenarios that can enhance the teaching of chemical engineering topics. Submissions must have clear learning objectives, outcomes, or similar statements. The fit within a typical chemical engineering (or closely related) curriculum should be clear. Problems may represent a new application of fundamental principles, substantive adaptations that enable effective pedagogical approaches, or new non-proprietary applications of software. Manuscripts should follow the same general guidelines as other CEE submissions, but should be submitted directly to
Dr. David Silverstein (david.silverstein@uky.edu)