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IMPLEMENTATION OF MATLAB GUIDE TEMPLATES FOR CHEMICAL ENGINEERING STUDENTS TO SOLVE COMPLEX MATERIAL AND ENERGY BALANCES

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Abstract

Chemical engineering involves activities that require specific skills, such as analyzing, calculating and simulating real problems to develop the profession adequately. During the training stage, students of the Chemical Engineering Degree must transform real problems into mathematical equations that respond to the demands of a system. As a result, a complex system of algebraic equations is involved, which students must be capable of solving and getting numerical solutions. In order to facilitate the resolution, a mathematical software called Matlab is employed.
In this regard, Matlab is a powerful tool widely used in engineering, but it is not very intuitive for users. The programming window is simple, and students should program in an empty editor using Matlab functions with a certain complexity. Moreover, the introduction of the proper Matlab functions and the mathematical equations and restrictions of real problems based on material and energy balances requires time that is not available in the classroom. To overcome these disadvantages, students from Chemical Engineering Degree are provided with Matlab templates. This guide allows students to solve material and energy balances using a specific methodology to obtain a mathematical solution.
These Matlab templates consist of two files: the first one, called *template.mlx* is developed using the *Live Script* mode. This mode allows solving the low interaction and possible customization of the Matlab programming environment. In this language, it is possible to include equations, comments and even images that allow a better understanding of the students. The second file is called steady_state_balances_solver.m. This file works as a *"black box"* and contains the *"solve functions"* needed to solve all equations introduced by students in the *template.mlx.*
Therefore, in addition to providing a way to solve complex algebraic equations in a more student-friendly programming environment, the use of templates gives students a better understanding of solving material and energy balances. Anonymous surveys were done by students to determine the degree of satisfaction and to determine possible improvements and solve the weaknesses of the new methodology proposed.

Keywords: *Matlab, guide template, chemical engineering, student-friendly, material and energy balances.*

1. Introduction

Chemical Engineer requires specific skills which involve analyzing, calculating and simulating real problems. In this field, one of the most essential tools is the use of material and energy balance. In most problems studied, mass and energy are always involved, as in reactors with chemical reactions. The employment of these balances in a steady state, which is obtained after analyzing the system, results in complex mathematical equations with a high number of both equations and unknown variables (Carbonell Alcaina et al., 2021). In this sense, mathematical software is highly recommended since the manual calculation is time-consuming and can lead to possible miscalculations.

Regarding mathematical software, Matlab is one of the most powerful and widely used in the field of engineering, allowing any mathematical problem to be adequately solved. Nevertheless, this software uses programming code to carry out any mathematical resolution thus is a requirement for every user who wants to use it. In this sense, chemical engineering students are beginners in programming code, and one of the challenges is to resolve materials and energy balances to face real problems. Therefore, how can they solve these complex algebraic equations with poor programing skills? One of the proposals is to guide students and provided tools to ease this mathematical calculation (Cardona et al.,

2021). Then, the question is: what tools can teachers provide to reduce this drawback in solving material and energy balances, considering that calculation is needed in chemical engineering?

The main objective of this study is provided to students a methodology in order to solve mathematically complex material and energy balance. The study does not focus on modeling skills, but on solving these algebraic equations to overcome the deficiency in students' programming skills. Therefore, the authors have developed Matlab files capable of solving these equations without the programming knowledge for the student. Furthermore, anonymous surveys have been developed in order to know the students' opinions and future improvements of the proposed methodology.

2. Methodology

As a first stage of this research, Matlab templates provided to chemical engineering students are described. Two Matlab files have been developed by chemical engineer teachers of Campus of Alcoy in order to solve complex algebraic systems that involve material and energy balances in a steady state. These files are called template.mlx and steady_state_balance_solver.mlx.

First, the algebraic equations modeling the system studied by students are introduced into *template.mlx* file. This file is divided into 6 main points, that is, 4 points for material balance and 2 points for energy balance. In Figure 1a) can be shown the template of Matlab that is provided to students, which allows the organization of the information introduced in this file. In addition, using the Matlab live version allows the students to add images, equations and comments that let them understand in a better way the system they are focused on. In Figure 1b) is shown an example of possible customizing of the file, giving freedom to the students to a better understanding of the problem. This step requires filling the file with the information previously explained in class.

Figure 1. Image of Template.mlx file: a) material and energy balances template provided to students; b) proposal for customization of the template file by the student.

a)

Mass and energy balances template

eq{1}=;

eq{3}=;

eq{5}=;

eq{9}=;

eq{11}=T0==25;

eq{13}=;

eq{15}=;

eq{17}=;

eq{19}=;

eq{21}=eq{29}=F3*(xD3*hD3e+xO3*hO3e+xN3*hN3e)-F3*(xD3*hD3s+xO3*hO3s+xN3*hN3s)-qA==0;

eq{23}=;

b)

Mass and energy balances template

Take into account all the independent material balance equations, the specified variables, the additional relations and the summation of the mole or mass fractions for each stream. Also take into account the energy balance equations.

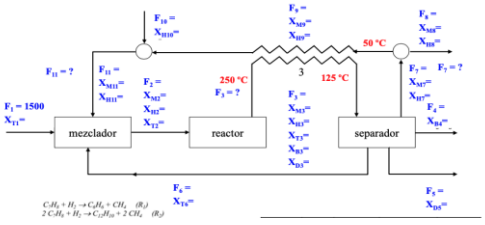
Write the equations following this example: eq{1}=F1==3; Write ; always at the end of the equations

Chemical reaction

$C_2H_6 + H_2 \rightarrow C_6H_6 + CH_4 \quad (R_1)$

$2\ C_2H_6 + H_2 \rightarrow C_{12}H_{10} + 2\ CH_4 \quad (R_2)$

Scheme of process



Questions:

a) Degrees of freedom analysis of BM and BE together.

b) Balances of Matter and (4 points) Energy balances to determine the heat (Q) exchanged between stream 3 and 9, as well as the outlet temperature of stream 9 (T9S).

(c) Matlab resolution of all variables.

Specified variables material balance

eq{1}=;

Additional relations material balance

eq{3}=;

Independent equations material balance

VC1

eq{5}=;

Summation of the mole or mass fractions for each stream

eq{9}=;

Specified variables energy balance

The next stage is to use the second file "*steady_state_balances_solver.m*". It works as a "black box"; thus students do not require to introduce any additional information. This file contains the solve function needed to solve all equations introduced previously by students into *Template.mlx*. Once the file has been executed in the software, a sentence asks the student for the name of the Matlab to be solved. The sentence specifies how to add the file name, which is without quotes and adding the extension (.mlx). An example of this sentence is shown below, where the file name that users (students) should add is written in red.

Steady-state balance file name (with extension and without quotes): **example.mlx**

The next information that "*steady_state_balances_solver.m*" file requires is the type of solution desired by users. In this sense, the student can choose between two options, that is, (1) numerical solutions and (2) analytical solutions. In general, a numerical solution is chosen as is exposed below.

Which type of solution do you prefer, numerical (1) or analytical (2)?: 1

Finally, the file solves the problem by giving mathematical solutions to the variables. In the next step, student has to interpret the solution from an engineering point of view.

To evaluate the usefulness of the methodology explained previously, a survey was conducted on the second-year students, since it is the first time they have used them. The anonymous survey was carried out during the first semester of 2022-2023, collecting 65 surveys. The satisfaction survey is detailed in Figure 3, in which questions have been divided into 4 main aspects. In terms of possible answers, 5 options were offered to students from totally agree up to an option for students that had a poor implication in the subject (option: I have not used them).

Figure 2. Satisfactory survey provided to chemical engineering students.

	MARK THE CORRESPINDING BOX WITH A X	Answers				
1. Usefulness Matlab guide files	1.1. Of the following didactic materials used in the course, how do you consider its level of ease of use?	VERY EASY	EASY	DIFICULT	VERY DIFICULT	I HAVE NOT USED THEM
	1.2. Of the following teaching materials used in the subject, how do you consider their usefulness?	VERY USEFUL	USEFUL	LITLLE USEFUL	NOTHING USEFUL	I HAVE NOT USED THEM
2. Adequacy of the guides to the resolution	2.1. Regarding the use of the Matlab template and the Steady State "solver", do you consider its use appropiate for solving material and energy balances?	VERY APPROPIATE	APPROPIATE	LITLLE APPROPIATE	NOTHING APPROPIATE	I HAVE NOT USED THEM
	2.2. Do you consider that the Matlab template and the Steady State "solver" help to understand material and energy balance problems?	TOTALLY AGREE	AGREE	LITTLE AGREE	NOTHING AGREE	I HAVE NOT USED THEM
3. Performance of the teacher in the implementation	3.1. Do you think the teacher has correctly explained the approach to the material and energy balance problems?					
	3.2. Do you think the teacher has correctly explained the use of Matlab templates and the Steady State "solver" for solving matter and energy balances?					
4. Student opinion	4.1. Do you think that Matlab Live improved the way of understanding the material and energy balance problems?					
	4.2. Regarding the Matlab template and the Steady State "solver", would you recommend its use to other classmates or even in other subjects?					
	4.3. After using the Matlab template and the Steady State "solver" in the course, what is the general level of satisfaction with the solving of matter and energy balances?	VERY SATISFACTORY	SATISFACTORY		UNSATISFACTORY	NOT SATISFACTORY

3. Results

The level of satisfaction with the methodology developed was obtained from studies surveys. The results are summarized in 4 main points following the survey structure (Figure 2).

The first main point aims to evaluate the usefulness of Matlab guides from the student's point of view. The authors have split this point into two questions: (1) the level of ease of use for files provided by teachers and (2) the usefulness of files in solving complex algebraic equations, which results are in Figure 3a.

Regarding the first question (1.1), students have considered the level of ease use of Matlab files as “very easy or easy” by 79%, being then the vast majority. It is an interesting and unexpected answer since students usually prefer different software, as can be Excel for its easiness. The main reason for it is the lack of skills in code programming on the part of students and the poor graphic environment of Matlab software, making it difficult to use. Nevertheless, according to these results, the guiding methodology seems to decrease more than 2/3 part of students' difficulty in solving these complex algebraic equations. The remaining students (18%) still consider using it “Difficult or very difficult”, whereas 3% confirm they have never used them. The authors should point out that this 3% is concordant with students who miss the subject. In the case of the second question (1.2), the usefulness of this methodology for students is quite evident with more than 90% of surveys with a “very useful or useful” selection. At least, for this first stage, students seem aware of the difficulty of resolving this problem without this software, since these files lead to making automatic the calculation of variables that are involved in the material and energy balance.

In the second point, the questions were aimed to find out if students considered appropriate the adequacy of the templates to solve and understand the material and energy balances (Figure 3b).

Considering the question about whether it is appropriate to use these templates for solving (question 2.1), it showed that 75% of students considered it “very appropriate” and 15% “appropriate”. Regarding the question related to the understanding of the problems raised using the templates (question 2.2), the results obtained indicate that students “totally agree” in 36% and “agree” in 37%, whereas 18% “little agree”. These results are a little expected because Matlab software and specifically the templates provided work as a “black box” resolving equations without any interpretation, giving the students the final interpretation. Although that teachers were concerned about this point, the results indicated that almost 75% of students considered that the template helped to understand the problems, which confirms the effectiveness of this methodology.

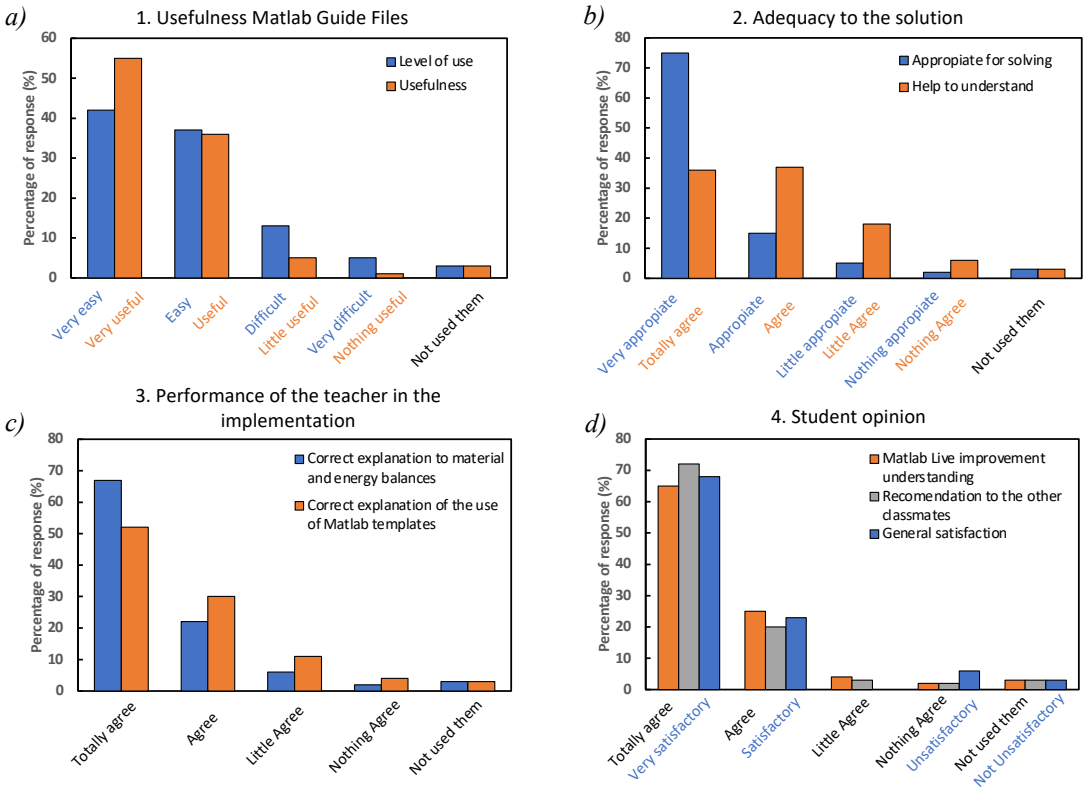
About the third point, it was a key aspect to ask students about teachers’ performance to implement the methodology described above. The results are summarized in Figure 3c.

In this point, two main aspects should be taken into account for the successful implementation of the methodology. The first question concerns the teachers’ correct explanation of material and energy balance problems (question 3.1). The 89% of the students surveyed answered both “totally agree” and “agree”, being a good approach for teachers and promoting student’s understanding of what is happening in the system under study. In this question, less than 10% “little agree” or “nothing agree”, which is quite low compared to the others. The second question was considered to determine if the procedure for using Matlab templates (question 3.2) was explained adequately by the teacher, since it is one of the central aspects of this methodology. The results showed the same trend as the explanation of the equations (question 3.1), reaching 82% with “totally agree” and “agree” from students. Considering the results obtained, the teacher’s role is adequate to solve material and energy balances using the Matlab templates as a resolution method.

To conclude this study, the student opinion is also evaluated in order to determine possible future improvements of the methodology exposed. In this last point, we were intrigued by the use of the new Matlab Live version, the possible recommendation of these templates to other students, and about the general satisfaction of the proposed methodology. These results are shown in Figure 3d.

The first question (4.1) was asked to determine whether customizing the template by students could improve the understanding of the problem, making the resolution more student-friendly. According to the results, students “totally agree” and “agree” in almost 90%. These results indicate that students feel more comfortable in software with a better graphic environment. In addition, the ability to add images of the problem statement, as well as to customize the format without the need to add % to be able to write in the software, can turn the template into a complete document to study for the exam improving the understanding of material and energy balances. Concerning to the second question (4.2), 92% of students would recommend using these templates to other students to solve these types of problems. This was somehow expected, considering the results obtained in the previous questions. Finally, the general satisfaction of students was requested (question 4.3). Based on the results, it was observed that this methodology seems to be satisfactory for 91% of students, whereas 6% are unsatisfactory. This highlights the methodology proposed by teachers in solving material and energy balances.

Figure 3. Results obtained in questions about: a) usefulness of Matlab guide files; b) adequacy to the solution; c) performance of the teacher in the implementation; d) student opinion.



4. Conclusions

As summary of our study, the use of Matlab guide template to solve complex algebraic equations of material and energy balance has been successfully implemented. Based on the research results, chemical engineering students considered very easy/easy the level of use and very useful/useful the Matlab templates provided. Besides, students assume that this methodology is appropriate for solving material and energy balances, helping to understand the problems under study according to 73% of students, as well as teacher performance is correct and highly valued using the templates. In general, students totally agree that the implementation of Matlab Live template improved the understanding of problems under study as well as found a very positive general satisfaction with a value of 91%.

Therefore, it is possible to conclude that the implementation of this methodology to solve material and energy balance was successfully accepted by more than 85% of students. These results highlight the usefulness of these templates to overcome the general disadvantage of students in solving complex equations.

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