Advances in Engineering Education

SUMMER 2010

On the Use of Interactive Texts in Undergraduate Chemical Reaction Engineering Courses: A Pedagogical Experience

DANIELA A. ASENSIO, FRANCISCA J. BARASSI, MARIANA T. ZAMBON,
AND GERMÁN D. MAZZA*
Departamento de Química
Facultad de Ingeniería
Universidad Nacional del Comahue
Buenos Aires, Argentina

ABSTRACT

This paper describes the results of a pedagogical experience carried out at the University of Comahue, Argentina, with an interactive text (IT) concerning Homogeneous Chemical Reactors Analysis. The IT was built on the frame of the *Mathematica* software with the aim of providing students with a robust computational tool. Students' performance was analyzed on the basis of parameters established by educational criteria. The use of IT can be strongly recommended in undergraduate Chemical Engineering courses.

Keywords: Interactive Texts - Chemical Reactors- Mathematica

INTRODUCTION

The development of new technologies in the domains of information and communication is one of the critical factors in understanding and explaining the social, cultural, politic and economic transformations that have taken place in the last two decades. The role of these new technologies in the process of social and cultural changes is particularly important where education is concerned.

The incorporation of the above quoted technologies to the present teaching practice indefectibly imposes a renovation of the teaching-learning process [1]. In this frame, the challenge is to apply the new technological elements in the teaching process without introducing resistances in the communication among students, between students and teachers and between individuals and groups.

* Author to whom mailing with regard to this work should be sent
e-mail: gmazza@uncoma.edu.ar

The student should be encouraged to accept the new technological tools and a certain feeling of affection toward their use should be promoted naturally.

Students should be encouraged to appreciate the different alternatives for carrying out the same tasks, to look for useful activities to make them think and for interactive exercises to relate knowledge within new contexts. In traditional university courses the lecturer presents the topic and students, in an almost passive attitude, listen and take notes. On the contrary, in our experience student activity is essential. The student (and not the teacher) should be the center of the teaching-learning process; he has to build and reach a consensus on the meanings of the different topics.

The progress of science and technology and the conception of modern education models have prompted the use of the computer as a powerful didactic resource. There are several teaching programs and software packages, which are available for a wide variety of curricular subjects, but the self-generation of programs applied to the specific needs of each subject remains each teacher's responsibility.

Last generation software that includes symbolic calculation allows producing interactive texts [2]. In these texts, numeric, symbolic and graphic instructions can be executed, and their results may then appear in the text. In this way, the student actively participates in the learning process, while discovering and understanding the different concepts. It is well known that an interactive text should not be printed, as the text will be modified in accordance with the examples generated by the user.

In this work we present an interactive text concerning Homogenous Reactor Analysis with a single isothermal chemical reaction, which was developed in the frame of the Mathematica software [3], as well as the results of the evaluation of the use of the mentioned text. The teaching tool presented here provides the basis for developing a first undergraduate course on Chemical Reaction Engineering (ChRE).

TEXT DESCRIPTION

The elaborated interactive modules concerning ideal homogenous reactors with a single isothermal chemical reaction [4, 5] deal with the analysis and design of the following chemical reactors: Batch Reactor (BR), Continuous Stirred Tank Reactor (CSTR) and Continuous Stirred Tank Reactors in series (SCSTR), based on the fluid-dynamic hypothesis of perfect mixing, and Plug Flow Reactor (PFR). The fluid dynamic hypothesis for the PFR is included in its denomination. Great emphasis is put on the problems that allow students to reach an appropriate management of the mass balances and to extend the treatment to the concept and optimization of Production and Net Profit [5, 6].

At the beginning, the interactive text is structured with the appropriate theoretical background and the practical questions and problems necessary for the student to discover and/or consolidate concepts. The data input for solving the problems is carried out by means of specific data sheets accessible through easy-to-use hyperlinks. The user may change the selected parameter values on the data input sheet. The text produces an immediate response and allows generating as many examples as needed by the user. After answering the questions in the text, the student may check if his answers are correct by opening hidden cells that show the right results. This feature allows the student to self-control his own learning.

The interactive text includes some specific programs that have been developed in the frame of the *Mathematica Software* in order to solve problems and case-studies. These programs include many different situations according to the intended level of knowledge.

The options offered by the text for solving problems related to each topic are shown in Table 1 for BR, and in Table 2 for CSTR and PFR. This version of the text does not include the possibility of handling variable volume for the BR and variable flowrate for the continuous flow reactors.

The particular kinetics is also a *Data Input* and must be chosen from a menu (Table 3), for a general reaction $A + \mathrm{b}\,B \underset{k_i}{\overset{k_d}{\rightleftarrows}} \mathrm{c}\,C + \mathrm{d}\,D$. Here, the stoichiometric coefficients, **a, b, c**, and **d** correspond to the substances ***A, B, C*** and ***D***; k_d and k_i are the direct and inverse rate coefficients respectively.

The results for any problem are presented in both analytical and graphic ways. The graphic outputs are built on the basis of Wickham-Jones suggestions for the generation of Graphics in *Mathematica*

XINPUT DATA	**RESULTS**
I) Existing reactor (Volume specified)	
Initial species concentrations Final species concentrations	Reaction Time and Production
Reaction Time	Species Concentrations and Production
Production	Species Concentrations and Reaction Time
Optimize Production	Species Concentrations and Reaction Time
Optimize Net Profit	Species Concentrations and Reaction Time
II) Design (Production specified)	
Species Concentrations	Reaction Time and Volume require d
Optimize Volume	Reaction Time and Species Concentrations

Table 1. Batch Reactor: Program options concerning the IT input and output data for an existing reactor (I) and for a reactor design problem (II).

INPUT DATA	RESULTS
I) Existing Reactor (Volume specified)	
Species Concentrations	Residence Time, Volumetric F low Rate and Production
Residence Time	Species Concentrations, Volumetric F low Rate and Production
Production	Species Concentrations, Residence Time and Volumetric Flow Rate
Optimize Net Profit	Species Concentrations, Residence Time and Volumetric Flow Rate
II) Design (Production specified)	
Species Concentrations	Residence Time, Volumetric F low Rate and Volume
Optimize Volume required	Residence Time, Volumetric Flow Rate and Species Concentrations

Table 2. Continuous Stirred Tank Reactor and Plug Flow Reactor: Program options concerning the IT input and output data for an existing reactor (I) and for a reactor design problem (II).

Irreversible Reactions ($k_i = 0$)		**Reversible Reactions**
$r = k_d\, C_A^{\alpha}$	$\alpha = 0, 0.5, 1, 2$	$r(C_A) = k_d\, C_A - k_i\, C_C$
$r = k_d\, C_A^{\alpha}\, C_B^{\beta}$	$\alpha = 1$ and $\beta = 1$	$r(C_A) = k_d\, C_A^2 - k_i\, C_C^2$
		$r(C_A) = k_d\, C_A^2 - k_i\, C_C\, C_D$
		$r(C_A) = k_d\, C_A\, C_B - k_i\, C_C\, C_D$
		$r(C_A) = k_d\, C_A\, C_B - k_i\, C_C^2$
Autocatalytic Reactions	**Kinetic Expressions including an inhibition term**	
$r = k_d\; C_A\; C_B$	$r(C_A) = \dfrac{k_1\; C_A}{1+k_2\; C_A}$; $r(C_A) = \dfrac{k_1\; C_A\; C_B}{1+k_2\; C_A}$; $r(C_A) = \dfrac{k_1\; C_A^2}{1+k_2\; C_A}$	

Table 3. Simple kinetic expressions considered in the program.

[7]. In the text, the students can find useful options for self-assessment and self-criticism of their work, which allow them to review and finally learn the concepts.

METHODOLOGY

The methodology for the application of the proposed interactive text in an undergraduate course of Chemical Reaction Engineering consists in developing the topic in a four-hour lesson in the presence of the lecturer and the teacher assistant at the Computer Lab. Students have the interactive text installed in the computers and a list of instructions for its management.

Students are encouraged to generate as many case-studies to be analyzed so to understand the effect of each variable. The comments made by the students are discussed in class and the lesson ends with a summary and conclusions.

USE OF THE INTERACTIVE TEXT

In this section we will present two case-studies to visualize the use of the proposed interactive text.

Study case I

The following reaction is carried out in a BR of V = 1000 liters:

$$H_2SO_4 + (C_2H_5)_2SO_4 \underset{k_i}{\overset{k_d}{\rightleftarrows}} 2\ (C_2H_5)SO_4H$$

The reaction proceeds isothermally at 23 °C (operation temperature), with reaction rate constants $\mathbf{k_d}$ = 7.02 10^{-4} liter /(mol min) and $\mathbf{k_i}$ = 1.41 10^{-4} liter/(mol min). The density of the solution can be considered essentially constant.

The initial concentrations of both reactants, H_2SO_4 and $(C_2H_5)_2SO_4$, were 5.5 M.

Additional Data:

- Total time for reactor charging, discharging and idle time: 30 min
- \$v = 0.1 \$/liter ($v: specific operating cost)
- Prices: H_2SO_4: 0.1 \$/mol $(C_2H_5)_2SO_4$: 0.1 \$/mol $(C_2H_5)SO_4H$: 0.4 \$/mol

a) Compute the daily Net Profit that will be obtained for the following cases:

a_1. the desired final conversion is x_{Af} = 0.5,

a_2. the reaction proceeds until the maximum Production of $(C_2H_5)_2SO_4$ takes place,

a_3. the reaction proceeds until the maximum of Net Profit takes place.

Additional information: The unconverted reactants are assumed to be reused with a negligible separation cost.

b) Compute the maximum Net Profit when the unconverted reactants are not recovered from the final solution.

c) Provide a summary of results in a table including the values of Production, Reaction Time, Conversion and Net Profit. Discuss the results, trends and draw conclusions.

In this case-study students strengthen the concepts related to the operation of a batch reactor as regards Production, Net Profit and the effect of the following variables on their values:

(i) the final conversion,

(ii) the possible recovery of unconverted reactants,

(iii) reaction time

As an example, two of the data input sheets (related with the problem initialization) are shown in Figures 1a and 1b. The data entered is highlighted in white.

The results as a fixed output format for the case in which the Net Profit is optimized are shown in Figure 2.

A plot of the output of the program, made by user request, is presented in Figure 3 to show the effect of reaction time on the Production value.

Study Case II

A simple irreversible n-th order reaction has the following kinetic expression:

$$r(x_A) = k_d\ C_{AI}^{n}\ (1\text{-}x_A)^n \qquad (1)$$

and will be first carried out in a BR.

It is known that the *reaction modulus*, τ, is defined for this case as

$$\tau = k_d\ t_r\ C_{AI}^{n\text{-}1} \qquad (2)$$

a) Derive an expression giving a generalized relationship between the fractional conversion of A (x_A) and the reaction modulus (τ) if it is possible. (Suggestion: Try with orders 0, 0.5, 1 and 2). The program will allow the user to check the results.

IndividualReactorVolume = yes	TotalVolume = no
IndividualResidenceTime = no	TotalResidenceTime = no
IndividualConversion = no	FinalConversion = no
ExistingReactors = $\begin{pmatrix} BR & no & no \\ no & no & no \\ no & no & no \end{pmatrix}$	NumberOfReactors = no
BranchFlowRate = no	FlowRate = no
Production = no	Optimize = yes
VolumeFunction = no	NetProfitComputation = yes

Figure 1a. Initialization sheet — Part I.

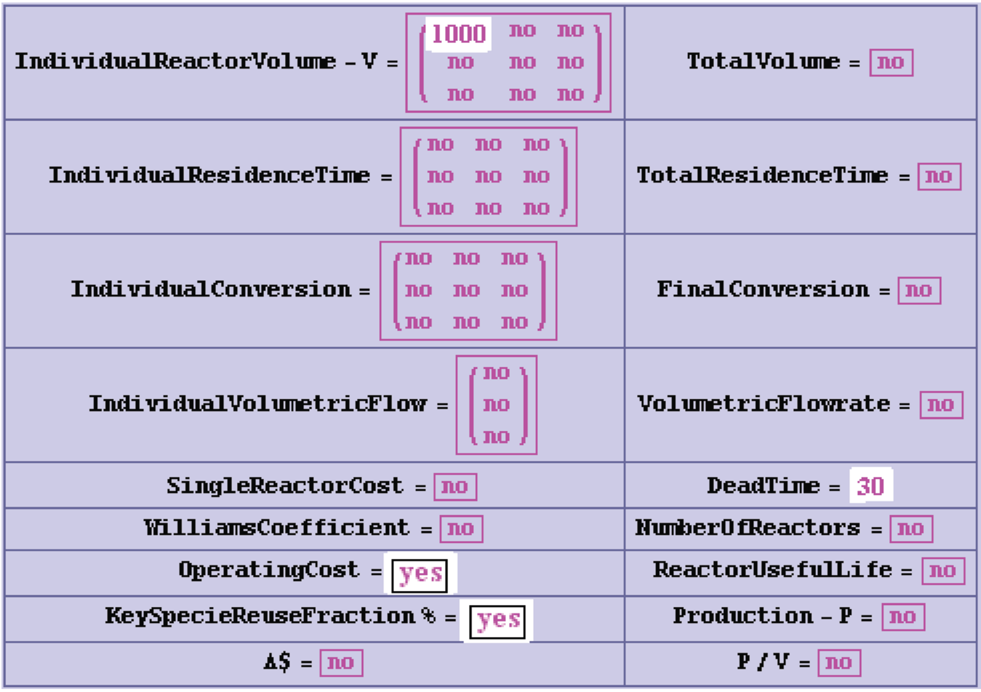

Figure 1b. Initialization sheet — Part II.

b) Give the values of ***n*** for which the key reactant **A** can be totally consumed for finite values of τ.

c) Plot the conversion of A as a function of the reaction modulus for different values of the reaction order **n**.

In this problem the student can analyze the variation of the conversion with the reaction modulus τ and with the variables occurring in its definition: temperature, initial concentration of A and reaction time.

The data input sheet for this case is shown in Figure 4.

It is necessary to point out here that the lecturer should provide students with an Instructions Manual for IT Use, which allows them to identify the Input Data Sheet to be chosen according to the case-study.

The results of part (a) are shown in Figure 5a, and those of part (c) are shown in Figure 5b. Figure 5c shows the response to Case II.b.

EVALUATION OF THE INTERACTIVE TEXT

In order to evaluate the Interactive Text proposed in this paper, an experimental study was carried out. In this study, an independent variable (*the Interactive Text*) is activated to analyze its effects on

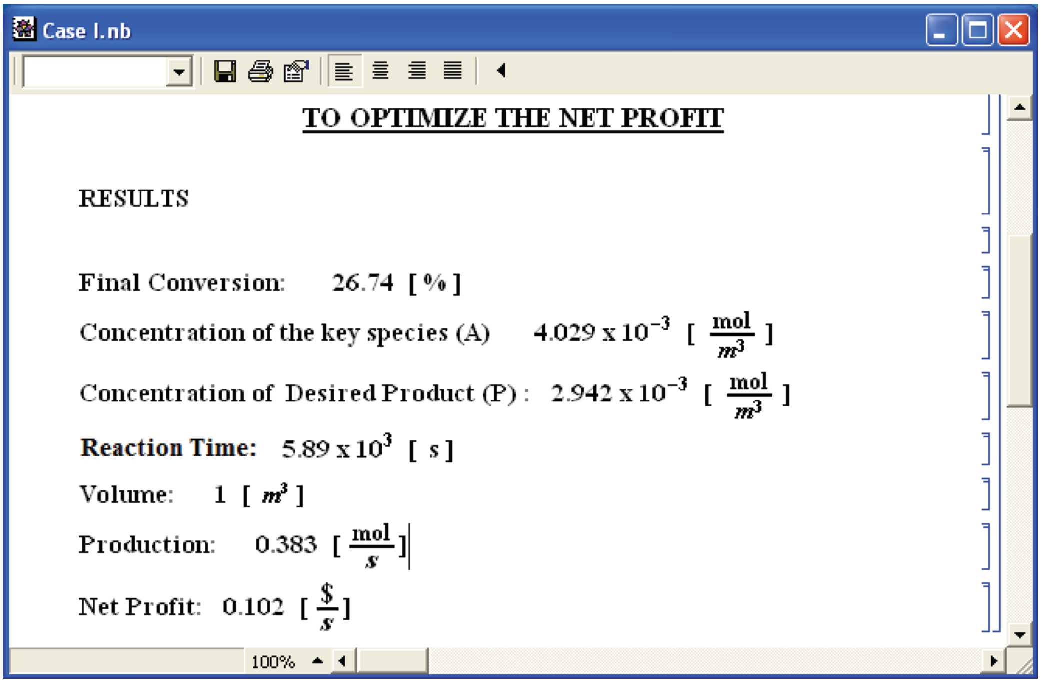

Figure 2. Output data sheet for Case I, sub-case b.

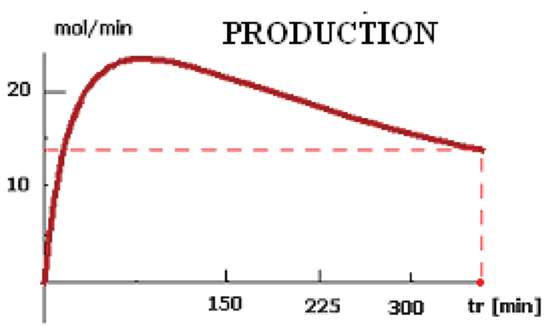

Figure 3. Production rate as a function of reaction time: Case I — sub-case a .

the dependent variable (*an appropriate incorporation of the knowledge about the topics developed at the cognitive structure of students*) under controlled conditions.

The results come from an experiment carried out with students of the Chemical Engineering undergraduate course at the National University of Comahue in the city of Neuquén, Argentina [4]. The modules of BR, CSTR and SCSTR involved in the interactive text dealt with in this paper were used.

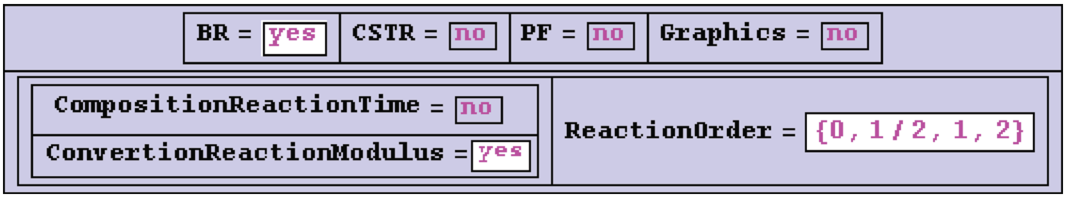

Figure 4. Initialization Sheet. Case II.

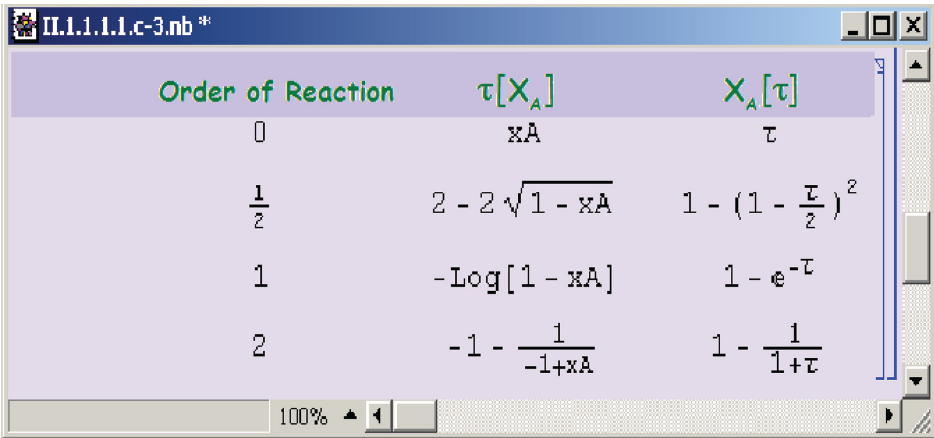

Figure 5a. Output data sheet for Case II.a

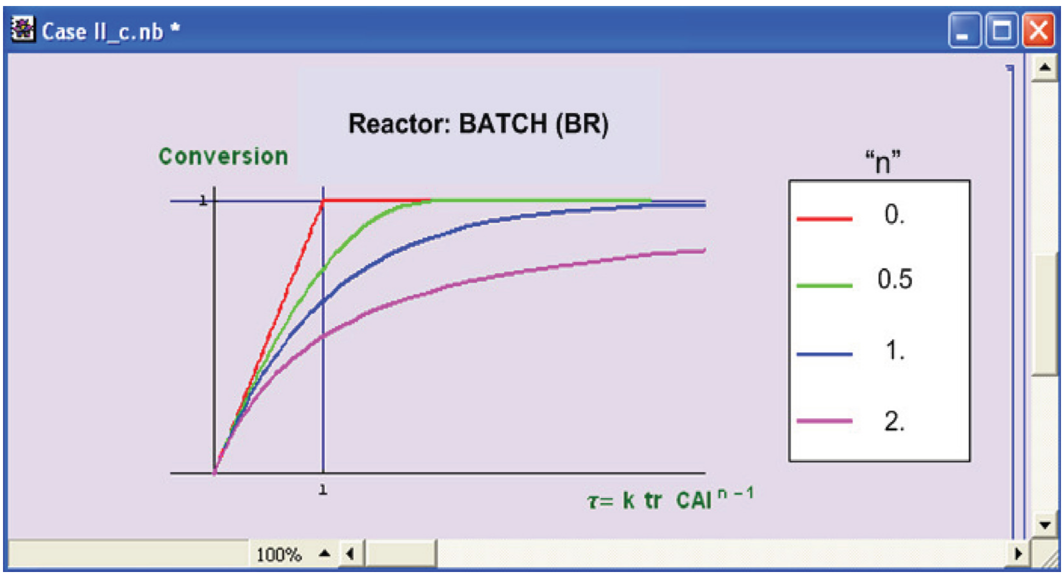

Figure 5b. Output data sheet for Case II.c

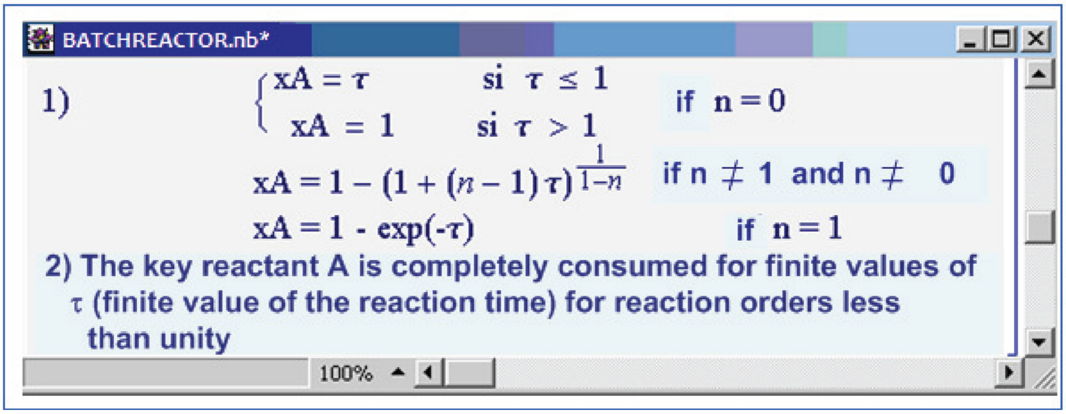

Figure 5c. Output data sheet for Case II.b

The experiment was evaluated with a personal survey at the end of the class, and a written test when finishing each subject.

ANALYSIS OF RESULTS

Two instruments are used for testing the results obtained from the pedagogical experience dealt with in this paper: *closed surveys* and *evaluation tests*.

The closed survey consists of a series of questions having a limited number of options and is based on analysis categories (AC). The AC can be defined as "situations and contexts, activities and events, interpersonal relationships, behaviors, opinions, perspectives about a problem, methods, strategies and processes" [8].

The selected ACs are detailed next:

Conceptual categories:

- 1.a. Theoretical Background
- 1.b. Examples
- 1.c. Task Difficulty

Methodological categories:

- 2.a. Understanding
- 2.b. Concept association
- 2.c. Question posing
- 2.d. Reflections on the IT subject

- 2.e. Summing up
- 2.f. Creation of appropriate mental representations
- 2.g. Satisfaction about working in group
- 2.h. Lecturer participation

2.i. Encouragement

Use of the Interactive Text:

- 3.a. Clarity of the Instruction Manual
- 3.b. Difficulty in handling the IT
- 3.c. User-friendly interface for solving problems
- 3d. Easiness to navigate

The statistic analysis was carried out on the basis of the closed survey included in Appendix I. The results are graphically shown in Figures 6, 7 and 8. The alternatives to answer the questions can be appreciated in the text of the survey, detailed in Appendix I

Abbreviations: ***satisf:*** satisfactory, ***very satisf:*** very satisfactory, ***interes.:*** interesting

A forty-five minute written test was given at the end of each unit of the subject. A typical exercise is taken from each unit based on the application of mass balances, Production and Net Profit (influence of the initial concentration and volume).

The results of the evaluation tests can be observed in Figure 9. The percentage of correct answers reached for each unit is shown for each student (E_j, in the abscissa axis).

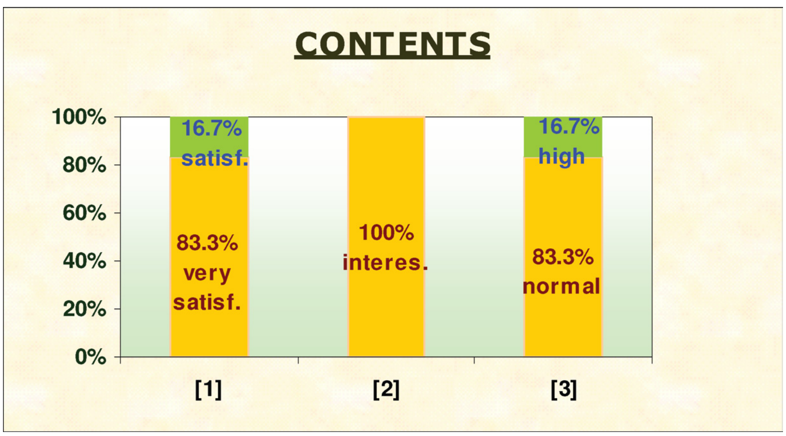

Figure 6. Contents: [1]: 1.a. Theoretical Background; [2]: 1.b. Examples; [3]: 1.c. Task Difficulty.

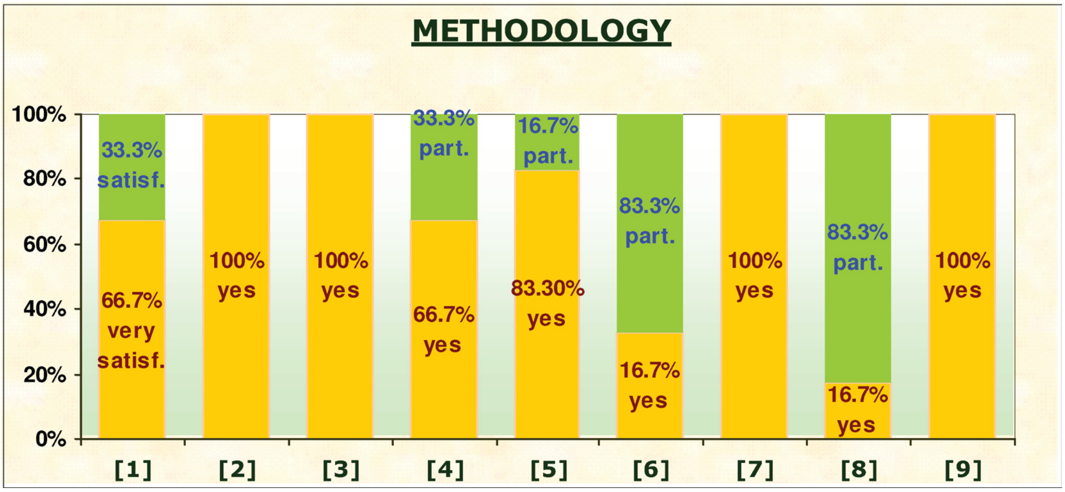

Figure 7. ***Methodology: [1]: 2.a. Understanding; [2]: 2.b. Concept association; [3]: 2.c. Question posing; [4]: 2.d. Reflections on the IT subject; [5]: 2.e. Summing up; [6]: 2.f. Creation of appropriate mental representations; [7]: 2.g. Satisfaction about working in group; [8]: 2.h. Lecturer participation; [9]: 2.i. Encouragement. Abbreviations: satisf: satisfactory,*** **very satisf:** ***very satisfactory,*** **part.:** ***partially.***

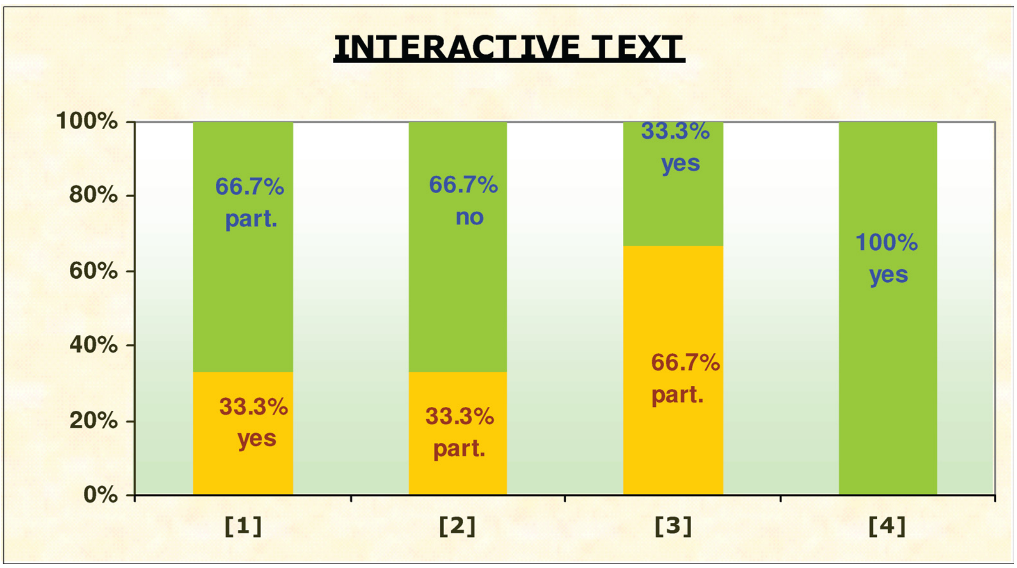

Figure 8. ***Interactive Text: [1]: 3.a. Clarity of the Instruction Manual; [2]: 3.b. Difficulty in handling the IT; [3]: 3.c. User-friendly interface for solving problems; [4]: 3.d. Easiness to navigate. Abbreviation: part.: partially.***

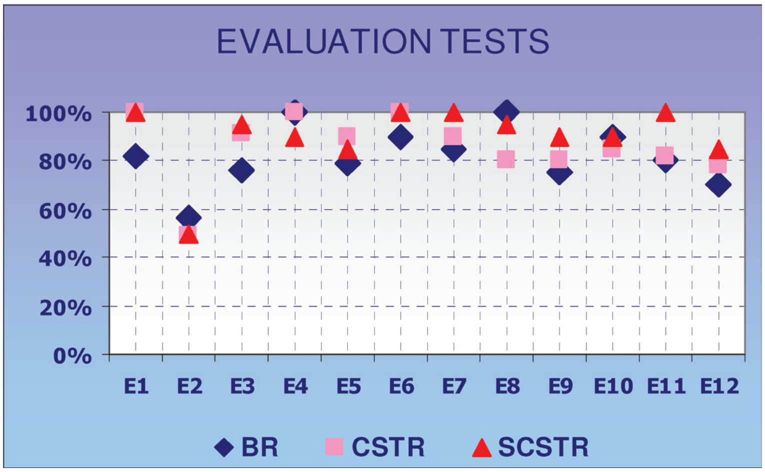

Figure 9. Evaluation Tests.

CONCLUSIONS

A significant degree of acceptance regarding the interactive text proposed here was detected from the observations made by students in the classroom. Mostly, students provided correct answers to the problems dealt with, and the instructions were easily followed. This is in good agreement with the conclusions reported by Nutall et al [2].

It is important to point out that at the beginning of the task there was a short period of general uneasiness that could be explained as a logic reaction of the students against a new methodology.

Students later realized that they had reached a motivation level higher than that of a traditional class for carrying out the same task, and they connected this motivation with the computer support. Students could reflect, draw conclusions and manage their own times. All of them remarked on the high level of interest they had experienced when studying the approached topics, since they had to discover different concepts by means of self- generated graphics and examples.

The results of the evaluation test show an average mark close to 85%, which is significantly higher than the results achieved in an undergraduate course carried out with the traditional teaching methodology.

It can be stated that the methodology acceptance - based on the positive level of the answers to the surveys and the analysis of the average performance facing the proposed exercises- is a factor that stimulates the adoption of the interactive text. It can be considered as a very important tool for university courses on ChRE and can play a major role in improving the efficiency of the teaching-learning process.

In this context, Interactive Texts can be easily integrated into the Chemical Reactor Engineering courses as the only way of teaching or, alternatively, they can constitute a valuable tool which can be combined with the traditional teaching method.

NOMENCLATURE

C_A	molar concentration of A, (mol m^{-3})
E_i	Each student acting in the pedagogical experience
k	reaction rate constant
n	order of reaction
P	Production of desired product
r	chemical reaction rate, (mol m^{-3} s^{-1})
t_r	reaction time (in batch reactors)
V	Volume of reactor, (m^3)
X_A	conversion of A, (−)
Greek Symbols	
τ	reaction modulus (defined by equation 2)
Subscripts	
A	key species A
d	direct reaction
f	final
i	inverse reaction
I	initial value of concentration for batch reactors

REFERENCES

[1] Litwin, E., Libedinsky, M., Liguori, E., Lion, C., Lipsman, M., Maggio, M., Mansur, A., Scheimberg, M. and H. Roig, 1995. *Tecnología Educativa. Política, historias, propuestas*. Ed. Paidós, Buenos Aires.

[2] Nutall H. E., White, K. and N. Vadiee, 2000. *A New Interactive Computer– Based Process Control Course*, AIChE Annual Meeting, Los Angeles, CA. Unpublished paper. *Wolfram Information Center:* www.library.wolfram.com

[3] Wolfram, S., 2003. *The Mathematica Book, 5th*. Edition. (Wolfram Media)

[4] Barassi F. J., 2004. Implementación de una metodología alternativa para el desarrollo de la enseñanza de la Ingeniería de Reactores Químicos. *MSc Chem. Eng. Thesis*, Faculty of Engineering, University of La Plata, Argentina.

[5] Barreto, G. F. and G. D. Mazza, 2002. *Reactores Homogéneos con Temperatura especificada*. Monography for un undergraduate course of Chemical Reaction Engineering. Chemical Engineering Department, Faculty of Engineering, University of La Plata, Argentina.

[6] Fogler, H. S., 1999. *Elements of Chemical Reaction Engineering*. 3rd Edition. Prentice Hall International.

[7] Wickham-Jones, T., 1994. *Mathematica Graphics, Techniques, Applications*. The Electronic Library of Science, Santa Clara, California.

[8] Flores, G. J., 1994, "Análisis de datos cualitativos", PPU, Barcelona, Spain.

AUTHORS

Daniela A. Asensio received her degree in Chemical Engineering from the National University of Sur, Argentina, in 2001. She joined the Faculty of Engineering at the University of Comahue in 2004 and has academic experience, working as Assistant, in the following courses: Chemical Reaction Engineering. She developed her research work at the Chemical Department of the University of Comahue as member of a research project in Modeling and Simulation of Heterogeneous Systems for the Analysis of Chemical Processes. Ms. Asensio's Ph.D. thesis in Chemical Engineering from the National University of la Plata will address *Simulation of Heat and Mass Transfer in Fixed Beds assisted by CFD*.

Francisca Barassi received her Academic degree in Chemical Engineering and her Master in Chemical Engineering from the National University of La Plata, Argentina, in 1970 and 1981 respectively, and her Academic degree as Specialist in Nuclear Engineering from the University of Buenos Aires in 1981. Mg. Barassi worked at the Mathematics Department at the National University of Comahue, Neuquén, Argentina, from 1972 until 1978. She worked at CASING SRL (Engineering Company) from 1979 until 1983, at the CNEA (National Commission of Atomic Energy) in the Engineering Management of the Nuclear Central Division from 1983 until 1993, and at the Heavy Water Industrial Plant in the Engineering Management of the Process Division from 1994 until 1995, and she joined the Faculty of Engineering at the University of Comahue in 1995, where she is currently Professor of Chemical Reaction Engineering.

Mariana T. Zambon received her degree in Industrial Engineering (Chemical orientation) from the National University of Comahue, Argentina, in 1987, and Ph.D. degree in Chemical Engineering from the National University of La Plata, Argentina, in 2010. She developed her research at the Chemical Department of the University of Comahue as member of a research project with strong experience in the field of educational topic applied to Chemical Engineers Education. Dr. Zambon was a Senior Process Engineer at the Arroyito Heavy Water Plant, Neuquén, Argentina from 1989 to 2001.

Professor Germán D. Mazza received a degree in Chemical Engineering and Ph.D. degree in Chemical Engineering from National University of La Plata, Argentina, in 1983 and 1993, respectively. From 1995–1996, Dr. Mazza was a postdoctoral research associate at the *Institut de Science et de Génie des Matériaux et Procédés*, France, at the laboratory of Professor Gilles Flamant. He has developed his research work for 23 years at the Chemical Engineering Department of the University of La Plata. From 2001 to 2004 acted as vice-dean at the Engineering Faculty, and he is currently Associate Professor of Chemical Reaction Engineering at the University of La Plata. In 2005, he joined the Faculty of Engineering of the University of Comahue, Argentina, where he is currently Professor of Chemical Reaction Engineering and Research Member of CONICET. He has published 32 scientific contributions on the subject of Fluidization, Heat Transfer and Analysis and Modeling of Chemical Reactors. Dr. Mazza has given over 30 presentations at scientific meetings.

APPENDIX: CLOSED SURVEY STRUCTURE

1. Contents

What do you think about the following characteristics of the IT?

1.a. Theoretical background

☐ Very satisfactory ☐ Satisfactory ☐ Quite satisfactory ☐ Not satisfactory

1.b. Examples

☐ Interesting ☐ Quite interesting ☐ Not interesting

1.c. Task difficulty

☐ Very High ☐ High ☐ Normal ☐ Low

2. Methodology

The methodology followed in the IT allows you to

2.a. *understand the topics ?*

☐ Very satisfactorily ☐ Satisfactorily ☐ Quite satisfactorily ☐ you did not understand it

2.b. *relate different concepts ?*

☐ Yes ☐ Partially ☐ No

2.c. *formulate your own questions on the subject ?*

☐ Yes ☐ Partially ☐ No

2.d. *draw conclusions?*

☐ Yes ☐ Partially ☐ No

2.e. *create appropriate mental representations?*

☐ Yes ☐ Partially ☐ No

2.f. *Do you think that it is interesting to work in groups?*

☐ Yes ☐ No

2.g. *Did you need the help of the lecturer during the class?*

☐ Yes ☐ No

2.h. *Do you think that this methodology motivates the student more than the traditional teaching method does?*

☐ Yes ☐ No

3. Interactive Text

3.a. *Did you find the Instruction Manual is clear?*

☐ Yes ☐ Partially ☐ No

3.b. *Did you have any difficulties in handling the Instruction Manual ?*

☐ Yes ☐ Partially ☐ No

3.c. *Is the interface of the text user-friendly for solving problems ?*

☐ Yes ☐ Partially ☐ No

3.d. *Is the text easy to navigate ?*

☐ Yes ☐ Partially ☐ No