> Class and Home Problems (CHP) present scenarios that enhance the teaching of chemical engineering at the undergraduate or graduate level. Submissions must have clear learning objectives. CHP papers present new applications or adaptations that facilitate learning in specific ChE courses. Submit CHP papers through journals.flvc.org/cee, include CHP in the title, and specify CHP as the article type.

BRIDGING THE GAP BETWEEN HAND CALCULATIONS AND CHEMICAL PROCESS SIMULATORS USING SPREADSHEETS

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BACKGROUND

Most design calculations in undergraduate separations courses involve solving a combination of mass/energy balances, mass transfer, and equilibrium equations. The teacher is responsible for a balanced schedule of theoretical lectures and practical workshops. Digital tools contribute to engaging students.[1,2] If computer software is integrated into the course, the teacher must decide between commercially available "task-specific" programs (e.g. AspenONE®, CHEMCAD®, etc.) and more general "equation solving" programs (e.g. Mathcad®, MATLAB®, Microsoft Excel®, etc.).[3] While process simulators are instrumental to chemical engineering practice, they have the disadvantage that the equations and the solution strategy are not always perceived by the students.[3-5]

The "Unit Operations of Chemical Engineering II" course at the University of Huelva (Spain) corresponds to the third year (second semester) of a standard Bachelor's Chemical Engineering program. The course deals with the design of equilibrium-staged and continuous-contact mass transfer operations, i.e. flash, batch and fractional distillation, gas absorption/stripping, liquid extraction, and leaching processes. Until last academic year, the theoretical lectures had always been supported by traditional problem-solving sessions consisting of solutions using graph paper and calculators, and by some computer workshops involving the parallel use of Aspen Plus® and Mathcad. The use of both software packages helped us mitigate the so-called "black-box" effect.[5,6]

Due to the lockdown period in the second semester of 2020, the course had to be adapted to a 100% virtual learning scenario. Consequently, its practical aspects needed to be enhanced because the established balance between theory and practice was no longer valid. Distance learning requires a more engaging environment than the one created by the mere utilization of traditional lectures and hand calculations. This scenario led the authors to reflect on the importance of
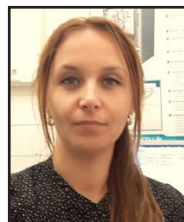
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developing suitable strategies, including the use of Excel described herein, when traditional face-to-face teaching is no longer possible.

Excel was chosen for different reasons: a) it is widely available and ideal for distance learning;[7-9] b) it is fully compatible with other free spreadsheet software; c) most students had some previous knowledge of the software, thus facilitating the instructional delivery;[10,11] and d) it will be one of the few calculation tools ubiquitously available to students once they graduate. The students were able to work from home, guided by the teacher who delivered instructions through a videoconferencing platform. The authors' experience is that students typically use Excel to carry out simple and repetitive calculations, but they do not know how to take full advantage of its capabilities in the study of chemical engineering. Upon completing the course, the students learned that Excel built-in functions (TREND, MATCH, INDEX, IF, etc.) enable very accurate results and provide nice graphical solutions.[11]

SPREADSHEETS AND MASS TRANSFER OPERATIONS

Excel has found extensive application in many chemical engineering subjects: mass and energy balances,[8] process simulation and control,[12-14] optimization,[10,11,15,16] chemical kinetics and reaction engineering,[17-19] heat transfer and transport phenomena,[20,21] phase equilibria and thermodynamics,[22-25] and unit operations.[26-28] In particular, Excel spreadsheets have been used as teaching aids in mass transfer separation problems.[3,4,7,29-31] In the latest edition of the book *Separation Process Engineering*,[32] Wankat has included the use of Microsoft Excel macros. The importance of this programming language is also discussed elsewhere.[17,33] By using predefined built-in functions, the students can take advantage of the power of spreadsheets for the design of mass transfer separations even if they are not skilled in computer programming. Such an approach allows the teacher to focus on the course contents. In this way the learning process is very efficient, provided that one is able to combine the built-in functions of Excel using a structured way of thinking. The ease of graphical analysis provided by Excel is valued in multistage operations problems because it allows the students to better visualize the problem, thus enhancing understanding.[3-7]

As long as the spreadsheet is clearly designed and appropriate comments within the sheets are included, Excel provides clear visibility at each step. This makes it easy to repeat the same long multiple-step calculations with different parameters,[29] thus facilitating the design of equilibrium-staged operations and reducing the workload. Through the process of entering inputs into particular cells and plotting the computed outputs, students gain an understanding of how commercial process simulators work.[29] However, unlike simulators, students still need to understand the solving algorithm in order to edit an existing worksheet to adapt it to a new case. The key for success lies in using a series of exercises that address the problem from different perspectives (using different specifications, unknowns, VLE data format, etc.). Thus, Excel may help to bridge the gap between traditional manual calculations and process simulators.[4]

EXPERIENCE IN A MASS TRANSFER SEPARATIONS COURSE

Over the last few years, the authors have become familiar with Aspen Plus and Mathcad software. However, this is the first time the authors have integrated Excel into a mass transfer separations course as a response to the teaching needs that arose. Previously published works on the use of spreadsheets in Unit Operations courses mainly focused on reporting a methodology for solving specific problems with the software. [3,4,7,26-31] However, we present a system of experiences centered on improving specific competencies. During 15 years of continuously teaching this material, the authors have identified a list of typical problems faced by students in mass transfer separation courses. Based on that, eight specific benefits of using Excel built-in functions in multistage operations design are presented and analyzed.

The course objectives were:

- To use Excel built-in functions and graphical representations to solve mass transfer separations problems, with special emphasis on the physical interpretation of the results.

- To demonstrate Information and Communications Technology (ICT) competencies related to the use of spreadsheets in engineering calculations.[9,10,33]

IMPLICATIONS ON THE STUDENTS' LEARNING

The following eight aspects can serve as guidelines to maximize the value of spreadsheet usage.

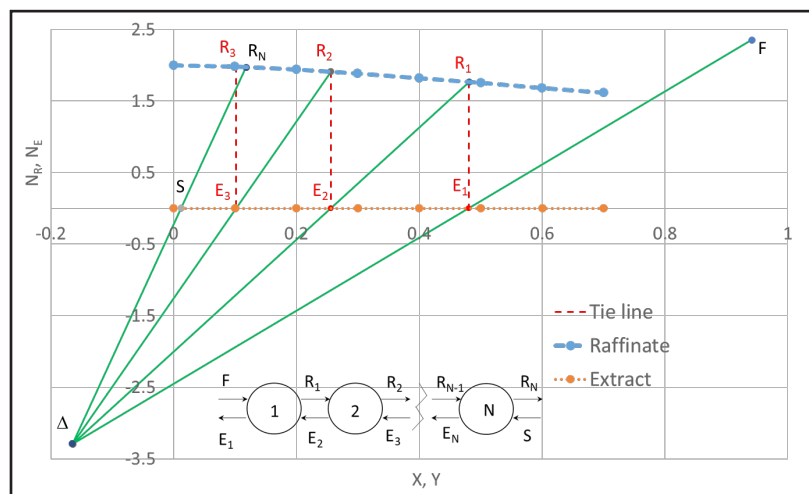### #1 Avoiding the Limitations of Using Graph Paper and Increasing Accuracy

"Fish oil (feed: 2000 kg/h solid; 800 kg/h oil; 50 kg/h benzene) is extracted with solvent (1600 kg/h benzene; 20 kg/h oil) in a multistage counter-current leaching process. The final raffinate must contain no more than 120 kg/h oil." This type of problem, illustrated in Figure 1a, can be addressed by a graphical approach, similar to the Hunter-Nash method

for liquid-liquid (L-L) extraction.[34] The method requires determining the so-called "operating point" (Δ) by the intersection of the straight lines FE_1 and R_NS in a Janecke diagram (Figure 1a).[35]

When solving the problem by hand, if the graph scales and/or orientation of the paper are not adequately chosen, the student will be unable to use the graphical method because the operating point lies too far from the area where the stages are plotted. If the student does manage to find the operating point (for example, by attaching an extra paper sheet), the solution lacks accuracy because the plotted lines deviate too much. With Excel the graph scales can be adjusted accordingly. Even if the operating point is located far from the area where the stages are plotted, the use of Excel is still valid because the student may localize analytically the coordinates $\Delta(X_\Delta, N_\Delta)$, as shown in Figure 1b. The procedure is explained later in point #3 Consolidating Basic Mathematical Concepts.

#2 Enhancing the Use of Different Types of Diagrams and Saving Time

Simple Cartesian equilibrium diagrams, such as the Janecke diagram for leaching (Figure 1a), or the McCabe-Thiele diagram for binary fractional

(a)

(b)

Figure 1. *(a) Graphical solution of a typical counter-current leaching problem, including a schematic representation of the extraction sequence; (b) Analytical solution of the operating point coordinates.*

distillation (see later in Figure 6, in point #6) are easy to plot using Excel. In a liquid-liquid (L-L) extraction problem, the graphical method is very often applied on a triangular phase diagram. Our experience is that many students do not perceive how to solve a L-L extraction problem using a right-triangle diagram because they are unsure about which two compositions (from the three possible: solute, carrier, and solvent) should be plotted. Consequently, they end up drawing an equilateral triangle on standard graph paper, which does not facilitate the scaling. In Excel it is not possible to plot equilateral triangles, so the student will have to cope with the use of right triangles. In Figure 2, for example, the solute and solvent weight fractions have been represented in the ordinate (y) and abscissa (x) axes, respectively. Of course, other options are also possible, thus varying the orientation of the LLE bimodal curve.[7] Moreover, the students will notice that using a right triangle is more convenient because sizing the x and y axes adequately allows better display of the solution.

#3 Consolidating Basic Mathematical Concepts

In the 2-stage, cross-flow L-L extraction problem shown in Figure 2, the required solvent flow rates, S_1 and S_2, can be determined given the mass flow rates and compositions of F, E_1 and E_2. Figure 3 illustrates the use of some basic analytical and geometrical operations (linear interpolation, linear regression, and intersection of straight lines) applied to that problem.

The first step is to find y_{R1} so that R_1 can be placed on the diagram. The relation between the raffinate and extract streams leaving the same stage "i", $y_{Ri} = f(y_{Ei})$, is given by the corresponding tie-line. Thus, for $y_{E1} = 0.395$ (cell B19 in Figure 3), $y_{R1} = 0.191$ (cell B22 in Figure 3) is found by linear interpolation using the equilibrium data table. Intentionally, for the sake of space-saving, some cells (F5, F6, etc.) referenced in the Excel procedure in Figure 3 are not in view. Using the TREND function, which interpolates a regression line passing through two given points, yields accurate results for the raffinate composition.

Further, it is necessary to locate the mixing point M_1 composition, which enables the user to calculate S_1 (assumed to be pure solvent, as in Figure 2) using the mass balance in Eq. 1:

$$y_{M1} = \frac{Fy_F}{F + S_1} \tag{1}$$

The coordinates $M_1(x_{M1}, y_{M1})$ are analytically determined by the intersection of the straight lines FS_1 and R_1E_1. The straight lines are calculated by using the Excel SLOPE and INTERCEPT functions that return the slope and intercept of a regression line passing through two given points, respectively. The same procedure can be used to find the operating point Δ (Figure 1b).
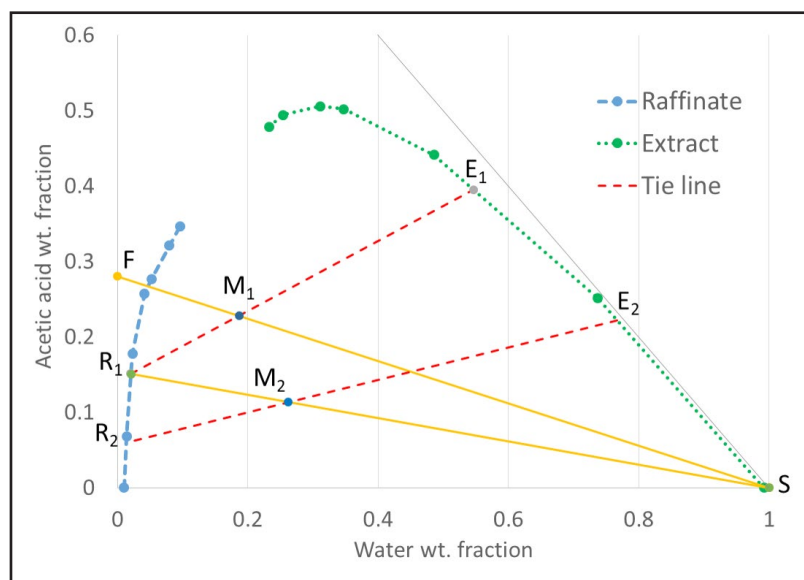

Figure 2. *A cross-current L-L extraction problem solved in a right triangle.*

**Figure 3.** *Specific use of the TREND, SLOPE and INTERCEPT Excel functions applied to the problem in Figure 2.*

#4 Enabling 'What-If' Analysis

The problem statement of a counter-current L-L extraction problem may ask the student to determine the number of equilibrium stages such that "*the final raffinate R_N must contain no more than, for example, 12 wt.% solute.*" The graphical solution for a problem of this type is displayed in Figure 4a. The dashed lines are the tie-lines that correspond to the equilibrium stages. In total, 3 stages are needed to satisfy the above requirement with the solvent flow rate specified by the problem (1800 kg/h). Even so, three stages yield a higher percentage of solute removal than what is required ($y_{R3} = 0.057 < y_{RN} = 0.12$). Excel may, thereby, assist in the analysis of potential alternative solutions.

The interactive nature of the spreadsheets allows "what-if" analyses in which the parameter values are changed and the results are immediately displayed.[4] For example, in the solution displayed in Figure 4a, there still remains scope for improvement, provided that the R_N solute wt.% does not exceed 12%. The number of stages is an integer variable. Thus, the students can "play" with the solvent flow rate in two ways: a) increasing the solvent flow rate (2050 kg/h) so that $y_{RN} = 0.12$ is reached with 2 stages (in Figure 4b); and b) decreasing the solvent flow rate (1625 kg/h) so that $y_{RN} = 0.12$ is reached with 3 stages (not shown). This open-ended approach empowers the students with skills to critically analyze a process.[29] Obviously, the final solution will need further economic analysis in order to find out which of the two options is better. This type of analysis contributes to bridging the gap between design, optimization and economics, thus giving the student a more complete overview of the chemical engineering discipline.

#5 Improving Creativity

McCabe-Thiele distillation problems require finding a $y = f(x)$ VLE function. Best fitting curves do not always yield accurate results, especially if the mixture deviates from ideal behavior. Direct interpolation using the data table is probably a better option.[3] Complete automation is possible using the existing built-in functions without the need for macros. The students are encouraged to seek the combination of functions that enables automation. Thus, this type of exercise helps students im-
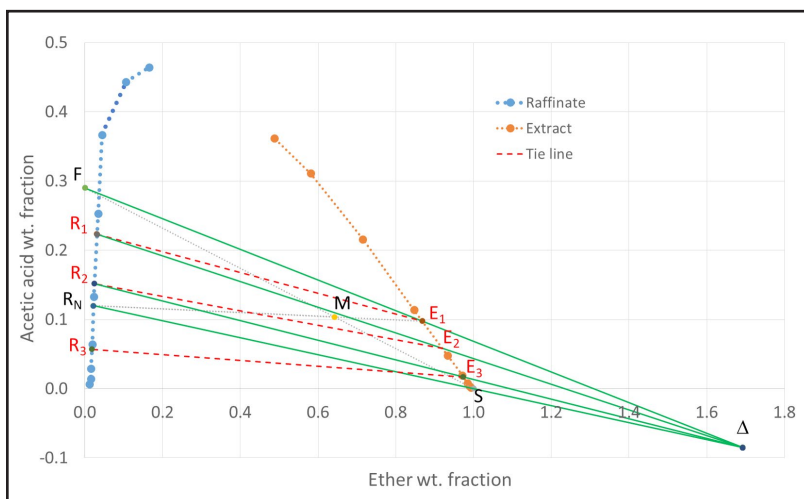
(a)
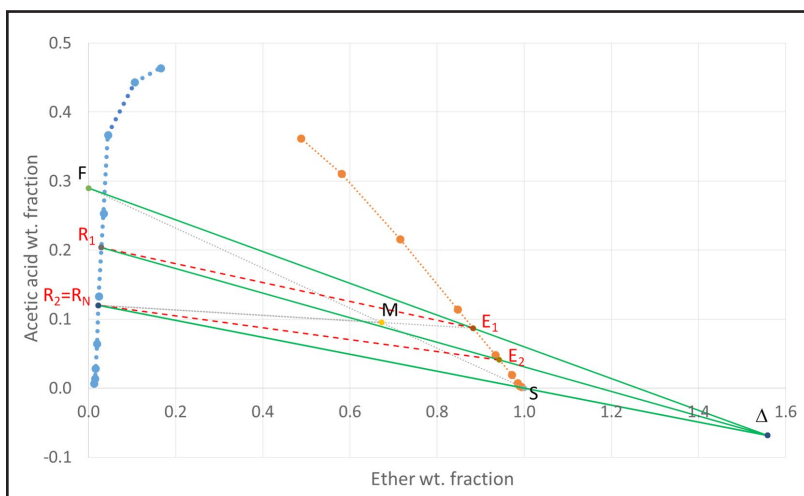
(b)

Figure 4. *(a) Problem solved with the specified solvent flow rate of 1800 kg/h; (b) Optimization process in order to achieve y_{RN} = 0.12 with 2 stages (solvent flow rate of 2050 kg/h).*

prove their analytical and structured (programming) thinking. For example, when stepping off the stages starting from the top, it is necessary to find the composition of the liquid leaving stage 1, x_{stage_1}. In a column equipped with a total condenser, the composition of the vapor leaving stage 1 is the same as the overhead product, x_D (cell N3, x = 0.950, in Figure 5). Thus, $y_{stage\_1} = x_D = 0.95$. One can use the MATCH function to identify the position in the equilibrium data table (not shown for the sake of space-saving) that corresponds to the value immediately below $y_{stage\_1} = 0.95$. The position is i = 9 (cell P4 in Figure 5). Then, the INDEX function allows reading the two y-values that satisfy $y_i < y_{stage\_1} < y_{i+1}$, and their corresponding x-values (cells Q4 to T4 in Figure 5). These values will be finally used to carry out linear interpolation (TREND function), yielding $x_{stage\_1} = 0.786$ (cell N4 in Figure 5). The use of the MATCH and INDEX functions is shown in Figure 5.

#6 Facilitating Step-By-Step Calculations (Multistage Operations)

The logic IF function can be used to decide, according to the optimal feed location, which of the two operating lines, either rectifying or stripping, is used to calculate the molar fraction of the vapor leaving a stage. Following the example from point #5, the rectifying section line (Figure 6) was used to obtain the composition of the vapor leaving stage 2, $y_{stage\_2} = 0.847$ (cell O5 in Figure 5). The optimal feed stage is based on the crossover point between the two operating lines (not shown for the sake of space-saving). The COPY and PASTE function allows repeating the same procedure until the condition $x_{stage\_6} < x_B = 0.05$ is satisfied, i.e. the liquid molar fraction leaving a plate (plate 6) is below the bottom product composition, x_B. The x_{stage_6} value is in cell N20, x = 0.024, in Figure 5. The graphical result is shown in Figure 6. For the sake of clarity, the rectifying section, VLE curve, and stripping section have been represented with solid, dotted and dashed lines, respectively. Stage 3 is the optimal feed location.

#7 Avoiding Inaccuracy Derived from Inadequate Fitting

Simple batch distillation requires the use of the so-called Rayleigh equation, Eq. 2

$$Ln\left(\frac{L_0}{L_f}\right) = \int_{x_f}^{x_0} \frac{dx}{y-x} \qquad (2)$$

where L_0 and L_f are the initial and final liquid charge in the still pot in moles, respectively; x_0 and x_f are their corresponding molar fractions; and y and x are the vapor and liquid molar fractions, respectively. Most often, the VLE data are provided in the form of a table, thereby requiring numerical integration. In the authors' experience students are quite reluctant to use numerical methods. If the students are left to solve the problem without any guidance, they usually opt for finding the best fit parameters of a high degree polynomial function. Moreover, they usually fit the whole data set provided, even if the solution lies within a narrow subinterval (Figure 7a). The students are not aware whether the obtained curve, in actuality, fits the data set or not. Thus, lack of accuracy often arises as a consequence of a poor fitting (dashed line in Figure 7a).

Excel enables an easy application of numerical integration, e.g. the simplest method, trapezoidal rule. Only data within the x-value interval from 0.100 to 0.420 were used in Figure 7. The TREND function can be used, if required, in order to find interpolated values corresponding to the starting and ending concentrations, $x_0 = 0.4$ and $x_f = 0.191$, respectively. Each trapezoid area is calculated in a separate cell so that the integral is computed using the SUM function within the entire interval of interest, thus providing accurate results (Figure 7b).

#8 Engaging Students, Especially During Distance Learning Activities

The use of Excel was, in general, well received by the students as a way to stay connected to the course during the forced virtual learning period. Excel's built-in functions are powerful enough to assist in the study of this matter in any possible distance learning scenario, or even in face-to-face courses when other software may be unavailable.[8,9]

To this point in the curriculum, the students had never approached a subject within which the entire collection of problems was solved with Excel built-in functions. Studying the contents was more appealing. Thus, the methodology attracted their interest in such a way that it improved their academic performance. In 2018-2019, using the traditional method, only 6 out of 11 students (54.5 %) passed the exam (5 or more points out of 10). In 2019-2020, with the use of Excel, 17 out of 20 students (85 %) passed the exam. Moreover, in 2018-2019, no one earned grades equal to or higher than 9 points out of 10, while in 2019-2020, 35 % of students performed at such a high level. From the authors' standpoint, the course objectives were achieved. As the students progressed through the course, they improved their competencies in the use of spreadsheets in engineering calculations. We think they are now better equipped to face other subjects that may also require calculations and graphical representations.

	L	M	N	O	P	Q	R	S	T
2	**Stage**	**Point**	**x**	**y**		Data used in interpolations			
3		Rectifying	0.950	0.950	i=	$x_i=$	$x_{i+1}=$	$y_i=$	$y_{i+1}=$
4	**1**	**Equilibrium**	**0.786**	**0.950**	*9	0.700	0.800	0.920	0.955
5		Rectifying	0.786	0.847	*=MATCH(O4;C$2:C$13;1)				
6		Rectifying	0.786	0.847	i=	$x_i=$	$x_{i+1}=$	$y_i=$	$y_{i+1}=$
7	**2**	**Equilibrium**	**0.554**	**0.847**	7	**0.500	0.600	0.814	0.874
8		Rectifying	0.554	0.701	**=INDEX(B$2:B$13;P7)				
9		Rectifying	0.554	0.701	i=	$x_i=$	$x_{i+1}=$	$y_i=$	$y_{i+1}=$
10	**3**	**Equilibrium**	**0.365**	**0.701**	5	0.300	0.400	0.631	0.739
11	**(feed)**	Stripping	0.365	0.506					
12		Stripping	0.365	0.506	i=	$x_i=$	$x_{i+1}=$	$y_i=$	$y_{i+1}=$
13	**4**	**Equilibrium**	**0.205**	**0.506**	4	0.200	0.300	0.500	0.631
14		Stripping	0.205	***0.275	***=IF(N14>B$34;D$23*N14+E$23;D$31*N14+E$31)				
15		Stripping	0.205	0.275	i=	$x_i=$	$x_{i+1}=$	$y_i=$	$y_{i+1}=$
16	**5**	**Equilibrium**	**0.079**	**0.275**	2	0.050	0.100	0.196	0.331
17		Stripping	0.079	0.092					
18		Stripping	0.079	0.092	i=	$x_i=$	$x_{i+1}=$	$y_i=$	$y_{i+1}=$
19	**6**	**Equilibrium**	**0.024**	**0.092**	1	0.000	0.050	0.000	0.196
20	**(reboiler)**	Stripping	0.024	0.012					

Figure 5. Specific use of the MATCH, INDEX and IF Excel functions applied to a fractional distillation McCabe problem.
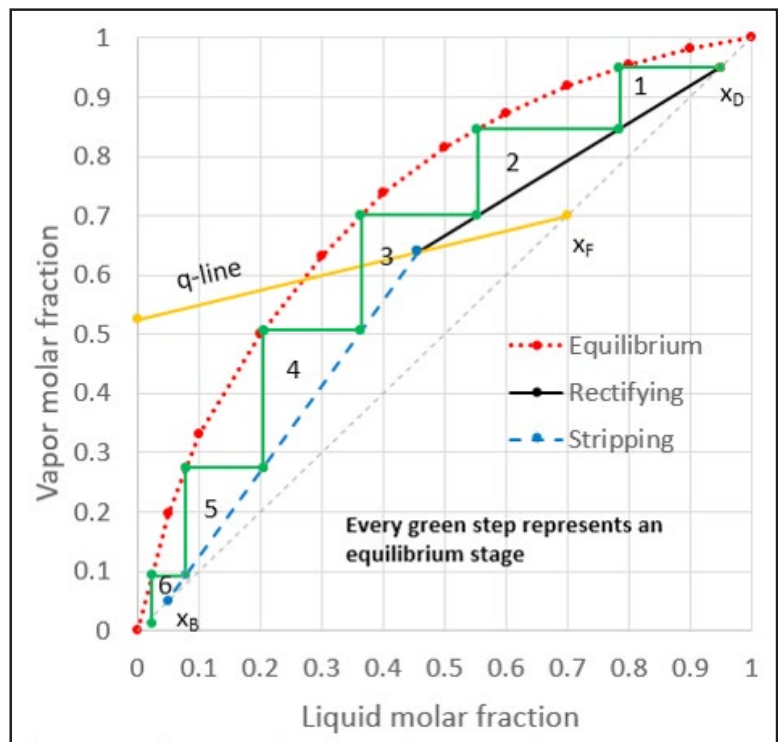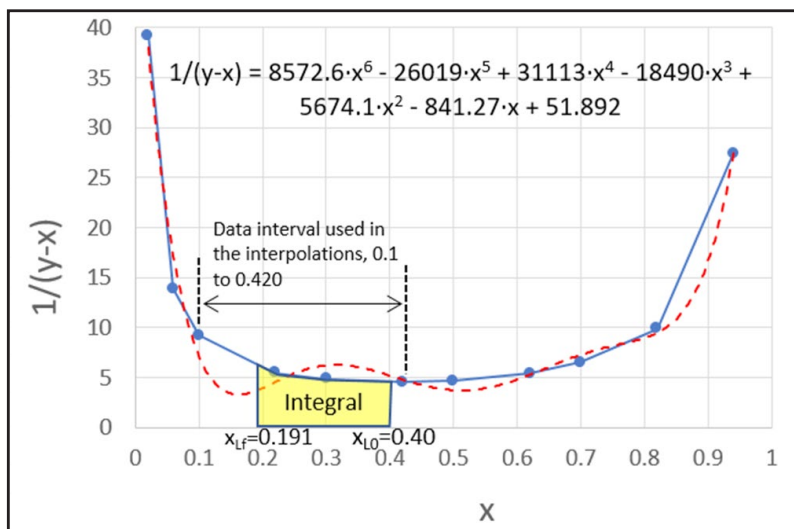

Figure 6. Example of graphical result corresponding to a typical fractional distillation McCabe problem.

(a)

(b)

Figure 7. *(a) Application of best fit curve (red dashed line) for the analytical integration of the Rayleigh equation. The blue solid line represents the linear interpolation between two consecutive data; (b) Numerical integration (trapezoidal rule) used in a batch distillation problem.*

Upon finalization of the activity, the students had to complete a survey that aimed to gauge their level of satisfaction with the integration of Excel into their learning process. They were asked to rate different items on a scale of 1 (totally disagree) to 5 (totally agree). It is worth noting that 19 out of 20 students assigned 4 or 5 points to the item "*The approach is important with a view to my professional career*," while 18 out of 20 students assigned 4 or 5 points to the item "*The software used can be applied to other subjects*." Also, 14 out of 20 students admitted that "*Solving the problems with software is more fun*." Much more interestingly, a blank space was provided for extra comments. We provide some below:

- *I think it is difficult to gain knowledge over distance.*
- *Microsoft Excel is very complete and adequate for solving these type of exercises.*
- *I am happy to learn other strategies to solve the problems rather than by hand.*

- *Using Microsoft Excel in this course has [caught] my interest in the subject.*
- *This experience has meant an advance for education. It should be integrated into the whole study program.*
- *It was difficult to apply the software (MS Excel) due to the virtual classes*
- *It enabled more accurate results and nicer plots.*
- *There are more powerful software packages than Microsoft Excel; however, until now I did not know that it was possible to perform complex calculations with a spreadsheet, and analyze the effect of variables.*
- *It was possible to automate the solving process.*
- *Good choice in times of COVID19.*
- *I want more courses like this, even if they are outside the curriculum.*

CONCLUSIONS

As a result of this approach, the students now realize that it is possible to use Excel built-in functions to solve unit operations problems in an easy and elegant way. If conveniently combined, these functions allow accurate graphical representation and calculations to be carried out, even without introducing VBA macros. Our designs were sustained by simple mathematical operations like linear interpolation and intersection between straight lines given by slope and intercept. Moreover, Excel avoided some frequent mistakes associated with these simple calculations. The students' motivation and academic performance were higher as compared to the use of traditional hand calculations. Manipulating data was very simple thanks to the use of "cells." Moreover, everyone had at least some previous knowledge of the software such that it was easier to deliver instructions. Excel enabled preliminary insights into the optimization process of the number of equilibrium stages in multistage separation problems. With scope for improvement, the authors feel confident about the validity of the proposed methodological approach and will continue to use it and improve it in the coming year. They also plan to extend the experience to similar Master's subjects.

ACKNOWLEDGMENTS

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