CHEMICAL ENGINEERING ANALYSIS THROUGH SYSTEMATIC MODELING AND OPTIMIZATION

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INTRODUCTION

With the rapid development of computing technology, computer-aided design and analytical skills are in high demand by STEM field employers. In this era of Industry 4.0, proactive data analytics are central to process operations and data-driven decision-making.[1, 2] With this background, our course in Chemical Engineering Analysis was redesigned to include analytics with advanced numerical methods. This course serves as an elective for our undergraduate majors and a requirement for our graduate program.

With the surging availability of massive data, chemical engineering graduates may face design, control, or operations optimization problems that involve handling data sets.[3, 4] Solving these problems requires proficiency in computer programming for data processing, analysis, visualization, modeling, and optimization. Optimization problems can be found everywhere in engineering, industry, and academia. However, many chemical engineering programs do not offer a course that discusses optimization.[3] It is vital to incorporate such concepts of systematic optimization in our curriculum to make our graduates competitive in today's market.

A growing number of employers believe their company is experiencing a widening skills gap in which the most in-demand hard skills are strategic thinking and analytical skills (48%), computer skills (46%), and project management (32%).[5] Our Chemical Engineering Analysis course bridges the skills gap for our graduates, enabling them to use fundamental data analysis techniques, skills, and modern engineering tools necessary for engineering practice.

The concept of skills is a multi-dimensional linking of education and experience.[6] Technology-enhanced learning opens remarkable new avenues for learning and skills development.[7] It is necessary to keep up with technological advances and changes in the work processes of industry.[8] Thus, the multi-paradigm numerical computing environment of MATLAB® was selected as the computational tool for this course. MATLAB is a popular computational tool used by students, academics, and industry researchers. Students may use their MATLAB skills to quickly adapt to other popular computing and analysis tools, such as those based in Python™ and R®.

This course aims to build a fundamental understanding of chemical engineering systems by developing mathematical and statistical models and digital computer simulations. It also aims to develop a systematic understanding and a critical awareness of process optimization and analysis of results.

COURSE DESIGN AND ORGANIZATION RATIONALE

The Chemical Engineering Analysis course is organized into three major sections with 10 modules shown in Table 1. Section I introduces the foundations of chemical engineering process modeling and MATLAB skill preparation. Section II builds on the foundation with advanced algorithms and computational methods using case studies in chemical

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engineering. Finally, Section III integrates algorithms and methods for tackling complicated case studies in chemical engineering. The modules incorporate several chemical engineering-related examples at both the undergraduate and advanced graduate levels.

TABLE 1
Three major sections with 10 learning modules in the Chemical Engineering Analysis course.

Sections	Modules	Topics
I	1	Modeling in Chemical Engineering
	2	MATLAB programming
II	3	Model fitting and spline functions
	4	MATLAB optimization toolbox
	5	Enhanced optimization
	6	Global optimization
	7	Optimal experimental design
III	8	Process integration and optimization
	9	Complex equation systems
	10	Data statistics and analytics

BRIDGING THE SKILLS GAP – DISTINGUISHING FEATURES

This course's most distinguishing feature is to apply systematic optimization for chemical engineering analysis to help students build their confidence for optimized data-driven decision-making. Students receive exposure to various model types and modeling methods throughout the Chemical Engineering curriculum. In particular, it was helpful for them to understand the importance and meaning of dimensionless groups. As illustrated in Figure 1, students must distinguish between the numerical values and their associated units. The Buckingham PI Method was introduced to correlate experimental data in dimensionless groupings of parameters and variables.[9]

Students also experience limitations of MATLAB's optimization solvers. For example, consider the optimization

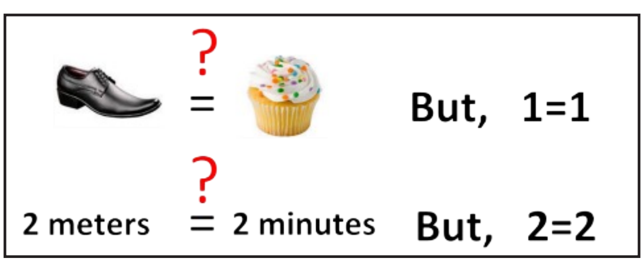


***Figure 1**. Data with or without units.*

problem with the objective function in Equation (1) and constraint in Equation (2):

$$f\left(x_1,x_2\right)=10\left(x_2-x_1^2\right)^2+\left(1.5-x_1\right)^2 \qquad (1)$$

$$-x_1+x_2\leq 0 \qquad (2)$$

The MATLAB code for minimization with the genetic algorithm (GA, a method to find global minima for highly nonlinear problems) follows:

```
[x f] = ga(@(x)(10*(x(2)-x(1)^2)^2+(1.5-x(1))^2),2,[-1 1],0)
```

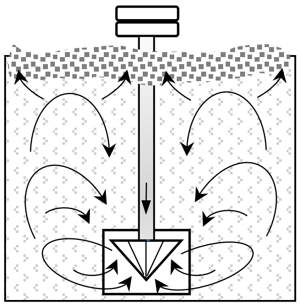
Using the default settings, MATLAB version R2020B returned an incorrect solution x = [1.0484 1.0494] and f = 0.2287 with $x_1 < x_2$, which does not satisfy the constraint in Equation (2). Thus, the genetic algorithm from MATLAB does not work for this optimization problem without experimenting with the optional settings for convergence criteria, which requires experience and expertise in the method. Office 2019 Excel's Solver® add-in has an option for an evolutionary optimization method employing a genetic algorithm, which gives an acceptable result of x = [1.0408 1.0408] and f = 0.2289, thus satisfying the constraint in Equation (2). Thus, students learn not to rely on any one of several existing commercial software tools and not to treat them as black boxes.

The natural next step is to instruct students on advanced topics that overcome the limitations of MATLAB software, including enhanced optimization methods, such as Lagrange's method, of converting constrained optimization to non-constrained optimization, conversion of inequality constraints to equality constraints, the penalty function method, and an enhanced constraints method to avoid the unwanted "zero" local optimal point.

As this course focuses on optimization techniques, they are demonstrated by case studies in model fitting, solving complex equations, and process optimization. The case studies reinforce concepts of data analysis, including programming, algorithms, digitalization of analog information from unstructured data, application of least-squares regression to noisy structured data, and data classification.

Students also learn to apply the statistical modeling technique of orthogonal experimental design (OED) to identify influencing factors, the levels of significance of each factor, and their combined effects. The robust and systematic OED method saves time and effort in experimental trials and optimization. For example, the OED L16 (4^5) applied in turbulence model development of a stirred flotation cell achieved a time saving of 98.4% effort with 16 trials, shown in Figure 2, compared to the total combination of 1024 trials from 5 factors at 4 levels.[10] By determining the critical factors from OED, students are introduced to analytical concepts of dimensional reduction besides the Buckingham PI method.

(a)



(b)

Experiment	Factor 1	Factor 2	Factor 3	Factor 4	Factor 5
1	1	1	1	1	1
2	1	2	2	2	2
3	1	3	3	3	3
4	1	4	4	4	4
5	2	1	2	3	4
6	2	2	1	4	3
7	2	3	4	1	2
8	2	4	3	2	1
9	3	1	3	4	2
10	3	2	4	3	1
11	3	3	1	2	4
12	3	4	2	1	3
13	4	1	4	2	3
14	4	2	3	1	4
15	4	3	2	4	1
16	4	4	1	3	2

***Figure 2**. OED method has been applied in turbulence model development. (a) A schematic of a stirred flotation cell; (b) OED L16 (4^5) table.*

BRIDGING THE SKILLS GAP – ASSIGNMENTS

To bridge the skills gap, the students completed the following four primary case studies to apply their training from this course:

1. Fit a model of a particle size distribution via different optimization methods in MATLAB. Equation (3) predicts the effect of specific comminution energy (Ecs) on the breakage index t_{10} (percentage passing an aperture of 1/10 of the original ore particle size).[11]

$$t_{10} = A\left(1 - e^{-bE_{cs}}\right) \qquad \left.\frac{dt_{10}}{dEcs}\right|_{Ecs=0} = Ab \qquad (3)$$

   The model's ore breakage parameters *A* and *b* are determined from laboratory Drop Weight Test (DWT) data, tabulated and plotted in Figure 3. The product *Ab* indicates ore hardness – the greater the *Ab* value, the softer the ore. The product *Ab* is the slope of the curve at zero energy input. To determine the ore hardness category tabulated in Figure 3, students find *A* and *b* using MATLAB's model-fitting tool optimization methods: fminunc, fminsearch, fmincon, and fsolve.

   This first assignment trains students on various MATLAB programming, modeling, analysis, and optimization features available in the MATLAB optimization toolbox. Students must deal with noisy data and apply data analytics to determine the goodness of the fit.

2. Optimize the location of a petrol and convenience station along the road winding among five communities, as shown in Figure 4. This assignment incorporates features of weighted optimization and constraints under the following conditions:

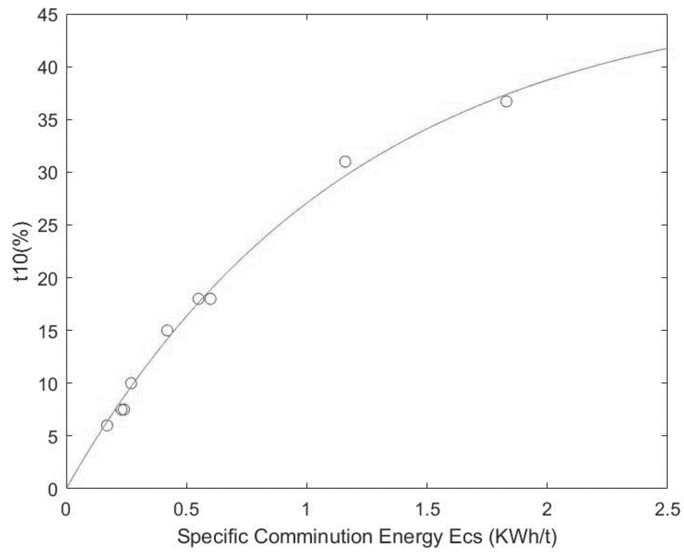
   a. Minimize the sum of distances from the station to all communities.

   b. Consider the community populations given in parentheses as distance weights in the optimization.

   c. Consider the population distance-weights, and constrain the distance between the station and community C to less than 20 miles. This additional constraint fosters a discussion of diversity, equity, and inclusion in engineering solutions that need to consider equitable access to the petrol resource among communities with diverse needs and circumstances.

Assignment 2 trains students to formulate optimization objective functions and constraints from real-world problems. This requires transforming the unstructured data in the form of a map into structured data for numerical analysis. The students then construct a

Ecs	t_{10}
1.83	36.7
1.16	31.0
0.60	18.0
0.55	18.0
0.42	15.0
0.27	10.0
0.24	7.5
0.23	7.5
0.17	6.0



	Very Hard	Hard	Mod. Hard	Medium	Mod. Soft	Soft	Very Soft
Ab	<30	30-38	38-43	43-56	56-67	67-127	>127

Figure 3*. Model fitting assignment: the effect of specific comminution energy on the breakage index t_{10}.*

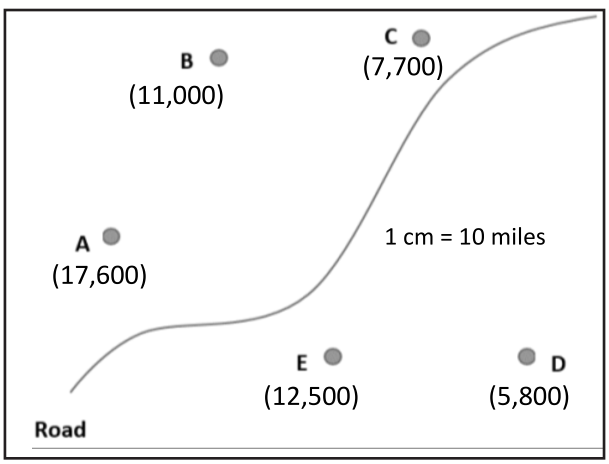


Figure 4*. Assignment 2: build a petrol station located on the road among five communities.*

function of the road's coordinates by a least-squares and interpolation model fitting exercise, using a polynomial, rational function, or cubic spline interpolation. This assignment gives them opportunities to work on different codes and compare the results.

3. Optimize a nodal network in a Cartesian grid to simulate steady-state two-dimensional heat conduction using the Finite Difference (FD) method. The following heat equation describes the temperature profile with constant thermal diffusivity:

$$\frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial y^2} = 0 \tag{4}$$

subject to boundary conditions of constant temperatures T_1 on three sides and T_2 at the top, as illustrated in Figure 5.

a. Solve the problem using the numerical finite-difference (FD) method for a grid of 4×4 nodes, as shown in Figure 5 with $\Delta x = \Delta y$, and draw a 2-D contour plot. The problem simplifies to a system of four linear equations:

$$\begin{aligned} 4T_{1,1} - T_{2,1} - T_{1,2} &= 2T_1 \\ 4T_{2,1} - T_{1,1} - T_{2,2} &= 2T_1 \\ 4T_{1,2} - T_{1,1} - T_{2,2} &= T_1 + T_2 \\ 4T_{2,2} - T_{1,2} - T_{2,1} &= T_1 + T_2 \end{aligned} \tag{5}$$

b. Increase the number of finite difference nodes (n) to $n \times n$ to solve the problem using the FD method, compare to the following analytical solution to reach an error tolerance of less than 0.01, and draw a 2-D contour plot.

As shown in Figure 5, the nodes are indexed on the grid using i = 0..(n-1) for the x-dimension and j = 0..(n-1) for the y-dimension. For assignment 3, students de-

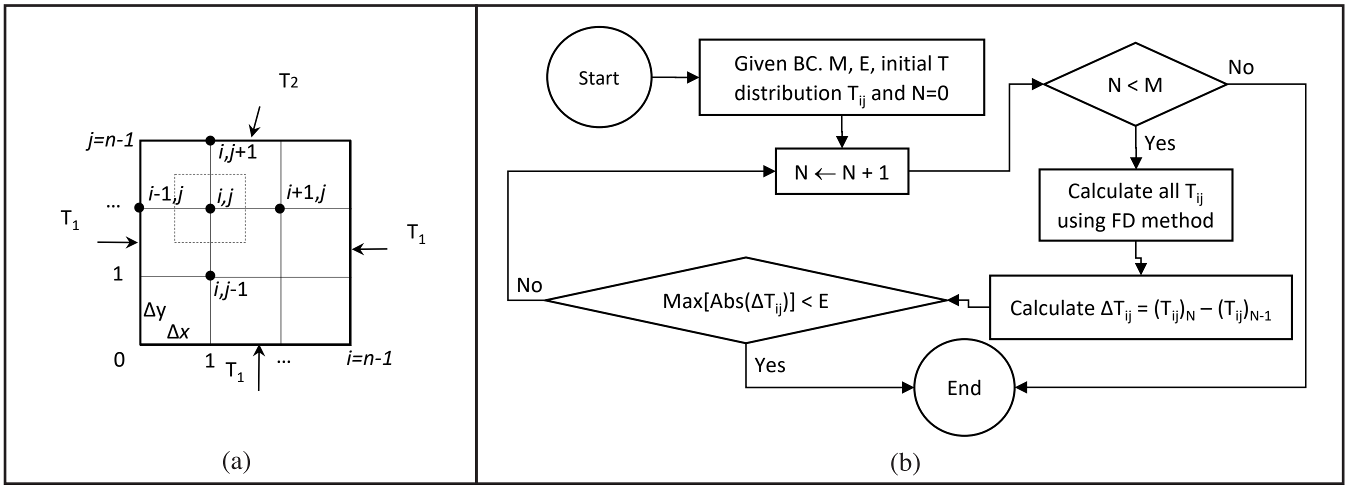


***Figure 5**. Assignment 3 to optimize a nodal network in a Cartesian grid to simulate steady-state 2D conduction heat transfer without internal heat resources. (a) The nodal network in a uniform Cartesian grid with i and j indexes for the x and y coordinates and n nodes in each dimension; (b) the numerical algorithm flowchart, where N is the iteration counter, M is the maximum iterations, and E is the error tolerance for convergence.*

termine the minimum number of nodes, or grid spacing, to match the finite difference solution with the analytical solution given in Equation 6.

$$\frac{T_{i,j}-T_1}{T_2-T_1} = \frac{2}{\pi}\sum_{k=1}^{\infty}\frac{1+(-1)^{k+1}}{k\sinh(k\pi)}\sin\left(\frac{k\pi i}{n-1}\right)\sinh\left(\frac{k\pi j}{n-1}\right) \quad (6)$$

The third assignment trains students on writing codes for implementing a numerical algorithm flowchart. They learned the FD (finite-difference) method for numerical solutions to boundary-value problems, logical operations, and program convergence using the tolerance value.

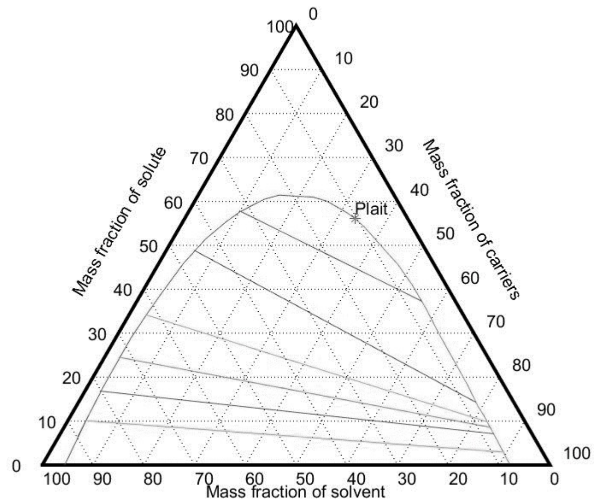
4. Apply an orthogonal experimental design to find the optimal parameters that minimize the operating costs in a counterflow solvent extraction flowsheet using a ternary diagram shown in Figure 6.
   a. Code the Hunter–Nash Graphical Equilibrium-Stage Method in MATLAB to get all data points on the ternary phase diagram, including the mixing points M and P, the extracts E1, E2, E3, the raffinates R1, R2, and R3, and their compositions in mass fraction.
   b. Given the following economic factors, apply an orthogonal experimental design to find optimal parameters that minimize operating costs to reach a final raffinate of less than 2%.
      - Mass of solvent ($15/kg)
      - Addition of carrier ($5/kg) for dilution (carrier usage is limited to max 200kg)
      - Number of stages ($1000/stage)

Students work in teams for this assignment and submit a written group report. In engineering education, interpersonal skills, teamwork, communication, and problem-solving skills are most frequently identified as necessary by engineers.[12] Assignment 4 also trains students to write the codes for solvent extraction using Hunter–Nash graphical equilibrium-stage method and apply the OED method to find optimal parameters that minimize the operation costs in the solvent extraction flowsheet. This assignment also requires the group to organize their digitized data into classes that include mass compositions, phases, and phase distributions at equilibrium conditions.

COURSE ASSESSMENT

This course requires students to apply math, science, and engineering principles and skills. Student learning can be enhanced by integrating theory with computational tools applied to case studies.[13] Our experience delivering this course taught us the need for in-class coding sessions with rapid and meaningful feedback to strengthen student retention and facility with MATLAB.[14] By providing students with just-in-time feedback, they know their limitations and take concrete measures to advance their skills and create deeper knowledge. Student feedback on the Spring 2021 course is summarized in Table 2. The course had eight students. The scores of all items equal or exceed 4.00 on a scale of 0-6, which means students generally agreed with each item. We also asked for informal student feedback on the course. Students liked the application of the analytical methods to real-world scenarios. They also liked the course format that allowed group work and weekly interaction with

(a)



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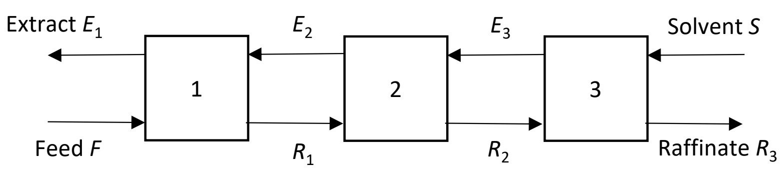

(c)

Feed	Solvent
$F = 300$ kg	$S = 100$ kg
$X_{FA} = 0.40$	$X_{SA} = 0.00$
$X_{FC} = 0.60$	$X_{SC} = 0.00$
$X_{FS} = 0.00$	$X_{SS} = 1.00$

Figure 6. *Assignment 4 to apply the OED method for finding optimal parameters that minimize the operation costs in solvent extraction flowsheet (a) The ternary phase diagram; (b) Counter-current three-stage solvent extraction circuit; (c) the feed and solvent amounts and compositions in mass fractions.*

TABLE 2
Student evaluations of the Chemical Engineering Analysis course - Spring 2021.
Responses range from 1 (Very strongly disagree) to 6 (Very strongly agree).

Items	Mean	Standard Deviation
The course had an open, respectful environment that supported learning.	5.50	1.00
The course included a way to exchange ideas with other students.	5.25	1.50
Instructions were clear, and help was available if I encountered problems.	5.00	1.41
The instructor clearly articulated expectations for this course.	5.00	1.15
The course assignments were a good measure of my learning.	4.50	1.29
The required materials were a necessary part of the course.	4.33	0.58
The course used appropriate and effective instructional methods.	4.25	1.71
The course provided a regular and helpful assessment of my progress.	4.25	1.26
The course was well organized.	4.00	2.16
Overall, I learned a lot in this course.	4.00	2.16

the instructor and class peers in a computing lab environment. As reflected in the mean score for the last item in Table 2, students reported being challenged by the modeling aspect of the course. They did not feel as confident in their ability to devise mathematical models as the computational tools. We plan to add more straightforward modeling exercises earlier in the course to give students experience and confidence in creating mathematical models for analysis and optimization.

CONCLUSIONS

Skills for data analytics are in high industrial demand and are becoming critical to our students' future career success. Our Chemical Engineering Analysis course helps bridge the skills gap by training students in programming algorithms, modeling, and analysis methods, including digitalization, regression, orthogonal experimental design, data structures and classification, and dimensional reduction. Students realize the importance of data analysis and learn modeling, MATLAB programming, and robust optimization techniques. This course also enables them to use data analysis techniques, skills, and modern engineering tools necessary for engineering practice. Significantly, this course builds their analytical skills within the framework of systematic optimization applied to chemical engineering analysis.

REFERENCES

1. Qin SJ and Chiang LH (2019) Advances and opportunities in machine learning for process data analytics. *Computers & Chemical Engineering*, 126: 465-473. https://doi.org/10.1016/j.compchemeng.2019.04.003.
2. Venkatasubramanian V (2019) The promise of artificial intelligence in chemical engineering. Is it here, finally? *AIChE J*. 65(2): 466–478.
3. Verrett J, Boukouvala F, Dowling A, Ulissi Z and Zavala V (2020) Computational notebooks in chemical engineering curricula. *Chemical Engineering Education*. 54(3): 143–150. https://journals.flvc.org/cee/article/view/116661
4. Ford H, Wilding KM and Bundy BC (2021) Applying an optimization mindset to engineering education: Junior level course project case study. *Chemical Engineering Education*. 55(4): 228-234. https://doi.org/10.18260/2-1-370.660-114933
5. Wiley Education Services & Future Workplace. (2019). *Closing the Skills Gap 2019*. Wiley Edu, LLC, Louisville, KY.
6. Rathelot R and van Rens T (2017) Rethinking the skills gap. *IZA World of Labor 2017*: 391 doi: 10.15185/izawol.391.
7. Zheleva S and Zhelev T (2010) Integrated Approach for Enhanced Teaching and Learning towards Richer Problem Solving Experience. In *Computer Aided Chemical Engineering* 28: 415-420. Elsevier.
8. Warsame AF (2017) *The Gap Between Engineering Education and Postgraduate Preparedness*. Ph.D. dissertation. College of Education, Walden University, Minneapolis, MN. Available at https://scholarworks.waldenu.edu/cgi/viewcontent.cgi?article=5289&context=dissertations.
9. Perry RH, Green DW and Maloney J (1984) *Perry's Chemical Engineers'* Handbook. 6th ed. McGraw-Hill, Inc., New York, NY.
10. Meng J, Xie W, Tabosa E, Runge K and Bradshaw D (2016) Turbulence model development for flotation cells based on piezoelectric sensor measurements. *International Journal of Mineral Processing*. 156:116-126.
11. Napier-Munn TJ, Morrel S, Morrison RD, and Kojovic T (1996) Mineral comminution circuits: Their operation and optimization. JKMRC Monograph Series, Queensland.
12. Craps S, Pinxten M, Saunders G, Leandro Cruz M, Gaughan K, and Langie G (2017) Professional roles and employability of future engineers. *Proceedings SEFI Annual Conference - Education Excellence for Sustainability, SEFI 2017*: 499–507.
13. Yenkie KM (2020) Enhanced undergraduate learning through integration of theory and computational tools. *Chemical Engineering Education*. 54(3): 129–136.
14. Alique D and Linares M (2019) The importance of rapid and meaningful feedback on computer-aided graphic expression learning. *Education for Chemical Engineers*. 27: 54-60. ❒