# AC 2012-4335: IMPLEMENTING PROBLEM-SOLVING LEARNING ENVIRONMENTS IN A KINETICS AND HOMOGENEOUS REACTOR DESIGN COURSE

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## Implementing Problem-Solving Learning Environments in a Kinetics and Homogeneous Reactor Design Course

### Introduction

The main task of a chemical engineer is to design and operate processes to transform raw materials into final products, particularly by the exploitation of chemical reactions at industrial scale. Reactor operation is at the heart of many chemical processes, while other unit operations and equipment are necessary to prepare the reactants for the reactor conditions or to separate the different components from the reactor effluent. For proper reactor design, chemical kinetics and reactor engineering must be considered. Chemical kinetics study chemical reaction rates, which must be obtained from experimental measurements; reactor engineering defines the type and size of the device within which the reaction occurs and its operating conditions (temperature, pressure, and the energy exchange with the environment) to achieve a reaction specific goal.

According to Felder[1], there are six pillars holding up the application of chemical reactor engineering: stoichiometry, rate laws, mole balances, energy balances, diffusion, and contacting pattern. At *Universidad de las Américas Puebla* chemical engineering (ChE) students develop the knowledge and skills to design and operate chemical reactors in two senior courses, the first one entitled Kinetics and Homogeneous Reactor Design (IQ-407) and the second one Catalysis and Heterogeneous Reactor Design (IQ408). Heterogeneous reactors using solid catalyzers are the most common reaction technology implemented on industrial scale; catalytic models are built using the same basic concepts that those used in homogeneous reactor design, for this reason it is indispensable that students acquire a solid knowledge from their first course of reactor design.

The first course (IQ-407) is focused on the first four pillars mentioned above and its outcomes include that students will be able to: 1) determine reaction rate expressions obtained from experimental data; 2) use basic concepts of kinetics, mass and energy balances, as well as principles from thermodynamics to design ideal homogeneous reactors; and 3) asses and propose reactor operation conditions to achieve a specific objective.
Practicing engineers are hired, retained, and rewarded for solving problems. Thus, engineering students should learn how to solve workplace problems[2]. In general, workplace engineering problems are substantively different from the kinds of problems that engineering students most often solve in the classroom; therefore, learning to solve classroom problems does not necessarily prepare engineering students to solve workplace problems[2, 3]. Therefore, we designed and implemented several problem-solving learning environments (a term that represents problem-solving instruction in a more open-ended way than problem-based learning) for the IQ-407 course.

Problems vary in different ways, so different kinds of problems call on different conceptions and skills[2-4]. Based on those differences among problems, different kinds of IQ-407 problems were developed such as story problems, decision-making problems, troubleshooting, strategic performance problems, and design problems. Since there exist different kinds of problems, which call on different skills, learning methods should also vary[3, 4]. That is why special attention was given to the building blocks (cases) of our problem-solving learning environments (PSLEs), since the intellectual functions of cases vary and consequently they support different kinds of problem solving[3, 4]. Furthermore, students develop metacognitive skills along the problem solving process, which is as important as finding the right problem solution; metacognition is the ability to understand, monitor and regulate our own learning process[5].

## Methodology

In order to know how students solving problems skills can be developed trough PSLEs implementation, we conducted a preliminary research in the course IQ-407. We designed, implemented and tested a block of problems categorized according to Jonassen[3] classification: story problems, troubleshooting and diagnosis problems, decision-making problems, and design problems. Each one of these problems was implemented for developing specifics skills or to improve the understanding of key concepts related to chemical reactor engineering. Finally, a design (open-ended) problem was used to assess the expected learning outcomes and student problem solving skills development.

Learning outcomes assessment was carried out, among other measures, by using a rubric designed to know the importance that students assign to each studied course outcome and their progress in achieving them along the course. In order to assess metacognitive skills developed by the students, a Metacognitive Awareness Inventory[6] (MAI) was utilized to obtain evidence about how those skills are identified by the students. According to Flavell[5], two main metacognition characteristics exist, learning monitoring and learning regulation.

Instructional materials were available on the course website and students and instructor were using Tablet PC's with selected instructional platforms for PSLEs implementation, which allowed working online simultaneously. Class population was integrated by four students, thus monitoring their individual progress along the course was pretty easy. Backups with the developed material were saved as electronic files, but the primary data source for this work was an in-depth interview with the students at the end of this initial implementation.

## Implementing problem based learning environments in IQ-407

Problem based learning is an instructional strategy in which learning is organized around authentic problems[7]. IQ-407 problem solving learning environments were based on Jonassen[3], thus different kinds of problems were implemented along the IQ-407 course. Since story problems objective is that students recognize variables and utilize algorithms, several story problems were used to teach and learn stoichiometry. Generally, students are familiar with the stoichiometric relationships from their previous chemistry lessons, but they are not able to generalize it or write these relationships as mathematical equations, which are required for modeling a reaction system. To support students to develop this ability, some story problems were implemented; students were asked to analyze, for different reactions, the relationship between each pair of components and its stoichiometric coefficient, for introducing basic concepts as reaction coordinate and conversion fraction[1, 8]; then they must to induce a conceptual model to describe stoichiometric relationships. An example of story problem utilized is described in Figure 1. Students were able to identify main concepts, select useful information, generate and verify the solutions to these kinds of problems.

The reaction

$$A + 2B \rightarrow C$$

is to be carried out in liquid phase within a continuous flow reactor. The feed stream contains A and B with $C_{A0}=C_{B0}=$ 2M and it is fed with a volumetric flow rate of 5 $dm^3$/min. If a 50% conversion from the limiting reactant is desired, determine the molar flow of each component at the reactor effluent.

Figure 1. Example of a story problem for IQ-407 course. Adapted from Fogler[1].

Kinetics is the second pillar of chemical engineering. As mentioned before, rate laws have to be determined from experimental data, so laboratory work was used to support this topic learning. Three different methods for obtaining kinetics parameters (reaction order, reaction specific rate and temperature dependence) from experimental data were discussed at classroom. Then, students developed laboratory work to collect data of concentration-time for three different reactions: saponification of ethyl acetate, decomposition of hydrogen peroxide, and hydrolysis of sucrose. As example, the problem context of decomposition of hydrogen peroxide is described below in Figure 2. In all cases, the appropriate method to determine every kinetic parameter was identified and applied by students.

Hydrogen peroxide can be decomposed spontaneously into water and oxygen according to the next stoichiometry:

$$2H_2O_2 \xrightarrow{MnO_2} 2H_2O + O_2$$

this reaction can be catalyzed by manganese dioxide. By using commercial product (aqueous solution at 3% $H_2O_2$) develop the experiment described into the laboratory manual to obtain data for produced oxygen vs. time. Repeat the experiment for two different temperatures. Analyze the obtained results and determine a kinetic expression by fitting the obtained experimental data. Report the global reaction order, the frequency factor and the activation energy for this reaction.

Figure 2. Example of a decision making/troubleshooting and diagnosis problem for IQ-407 course.

When students were able to write stoichiometric relationships and determine reaction rate expressions, then chemical reaction engineering was introduced. The reactor design equations are built from mole and energy balances, the proper solution of this equations allows defining design variables or operating conditions for reacting systems. In IQ-407 three types of ideal homogeneous reactor were analyzed: Batch Reactor, Continuous Stirred Tank Reactor (CSTR) and Plug Flow Reactor (PFR). For this topic we built a block of cases with a progressive difficulty, most of them designed as troubleshooting and diagnosis problems, which present a higher complexity level and requiring a better knowledge of the subject. First, problems with single reaction occurring in single phase within a single reactor were studied (story problem). After that, we analyzed how to improve the achieved conversion by adding a second reactor, connected in series or parallel with the first one (decision making/troubleshooting and diagnosis problems allow students selecting one or more satisfactory answers). Traditionally, problems with a single reaction are used to teach the whole course, but it is known that single reaction system is a particular case in reaction engineering; therefore problems with multiple reactions[8] were introduced for each topic along the course, in order to foster students' knowledge transfer to any kind of reactor and any number of reactions. A decision-making problem example is exhibited in Figure 3.

There are two CSTRs available to process 80 L/min containing 0.5 M of A and 0.1 M of B, the first one with a 5 $m^3$ volume and the second tank with $2m^3$ volume. The desired product C may continuing reacting to a side product with no commercial value. The important reactions are:

$$A + \frac{1}{2}B \rightarrow C$$

$$C + \frac{1}{2}B \rightarrow D$$

The kinetic laws for each reaction, which are referred to component B are:

$$\left(-r_B\right)_1 = k_1 C_A C_B^{\ 0.5} = 0.0068 \frac{lt^{0.5}}{\min * mol^{0.5}} C_A C_B^{\ 0.5}$$

$$\left(-r_B\right)_2 = k_2 C_B C_C = 0.0745 \frac{lt}{\min * mol} C_B C_C$$

Determine the proper order to install both reactors.

Figure 3. Example of a decision-making problem for IQ-407 course. Adapted from Tiscareño[8].

## Problem solving learning environment assessment

The initial implementation of the PSLEs in IQ-407 was exploratory, intended to provide formative evaluation along the course. However, a deep analysis for the final problem solution was conducted. The final project was assigned over the last week of the 2011 fall semester;

students had a period of one week to develop their proposal. Students were asked to carry out a formal presentation of their problem solution methodology, the obtained results and their final conclusions. The presentation was video recorded to be further examined. The analysis of this presentation allows identifying students ability to solve workplace problems as well as their skills to argue their decisions.

Problem definition is the first important stage to arrive at the correct solution; students mentioned that they needed to make the process diagram (by drawing a graphical representation of the problem) to identify the available data and the missing information. After that, their strategy for problem solution involves break the problem into two sub-problems: mathematical model development and then analysis of alternatives. To develop the mathematical model students worked together as a team (each one construct their own model but it was reviewed by all of them for validation) and they worked individually to evaluate alternatives for process operation. Since the problem was open ended, a number of alternative solutions can be generated, for this reason students had to define a methodology to constrain the number of scenarios to be evaluated. Each student generated at least three suitable solutions. Along students' presentations, instructor conducted some key questions to let students construct arguments for supporting their selection. At the presentation closure, every one of the students said that it was pretty difficult to select "the optimum operation conditions" or "the better solution" because it is necessary to evaluate some other aspects (e.g., economic or environmental) not available in the tested design problem to make a final decision. It can be noted that most knowledge and cognitive processes categories of the revised Blooms' taxonomy[11] were distinguished during this presentations: factual, conceptual, procedural, and metacognitive knowledge, as well as cognitive processes such as remember, understand, apply, analyze, evaluate, and create.

As stated before, this final design problem was designed to evaluate the expected learning outcomes. In a general way, students were able to organize and recognize useful information, get the missing data, develop a mathematical model to represent the problem statement and evaluate different scenarios to achieve the specified goal. In order to identify the students' perception on the importance and the progress achieved by them for each studied course learning outcome, a final survey was carried out. These learning outcomes assessment results are exhibited in Figure 4. The dark gray bars indicate the importance (in a scale from 1: "none" to 5: "a lot") that students assign to the course learning outcomes, while the light gray show the progress achieved by them regarding achievement (in a scale from 1: "none" to 5: "a lot") of course learning outcomes according to their own perception.

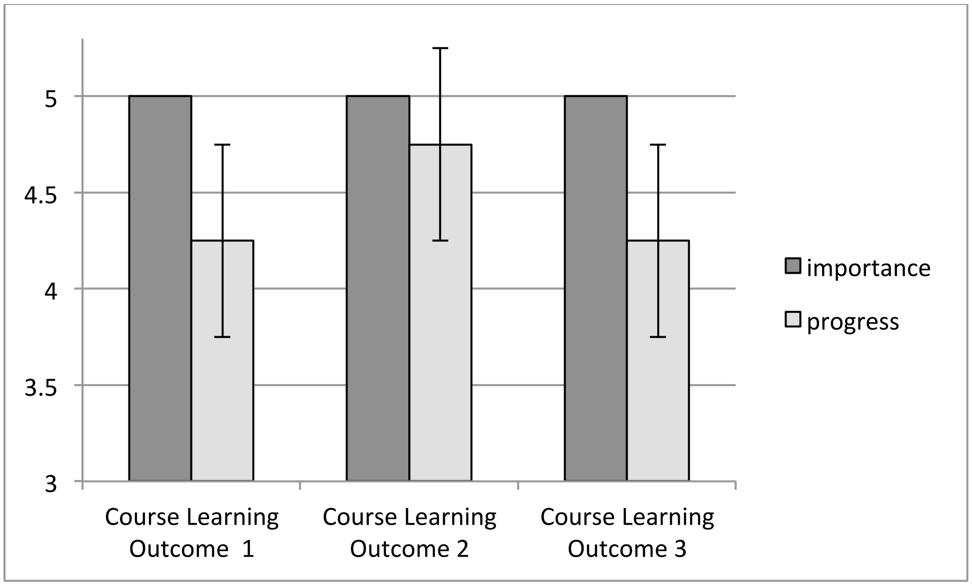


Figure 4. Course learning outcomes (students will be able to: 1) determine reaction rate expressions obtained from experimental data; 2) use basic concepts of kinetics, mass and energy balances, as well as principles from thermodynamics to design ideal homogeneous reactors; and 3) asses and propose reactor operation conditions to achieve a specific objective) importance and student progress in achieving them.

As can be observed from the obtained results, students think that studied course learning outcomes are very important; this perception can be associated to the fact that reactor engineering is precisely the main difference from other engineering programs. Regarding their perception on their progress in achieving course learning outcomes, it was the second outcome (use basic concepts of kinetics, mass and energy balances, as well as principles from thermodynamics to design ideal homogeneous reactors) from which they perceived their greatest progress. In the case of course learning outcomes 1 and 3, the importance and student progress in achieving them were significantly different ($p<0.05$). It can be observed (Figure 4) that students felt less confident with their progress in these two learning outcomes; this result can be attributed to the fact that experimental data obtained from laboratory work do not always fit perfectly, and in most cases students feel disappointed with this mismatch. For the learning outcome 3, we assume that their perception was related with their final remarks on their project presentation; they think that additional tools are required to complete a thorough process evaluation.

**Metacognitive skills development**

In order to assess how and which metacognitive skills were recognized by students, the MAI[6] was applied. Key questions are suggested by Schraw and Dennison[6]. The rubric to evaluate the metacognitive skills was designed using a Likert scale, from which students can choose between three parameters “Yes”, “Sometimes” and “No”. For metacognitive knowledge (also called metacognitive awareness) assessment, the following questions were included: a) I can motivate myself to learn when I need to; b) I am good at judging how well I understand something; c) I focus on the meaning and significance of new information; and d) I learn more when I am interested in the topic. The obtained results are exhibited in Figure 5. According to students' answers, they are conscious about the metacognitive skills required for monitoring their learning process; they can motivate themselves to learn, especially when they are interested on the topic, but they face some difficulty identifying and understanding new information.

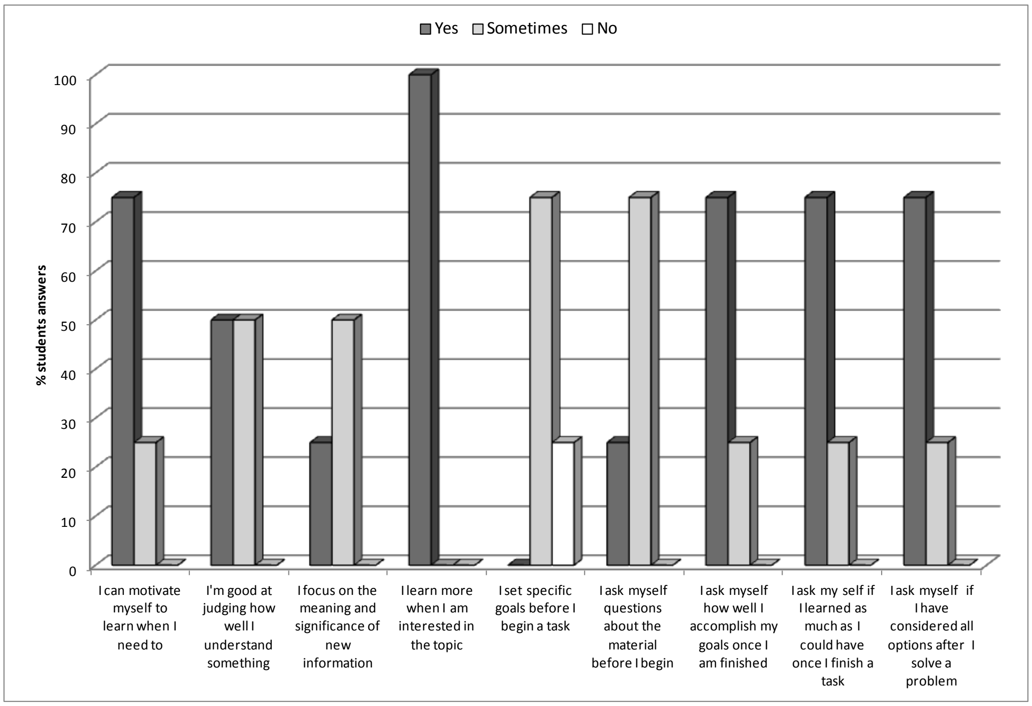


Figure 5. Metacognitive skills assessment results

For metacognitive regulation assessment the next questions were considered: e) I set specific goals before I begin a task; f) I ask myself questions about the material before I begin; g) I ask myself how well I accomplish my goals once I am finished; h) I ask myself if I learned as much as I could have once I finish a task; and i) I ask myself if I have considered all options after I solve a problem. Students recognized (Figure 5) that they do not always set specific goals or analyze the available material before they begin a task. However, they emphasize on questioning about the consistence of their problem solution (questions g, h, and i). It is clear that students recognized both metacognitive processes, learning monitoring and learning regulation. Although they were more conscious about the second one.

## Final remarks

Implementing PSLEs in the IQ-407 class represented a challenging transition for both instructors and students. Implementation of any curricular change is a diffusion and adoption of change problem[7]. In this initial implementation, IQ-407 students and the instructor were challenged to develop new approaches to teaching and learning that had different expectations. In the case of students, these expectations defied their well-developed study strategies. During the Spring 2012 semester, we are collecting further research data in the course IQ-408 by means of multiple data sources to assess content understanding, problem-solving skills, and self-regulation skills among the students enrolled in the course. Based on the experiences in this first PSLE implementation, we have added several scaffolds to help IQ-408 students better comprehend and solve the problems. Each student is being responsible for populating a *OneNote* page for each problem. Their responses are being guided by a series of content and metacognitive scaffolding questions with the help of Tablet PCs and associated instructional platforms. We hope that students' efforts will be even more concerted and rigorous.

## Acknowledgments

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APPENDIX A: Final problem

The process flow sheet for the hydrodealkylation of toluene to obtain benzene is shown in Figure 6:

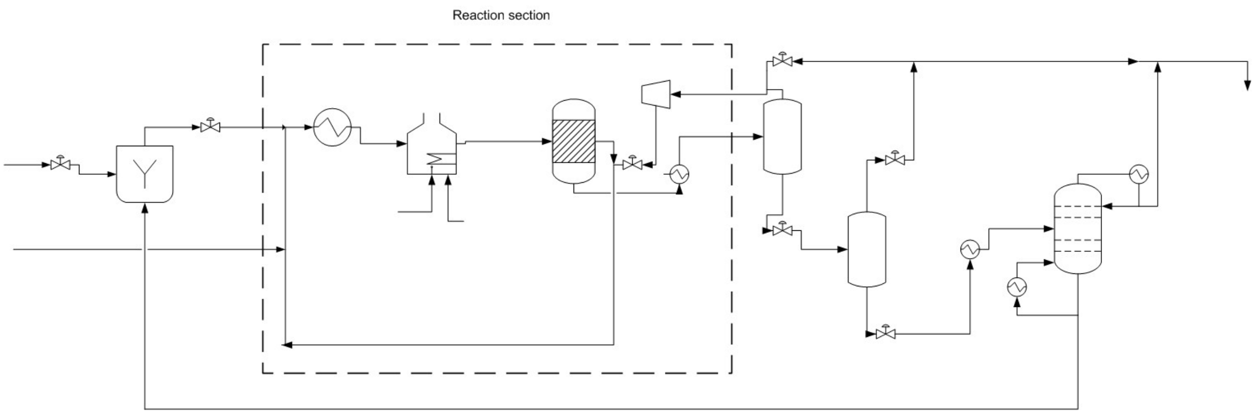


Figure 6. HDA Process Flow sheet. Adapted from Turton et al[9].

The process synthesis depends on reactor design, because of the selected operating conditions for this unit define the utilities requirements to prepare raw materials for the reactor conditions, and the reactor yield defines the use of separation units for product purification and/or for recovery the unreacted compounds. For the study case, reaction can be carried out in a catalytic fashion using a packed bed reactor (PBR) or by homogeneous reaction by using a plug flow reactor. Both alternatives are discussed by Turton et al[9]. Following reactions take place in gas phase within the reaction unit:

$$Toluene + 2Hydrogen \rightarrow Benzene + Methane$$
$$2Benzene \leftrightarrow Diphenyl$$

As process engineer on charge, you are asked to develop a process analysis to define the reactor volume required and its operating conditions, if a PFR is used to process 376 lbmol/h of toluene, taking into account the following operating constrains:

| | |
|---|---|
| Temperature range | 700-950°C |
| Operation mode | isothermal |
| Pressure range | 300-700 psia |
| Operation mode | isobaric |
| Reactants ratio $H_2$/Toluene | >2 |
| Composition of feed fresh Hydrogen stream | 95% mole $H_2$ and 5% $CH_4$ |
| Selectivity of desired product/ byproduct | >10/1 |
| Toluene conversion | <0.75 |

The rate reaction laws are described by following expressions[10]:

$$r_1 = k_1 P_T P_H^{0.5}$$
$$r_2 = k_2 P_B^2 - k_2' P_D P_H$$

$$k_1 = 3.686x10^6 exp\left(\frac{-90800}{RT}\right)$$
$$k_2 = 9x10^4\ exp\left(\frac{-90800}{RT}\right)$$
$$k_2' = 2.553x10^5\ exp\left(\frac{-90800}{RT}\right)$$

Where reaction rates have units of lbmol/min $ft^3$, partial pressures are in psia, activation energy is in Btu/lbmol and temperature is in °R.

1. - Develop the proper mathematical model, involving the mass and mole balances, the reaction rates expressions, the stoichiometric relationships, etc., for modeling system performance.

2. - Solve that model by using the polymath™ software, analyze different scenarios to define the effect of following variables on toluene conversion and its selectivity to benzene:

- Feed reactants ratio; hydrogen/toluene
- Operating temperature
- Operating pressure

a. Describe the used methodology to define the studied scenarios
b. Analyze the obtained results. In order to support your conclusions, analyze the behavior of all design variables (reactor volume, volumetric flow, residence time, spatial time, concentration of each component along the reactor…).
c. Based on such analysis propose a reactor design, justify the selected operation conditions.

This problem was adapted from different sources[9, 10].