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MATLAB as a tool as Analysis and Problem Solving Competency Development in Chemical Engineering Degree using MATLAB

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Abstract

Analysis and solving problems is a Chemical Engineering student capability. In order to develop this ability, activities that encompass problem-solving by students may involve problems in real-world settings.

In Chemical Engineering degree, MATLAB is a numerical software package that helps in the process of designing, evaluating and implementing a strategy to answer an open-ended question or achieve a desired goal. In this context, Matlab is software used in process simulation. Several lectures of Escuela Politécnica Superior d'Alcoi presented an innovation and improvement educational research project (PIME) in order to used MATLAB, like coordination teaching tool between some subjects.

The principal purpose of this work is the students improvement using, as has been mentioned previously, MATLAB in a problem-based learning methodology. This methodology allows a more effective coordination in the degree. The present paper presents a real- world problem and the common elements of most problem-solving contexts and how is designed to function across all disciplines.

Keywords

Analysis and solving problems, problem-solving learning, MATLAB, coordination

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1. Introduction

Due to the profound change that must take place in learning in the university context, the most important step is education-based training and evaluation for competencies. The UPV, in line with the Bologna process has launched a number of strategies for evaluating them, starting with generic competencies, linked to numerous subjects of university degrees (V. Yepes, 2014).

The generic competencies that have defined the UPV are:

- Understanding and integration.
- Implementation and practical thinking.
- Analysis and problem solving.
- Innovation, creativity and entrepreneurship.
- Design and project.
- Teamwork and leadership.
- Ethical, environmental and professional responsibility.
- Effective communication.
- Critical thinking.

In the present case, the generic competency to be treated in this work is the competence of Analysis and Problem solving. According to the UPV, this competition can be defined as "analyze and solve problems effectively, where significant elements are identified and defined". Three levels of complexity can be established: first demonstration proficiency, problem solving using knowledge learned in the classroom or in books. A second level, which is developing its own criteria in order to solve the problems, using reflection and experience. And a third, more developed, when the student is able to develop and propose solutions in unusual and unfamiliar topics (A Villa, 2007). In the Degrees, the required

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levels would be the first two, the first level for years 1st and 2nd and the second level of development would be taken into 3rd 4th. The next level would correspond to Master studies.

The subjects need a coordination following EEES framework (C. Armengol, 2009). This coordination must be addressed both horizontally and vertically level, focusing on coordination of content and evaluation of specific and generic subject competencies of the same course or specialty, and ensure the correct distribution of resources (D. Cazorla, 2010; JF Morales, 2013). This requires a lot of dedication on the part of academic committees of Degree and this complex work must be well planned, so that the creation of tools to facilitate the coordination work will be needed (Y. Garcia, 2013).

In the case of Engineering, the use of mathematical models that describe the behavior of processes is an important part of the basic knowledge that a student must possess (S.C. Cardona, 2014). In engineering, the use of mathematical software for student training (J.M. Gonzalvez, 2013) is necessary and essential. Because the market there are many software for solving mathematical models, a wide dispersion of software for the same purpose appears, a student manages different software for each subject to solve problems in various areas, but actually use the same numerical method (e.g., solving ordinary differential equations). One consequence of using two or more software for the same purpose during the degree is that the student doesn't dominate any of them, because the time is limited.

This lack of teacher coordination in the use of software could cause great uncertainty to students about the purpose of the mathematical tools and that reduce time for learning the contents of each subject.

Therefore, the use of the same general purpose mathematical software can be a tool of coordination and integration of the contents of many of the degree subjects and this tool could enhance a working method based on problem-examples (Maria-Fernanda Lopez-Perez, 2012.2013), to strengthen the general competency develop.

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A Project for Innovation and Educational Improvement of several teachers has been raised for real coordination in the Degree of Chemical Engineering, and enhance analysis and problem solving competency. The purpose of the project entitled "Using MATLAB as a teaching strategy and horizontal and vertical coordination between subjects Chemical Engineering Degree" is the use of this software as a teaching tool that serves as a link between subjects. To improve coordination between the subjects and pose a teaching methodology based on problem solving is the main objective.

2. Proposed methodology: integration of different teaching methods

In this Project, working method based on problem-examples that reinforce contents that are important in the application of chemical engineering, using MATLAB as an integration tool is the main objective.

For this, several tasks were developed:

1. Involve Chemical Engineering Degree lectures using single mathematical software in their subjects in the complex mathematical calculations.

2. Convert the student in an advanced user in MATLAB.

3. Develop a learning methodology based on transversal problems that allows students to achieve the analysis and problem solving competency.

4. Promote coordination of the contents of different subjects, both horizontally and vertically in the different courses. The coordination provides greater cohesion to the degree.

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3. Discussion of the proposal and results

3.1 Participation of interested lecturers

The next step was to involve different lectures who teach at the Chemical Engineering Degree to participate in this coordination project using MATLAB. This mathematical software would be used in problem solving and also should coordinate the subject contents by solving a complex problem in order to the competency.

The subjects were a total of eight (Table 1), from the first year to fourth, where the required level of knowledge and the mathematical complexity increased.

Table 1. Subjects into Coordination project using MATLAB.

Subject	Character	Year	Semester
Maths II	Basic formation	1	B
Calculation methods	Obligatory	2	A
Chemical Kinetics	Obligatory	2	B
Mass transfer	Obligatory	2	B
Chemical reactors	Obligatory	3	A
Experimental Chemical Engineering II	Obligatory	3	A
Analysis and simulation of processes	Obligatory	3	B
Biological wastewater treatment	Elective	4	B

Therefore, all subjects were adapted for the teachers. The teacher used MATLAB to solve problems. Because some teachers did not have the sufficient level mathematical software, several workshops were conducted. Three workshops were supported by the Instituto en Ciencias de la Educación (ICE) and were taught by a degree of Chemical Engineering, teacher with high knowledge in MATLAB.

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3.2 Students as advanced users in MATLAB.

In some subjects, during the degree, (Experimental Engineering I, II, and III) students have planned MATLAB workshops. In these workshops, a manual are given to students, with the most representative MATLAB functions in order to be used in solving the problems of the course.

These workshops offer the possibility that students learn MATLAB along the degree, which facilitates students reach educational competencies. Therefore, the basic contents assimilation in the subjects of the degree is improved. Also, better cohesion in the development of the title is achieved. Finally, students will learn, along the title, an advanced level in numerical/symbolic software, which will provide added value the degree; professional market appreciates this knowledge.

3.3 Analysis and problems solving competency development

All tasks that have been discussed above must be reflected in the contents of the degree subjects. Chemical engineering examples or problems will increase difficulty while students advance in their studies to achieve the competencies.

Therefore, for the development of Analysis and problems solving competency, problem-based learning methodology were used. This type of learning has the highest "learn to solve problems by solving problems". These problems must be appropriate to the level of the course, and should career of management statements, should be motivating to the formation and development of concepts is facilitated.

Students perceived cohesion of content and true coordination when the concepts are related to real examples along the courses, students could also understand the concepts in a more effective way, increasing their motivation to the subjects.

First, a complex problem that is resolved in semester B during 4th course was chosen. That problem was the design of a Sequencing Batch Reactor SBR.

This problem is very complex, since the design of such reactors implies knowing:

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- Bacteria that remove contaminants, respiration and kinetics of microorganism growth.
- Kinetic of biodegradable organic matter.
- Oxygen transfer process from the gas phase to the liquid

Therefore, in reactor design the student must possess concepts studied in many of the above subjects. This subjects and concepts coordination is very difficult.

The problem statement might be:

"In a milk company in ---town, SBR reactor is going to be installed for removing pollutants that discharged into the wastewater sewer. The discharge flow is 200 L/d and the control parameters discharge must be below discharge limits. Design the reactor (volume) and operational parameters".

As you can see the statement is completely open, so that each teacher can adapt it to your needs and purposes.

To better understand how the problem arises, we will be developing subject by subject, what are the problems associated with the design of the SBR and that can be resolved in each of them, their complexity and how to relate with others.

Remember that for 1st and 2nd course, analysis and problem solving competency include identify and analyze a problem to generate alternative solutions. For 3rd and 4th course the level of results required increases, in which the student must use the experience and judgment to analyze the causes of a problem and build a more efficient and effective solution.

In the first course students will deal with concepts that should have to design the bioreactor. The subject Math II; as is well known is a discipline that sometimes is a stumbling block for students. Math is difficult, but also students do not see the useful in the real live. In the present case, solving systems of differential equations are needed for the development of

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SBR reactor design, because it is a batch process where the variables change over time. One of the thematic units in Math II is ordinary differential equations and their analytically solving.

When the math concepts have been explained, the problem can be presented to the student. But, this problem should be presented as a real situation, the teacher explain the importance of wastewater treatment and the used reactors for this purpose. The lectures teach wastewater problem can be the math lecture or a person familiar with wastewater matter. Some videos of biological reactor operation could be presented. The video length would be a maximum of 15 minutes, because the subject can't be invalidated.

At this point the teacher will give the bacteria growth differential equation, oxygen and pollutant variation differential equations. Such processes can be modeled and are ordinary differential equations which can be solved analytically (Laplace). At the first the teacher uses only a variable, it can bacteria, for later, offers the students a more complex problem , which varies not only bacteria variable, but also the substrate and oxygen, then the teacher presents the complete system of ordinary differential equations (Eq. system 1).

$$\frac{dS_1}{dt}(t) = -\frac{1}{Y_1}\mu_{max\,1}\frac{S_1}{K_{S1}+S_1}X_H \qquad S_1(0) = S_{01}$$

$$\frac{dX_H}{dt}(t) = \mu_{max\,1}\frac{S_1}{K_{S1}+S_1}X_H - rO_2\big|_{endoH} \qquad X_H(0) = X_{0H} \qquad \text{(Sist. Eq. 1)}$$

$$\frac{dC}{dt} = Kla\cdot\left(C^*_{O_2} - C_1\right) - \frac{1-Y_1}{Y_1}\mu_{max\,1}\frac{S_1}{K_{S1}+S_1}X_H - rO_2\big|_{endoTOTAL} \qquad C(0) = C_0$$

Where S1 is substrate, X_H are heterotrophic bacteria and C is oxygen concentration.

All constants numeric value is provided, because the aim objective is the system resolution and not the physical concepts.

When students solve the problem on the paper manually, the problem should be solved with MATLAB, with the relevant functions, dsolve or ODE. The teacher has seen a very simple resolution and a real application of the subject.

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The next subject is Calculation Methods in Chemical Engineering (2nd year, semester A), where equations and systems of ordinary differential equations are solved numerically by the methods of Euler, Runge-Kutta and multistep. In this point, both subject, Math II and Calculation Methods are related. The same problem can solve with MATLAB, now numerically, once students have learned to solve systems manually. It is interesting that students learn to do with MATLAB and can see the savings in time. In these two subjects they have learned concepts and have got a way of solving systems with MATLAB. Students have also seen the usefulness of the concepts learned.

In this moment, students have seen the mathematical part of the SBR reactor design, so that engineering concepts can be introduced. In order to make a mathematical model, where there are chemical reactions, the reaction rate has to be studied to obtain a kinetic equation where relates the reaction rate with operational conditions and composition.

$$-r_A=[K(T)][f(C_A,C_B,\ldots) \qquad \text{(eq. 2)}$$

$-r_A$ is reaction rate (mol/l.·h), K is a constant (is Temperature function) and C_A, C_B, reactive concentration.

Calculation of the kinetic constant and the reaction order are described in this subject. MATLAB is used in this subject to solve these problems, using interpolation as polyfit or linearizing. Students have experimental data to kinetic equation resolve, e.g. Organic matter reduction for bacteria action.

There are several models, such as: the first order model Monod. Specific rate constant (usually expressed by k) is obtained in first order kinetics, while for the model Monod, three constants have to be evaluated: the affinity constant (Ks), the specific rate (μ_{max}/Y) and finally, the maximum growth constant (μ). In this part, the teacher would give students experimental data (substrate concentration versus time), and students could use the equations presented above to obtained these constants using MATLAB.

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Limiting SBR operational parameters is oxygen transfer because the most treatments are aerobic. Therefore, students have to know the chemical reaction mass transfer concepts. This knowledge is introduced in Mass Transfer subject (2nd year, semester B). Gas diffusion into a liquid in irreversible reaction models are explained in this subject. The model describes the diffusion through the film and can be obtained from oxygen matter conservation equation. The resulting equation has more than one independent variable and a differential equation in partial derivatives appears. In this part, this subject relates to the kinetic subject. When teachers, responsible for the two subjects are coordinated, can relate both subject, giving cohesion to the degree contents; thus students relates concepts that otherwise notices as separate issues.

Now, this equation have to be solved by numerical method, based on finite differences, therefore, this part of the problem is also related to Calculation Methods subject, so the teacher must be coordinated and should teach similar examples. Naturally, the numerical resolution method is not explained in the subject, but MATLAB is used to solve the problem. When teacher coordination exists, students have worked with numerical methods in order to solve similar problems and have the MATLAB codes (remember students have a MATLAB manual that can be used along the degree). No time is lost mathematical problem solving. When the coordination does not exist, Students does not relate both subject, and most of times must remember the concepts again, and starts with a new MATLAB program. In this step, much time is wasted in mathematical operative methods, and the problem is not focused on the part of chemical engineering concepts and gas-liquid diffusion. The student loses time and effort to solve the problem mathematically and neglects the chemical issue.

In this subject, the teacher should transmit the importance of the oxygen diffusion processes into a biological reactor, the oxygen concentration profiles in the liquid film for different times to reach steady state and as the oxygen amount that is transferred per unit of time and area. Thus, the student can understand the importance of the oxygen that microorganisms need for their metabolism and catabolism.

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In these two years (1st and 2nd year) basics concepts in the reactor design with chemical reactor, kinetics and mass transfer have been taught, with mathematical resolution using MATLAB. A basic MATLAB program is made as templates in order to students solve similar problems.

In the third year, the problem is focused on SBR reactor design and simulation process. The reactor design problem is continued in Chemical reactor subject (3rd year, semester A). In this subject, the concept of reactor size calculation is introduced from a kinetic equation. When the kinetic constants and reaction order is known, the reactor size can be calculated. The teacher provides experimental data and students have to calculate the time using interpolations and integers. These calculations are very simple with MATLAB, and have seen in Math I. Students only focuses on reactor design concepts In the SBR example, student calculates the decay time of the substrate and after SBR volume.

This subject is taught in the same time that Experimental Chemical Engineering II (3er year, semester A), and the two first class sessions are dedicated to second MATLAB workshop. Students learn new concepts, MATLAB functions, and new methods for using in the subject problem solving. In this subject, the concepts studied in Chemical Reactors subject is design a biological reactor with experimental data. Students make experiments to determine COD variation (Chemical oxygen demand) in an aerobic reactor. In this way, students become familiar with a real process in a laboratory scale reactor. But at this point, two subjects are being offered at the same time (semester A) and the laboratory practice may make before theoretical session. This is a problem that should be studied. In the laboratory practice and Chemical Reactors subject, the same MATLAB tools and functions are used.

Besides, transfer mass laboratory experimental are made in Experimental Engineering laboratory practices, where oxygen transfer gas-liquid coefficients are calculated through MATLAB parameter fit. It is very important that students see a connection between all subjects and a relationship with their professional life in the future.

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In 3th year, semester B, students are faced with the subject Analysis and Simulation Process (3rd year, semester B). Bioprocess Technology also is offer in this semester, and student is introduced in biochemistry process, microorganisms kinetic (Monod) that knows from Chemical kinetic subject.

In Analysis and Simulation Process, students work with appropriate mathematical model to a hybrid respirometer. Although this example is not a SBR reactor, the respirometer is a biological reactor works in batch. Six nonlinear ordinary differential equations describe this model, and are coupled together. Oxygen, biomass and substrate concentration are model dependent variables and the time is the independent variable. An additional difficulty in this mathematical model is how the substrate injection in the aerated reactor is modeled. This injection is usually done in the pulse form, and can be repeated over time.

When the mathematical model is raised and the biokinetic parameters are known, the biological system can be studied through variable data or operation conditions modification:

- Change recirculation flow between tanks
- Change oxygen transfer rate
- Change substrate amount in the injection, time injection

The results of the simulation allow a success in experimental design, because this experiments last long and a make a prediction of the system behavior is very interested.

MATLAB is naturally the software used to solve the problems but SIMULINK help (MATLAB environment) in the simulation problems. In this semester, the mathematical operations are more difficult than other years and thus students' knowledge about the MATLAB has been incorporating during all the previous years. Thereby, students only spend time in problem solving. The teacher saves re-explain the mathematical calculations.

And finally, students arrives to Biological Treatments subject (4th year, semester B). In the 4th year, semester A, Chemical Engineering Degree has a problem, because there is not any subject related with the SBR reactor. This weakness in the coordination should be remedied because students quickly forget the mathematical functions, subjects…

In Biological Treatment subject, SBR concept and biological wastewater treatments are learned. The mathematical models are more complete than previous (9 differential equations). The model adds all previously knowledge acquired (kinetic constants, matter transfer processes, simulation concepts…). The biological meaning is given in this subject.

Now, student is able to solve the SBR problem, is able to designs a SBR reactor and is able to optimizes the operational parameters. Student is able to use company data provided, and is able to look for the information he needs. The main aim, General competency, is reached: Student uses the experience and criteria to analyze a problem causes and build an effective solution.

4. Conclusions

In this paper we have presented a methodology of problem-based learning for the Chemical Engineering degree to enhance General competency, "Analysis and Problem Solving". Several Subjects have been coordinate using MATLAB as a link. The first step is to start with a problem that can be developed throughout the subjects of the degree. The main objective is more and more subjects are incorporated and develop a common project all of them.

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