# WEB TOOLS FOR CHEMICAL ENGINEERING EDUCATION COUPLING FUNDAMENTALS WITH PROCESS DESIGN

## *The Distillation Case Study*

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Abstract: In this paper the “Unit Operations and Separation Processes” area of a virtual platform called LABVIRTUAL (http://labvirtual.eq.uc.pt) is presented. The objective is to support the study of students engaged in a Chemical Engineering degree, especially in Portuguese-speaking countries. It is argued that these web tools support the autonomous study of the students, contributing to develop their critical and creative thinking, and enabling more practical approaches to the different chemical processes. Moreover, it is shown how coupling, in the same platform, sections directed to basic concepts/mechanisms, with sections directed to process design, contributes to knowledge integration and to a better understanding of the design methodologies for each process.

## 1 INTRODUCTION

In recent years, there have been many changes in teaching methodologies, namely in Engineering Education. Throughout Europe, the Bologna process required deep transformations in higher education curricula and courses organization. One of the consequences of the Bologna process is the reduction of lecturing hours to allow more time for the students to develop important skills such as: self learning, critical thinking, teamwork and knowledge integration between the different subjects. Furthermore, in parallel to the scientific and theoretical background, engineering students need to develop a more practical training. These fast changes and the rise of new technologies at the world scale have been inducing changes in teaching methodologies, having in mind the need to avoid dependent learners in the classroom (Bell and Fogler 1998, Shacham et al. 2009 and Hasna 2010). Additionally, it is also important to take advantage of the new skills, namely competences on informatics, the students possess nowadays. To achieve these objectives a demand for web and computational tools to support learning and teaching activities in Engineering education is increasing.

Some authors (Bell and Fogler 1998, Henry 2005, Streicher et al. 2005, Felder 2006, Edgar 2006, Henry et al. 2008, Shacham et al. 2009 and Garcia-Herreros and Gomez 2010) support that these tools contribute to engaging students and to the development of active learning attitudes. Web tools can facilitate the development of additional teaching strategies for simulation, demonstration, experimentation, operation, etc. Therefore, using different and complementary resources, the dynamics in the classes can increase (Bell and Fogler 1998, Felder 2006, Shacham et al. 2009 and Hasna 2010). The Chemical Engineering Departments of both the Universities of Coimbra and Porto have developed a virtual platform called LABVIRTUAL (http://labvirtual.eq.uc.pt, Rasteiro et al. 2009), with a wide scope, directed to the teaching of Chemical Processes, aiming at complementing and supporting the student’s study and help in developing his autonomy. The integration of the different Chemical Engineering subjects was the main goal. LABVIRTUAL brings together contents (multimedia libraries), simulators, virtual experiments and remotely controlled experiments, as well as links to other sources, aiming at getting the student acquainted with the subject under study.

The Chemical Processes area comprises four sections: Unit Operations and Separations, Chemical Reaction, Process Systems Engineering (PSE), and Biological Processes. These sections present funda-

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mental concepts and applications aimed at leading the students to understand, for instance, how different operating conditions result in different process designs, or which alternatives are available for a certain process. Whenever possible, process integration is also addressed. Moreover, each section includes case studies illustrating some of the features of the applications developed. These tools can be used in a wide range of disciplines in a Chemical Engineering degree curriculum, and be accessed either in classroom or at home.

This article focuses in more detail on the features of the Unit Operations and Separation Processes area of LABVIRTUAL. A special attention will be given to the tools developed to study the Distillation process, including the simulation and web methodologies adopted. Moreover, we will stress how fundamental insight of the underlying mechanisms is addressed in this platform, and integrated later to a better understanding of the design methodologies of each chemical process. Leading the students to establish this connection is most important for the effective understanding of the different chemical processes, and has been accomplished with success in this platform.

## 2 WEB METHODOLOGIES

The Web infrastructure of the Virtual Laboratories of Chemical Processes is based on standard open-source software. This approach allows similar functionalities to existing commercial software, with good flexibility for the specific needs of the portal. A Virtual Server is used that can integrate contents from various sources and present these contents in a consistent way to the user. Most of the materials available are stored in a Content Management System (CMS), for flexibility and to simplify the inclusion of new material. Joomla! was used for this task. Predefined presentation templates simplify the addition of new contents and the management of several kinds of information.

The integration of simulators and data acquisition systems with the Web portal is a critical point. The simulations are entirely run on the server and the user just needs a regular browser to access and interact with the platform. Since, as referred, the CMS used allows the construction of customized templates for the presentation of information, the integration with the simulators is made by developing forms to visualize and manage real-time data, and for the insertion of input parameters used by the simulators to run calculations and for presentation of the results to the users. This layer validates the user input and executes a system call to autonomous simulation codes. As a result of a successful simulation, graphical and numerical results can be returned, to be displayed on the web page. The communication between the computational applications and the web platform itself is done through a simulation gateway using a CGI (Common Gateway Interface) protocol.

## 3 DESIGN OF DISTILLATION PROCESSES

Distillation is one of the most used separation processes in the manufacturing of chemical products, generally speaking. Thus, this subject must always be present in any Chemical Engineering curriculum. The underlying principle of a separation by distillation is the difference in volatility of the different components in the feed mixture. Therefore, a good understanding of vapour/liquid equilibrium is essential to understand the design of distillation equipment. In the Chemical Engineering curricula this subject is usually taught in a course of Chemical Thermodynamics.

In the platform LABVIRTUAL we have integrated fundamental subjects with the design of process equipment. This is the case in the section of "Unit Operations and Separation Processes", where we start with the area of basic principles (Heat and Mass Transfer and Chemical Thermodynamics) in parallel with the area of Unit Operations design. Figure 1 describes this arrangement.

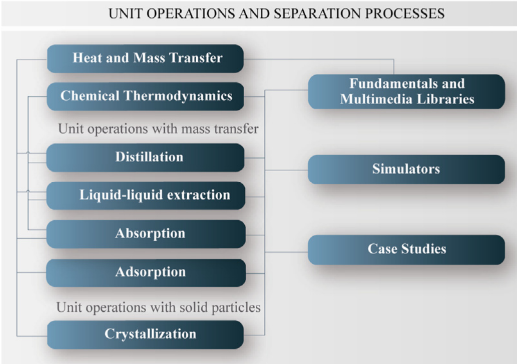


Figure 1: Scheme of the Unit Operations and Separation Processes area (from Granjo et al. 2009).

### 3.1 Basic Principles – Vapour/Liquid Equilibrium

The "Chemical Thermodynamics" area addresses, in general, the subject of the equilibrium of phases. In the case of vapour/liquid equilibrium (VLE) it is split in two parts: pure substances and mixtures. In the VLE Fundamentals of pure substances' section, the significance of temperature and pressure diagrams, the concepts of vaporization, vapour pressure, substance's fugacity and critical properties are explained. Regarding the VLE of mixtures the binary composition diagrams (Txy) and (Pxy) are studied and common VLE problems are addressed: bubble point pressure and temperature, BUBLP and BUBLT; dew point pressure and temperature, DEWP and DEWT, and isothermal flash.

Regarding VLE of mixtures, particularly important for the design of distillation processes, homogeneous and heterogeneous methods can be used. The VLE simulator carries out calculations of BUBLP, BUBLT, DEWP, DEWT and isothermal flash for mixtures, from a database with 25 substances. The following important thermodynamic model options are included for the heterogeneous methods: the ideal liquid and the perfect gas behaviour; the UNIFAC method to model liquid non-ideality and perfect gas; UNIFAC and the virial equation of state to predict liquid and vapour non-idealities.

These simulators are directly connected to case studies, to help the users to approach the simulator in the correct way and to enhance their learning experience. The main purpose is to allow discussing the need of using methods of non ideal behaviour of both liquid and vapour phases, which is mainly determined by the type of mixture and the operating pressure and temperature. For some of these case studies the results obtained are compared to those in the literature, as shown in Figure 2.

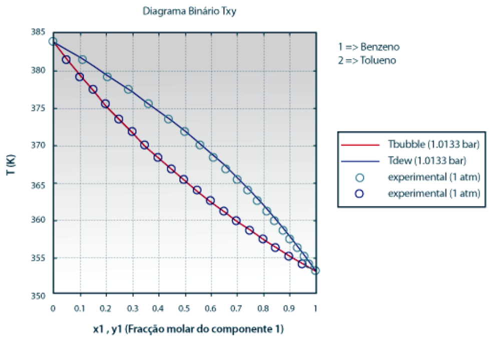


Figure 2: Txy diagram for a binary mixture (benzene/ toluene) produced with the VLE simulator - comparison with experimental data (legends in Portuguese).

## 3.2 Distillation Simulator

The area "Models Used in the Simulation" describes the general case of distillation of a mixture with any number of components. The shortcut methods are discussed with reference to the Fensk, Underwood, Gilliland and Kirkbride equations (FUGK) (Seader and Henley 2006). As far as the rigorous methods of calculation are concerned, the Wang-Henke (WH) method is covered (Wankat 2007 and Seader and Henley 2006). Empirical correlations and heuristics incorporated in the Distillation simulator to design and dimension tray distillation columns are also addressed (Wankat 2007).

The Distillation Simulator, which has been developed in MATLAB, allows the design of a distillation column with one feed stream; two liquid products (residue and distillate) streams; saturated reflux; total condenser; adiabatic stages and constant pressure. There are no limitations to the feed thermal state and the user can specify the temperature ($T_F$) or the feed thermal condition. The feed components database is the same as for the VLE simulator. Also, the thermodynamic models options are the same as for the VLE simulator. To carry out the simulation calculations two strategies are available.

Three mixtures are treated in the Case studies section: i-butane/n-butane/pentane/hexane; benzene/ methyl-cyclohexane/toluene and ethanol/water. With the first two examples it is pretended to show the influence of some of the distillation operating variables (e.g. reflux ratio, pressure) for a system with a non-ideal behavior, in the first example, and for a system close to an ideal behavior, in the second example. In the case of the ethanol/water mixture it is examined the impact on the distillation process of a mixture which exhibits an azeotropic point.

The user can experience as well the influence of several variables on the column dimensions and features, for instance, how changes in the operating pressure or on the feed conditions influence the column design and energy balance. Moreover, the user is also directed to evaluate which is the best thermodynamic model to describe VLE for each set of components, that is, for each feed.

### 3.2.1 Example of the Use of the Distillation Simulator – Distillation of a Mixture of Hydrocarbons

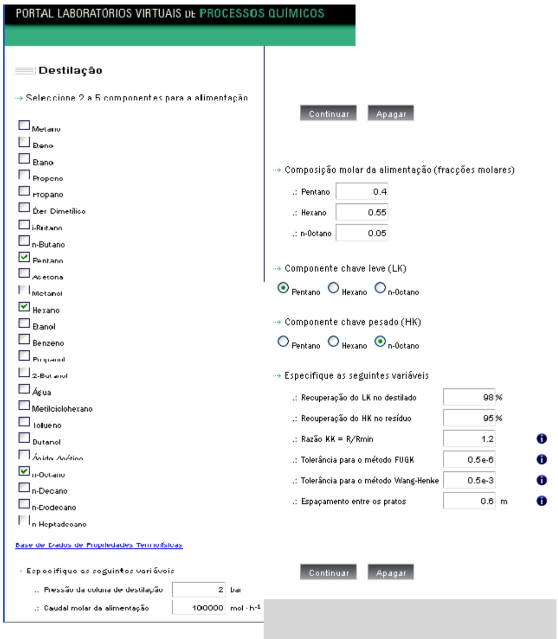
This example corresponds to one of the case studies in the distillation section and illustrates the use of the distillation simulator to design a continuous fractionating distillation column to separate a mixture of hydrocarbons (n-pentane – $nC_5$, n-hexane - $nC_6$ and n-octane - $nC_8$). The main separation aimed at is between $nC_5$ and $nC_6$, $nC_8$ being considered a contaminant. The feed stream has got,

Table 1: Summary of the design results for the distillation column to separate $nC_5$, $nC_6$ and $nC_8$.

$x_{D,LK} = 0.934$; $x_{D,HK}=0.066$;
$x_{B,LK} = 0.014$; $x_{B,HK}=0.9$;
LK recovery in distillate = 98%;
HK recovery in residue = 95 %
Residue molar flow rate (B) = 58 $kmol \cdot h^{-1}$
Distillate molar flow rate (D) = 42 $kmol \cdot h^{-1}$
Equilibrium stages, N = 22
Feed stage, $N_F = 10$
Reflux ratio, R = 1.63
$T_D = 332$ *K*; $T_B = 367$ *K*.
Heat duty in condenser = -781 k*W*
Heat duty in reboiler = 810 *kW*
Column height = 21.4 m
Column diameter = 0.99 m

$x_{D,LK}$, $x_{D,HK}$ are the mole fractions of light-key and heavy-key components in the distillate, respectively.
$x_{B,LK}$, $x_{B,HK}$ are the mole fractions of light-key and heavy-key components in the residue, respectively.
$T_D$, $T_B$ are the distillate and residue temperatures, respectively.

in mole percentages, 40, 55 and 5% of $nC_5$, $nC_6$ and $nC_8$ respectively ($nC_5$, is considered as the light key (LK) while $nC_6$ is the heavy key (HK)). The column operates at 2 bar. In the results presented here it is assumed that the feed stream enters the distillation column as a saturated liquid, and that both the liquid and vapour phases are taken as non-ideal (UNIFAC and virial equation being used, respectively, for the liquid and gas phases, Poling et al. 2001). The recovery targets have been established as 98% of the LK in the distillate and 95% of the HK in the bottom product. The operating reflux ratio (R) is assumed to be 1.2 times the minimum reflux ration ($R_{min}$). Figure 3 presents an image of the input form for the distillation simulator for this case study.



Destilação

→ Seleccione 2 a 5 componentes para a alimentação

☐ Metano
☐ Eteno
☐ Etano
☐ Propeno
☐ Propano
☐ Éter Dimetílico
☐ i-Butano
☐ n-Butano
☑ Pentano
☐ Acetona
☐ Metanol
☑ Hexano
☐ Etanol
☐ Benzeno
☐ Propanol
☐ 2-Butanol
☐ Água
☐ Metilciclohexano
☐ Tolueno
☐ Butanol
☐ Ácido Acético
☑ n-Octano
☐ n-Decano
☐ n-Dodecano
☐ n-Heptadecano

› Especifique as seguintes variáveis
.: Pressão da coluna de destilação 2 bar
.: Caudal molar da alimentação 100000 mol · h-1

→ Composição molar da alimentação (fracções molares)
.: Pentano 0.4
.: Hexano 0.55
.: n-Octano 0.05

→ Componente chave leve (LK)
● Pentano ○ Hexano ○ n-Octano

→ Componente chave pesado (HK)
○ Pentano ○ Hexano ● n-Octano

→ Especifique as seguintes variáveis
.: Recuperação do LK no destilado 98 %
.: Recuperação do HK no resíduo 95 %
.: Razão KK = R/Rmin 1.2
.: Tolerância para o método FUGK 0.5e-6
.: Tolerância para o método Wang-Henke 0.5e-3
.: Espaçamento entre os pratos 0.6 m

Figure 3: Input form to the distillation simulator: example for the case study (in Portuguese).

Table 1 shows the solution of this design problem, giving the specifications of the resulting distillation column, which must have 22 theoretical stages (including the reboiler) the feed stream being introduced in the 10th stage from top. The recoveries of both the LK and HK have met the specifications required. The column is expected to have a total height of around 21 m with a diameter around 1 m.

Figures 4 and 5 are examples of the output graphs from the simulator, showing how the liquid composition and temperature vary along the column. The students are guided to criticize these results by observing, for instance, that the composition profiles vary smoothly along the column, the same happening to the temperature profile, which is an indication of a well designed column where the feed stream is being admitted at its optimal location. Moreover, they can also verify that the heaviest component ($nC_8$) almost disappears in the rectification section (stages above the feed). At a later stage the students can be guided to evaluate, easily, the influence of changing certain operating parameters, such as the reflux ratio, operating pressure, feed temperature or the feed location, on the column design. Another feature that can also be tested by the students is the influence of the thermodynamic model selected to describe the liquid and gas phases on the output results (design of the distillation column). They can choose between ideal gas and liquid phases, ideal gas and non-ideal liquid phase and non-ideal gas and liquid phases. In this way they can perceive better that for some mixtures, as is the case for the example presented, the hypothesis of ideality does not affect the final equipment design. For other mixtures, like for instance azeotropic mixtures (see Granjo et al. 2009), or for very severe operating conditions, ideality is a completely invalid hypothesis.

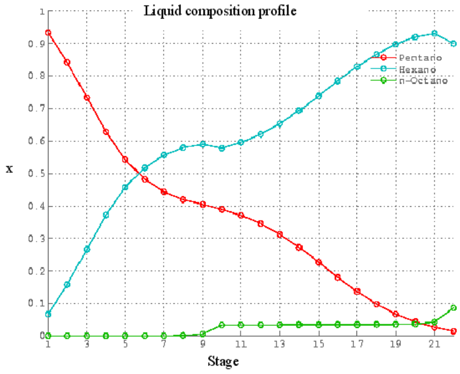


Figure 4: Liquid composition (mole fraction – x) profile – optimal feed location (10th stage).

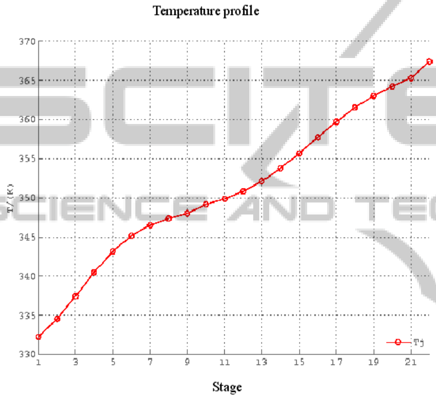


Figure 5: Temperature (T, K) profile – optimal feed location (10th stage).

Furthermore, the students can also compare the validity of different models for the design of a distillation column, going from approximate and short-cut methods to rigorous design methodologies (Wankat 2007 and Seader and Henley 2006). This case study can be used in the classroom to illustrate the influence of the aforementioned aspects on the design of a distillation column, serving as the basis for a discussion with the students. Additionally, the students can later go to the laboratory and perform lab trials which they will be asked to compare with the simulated results.

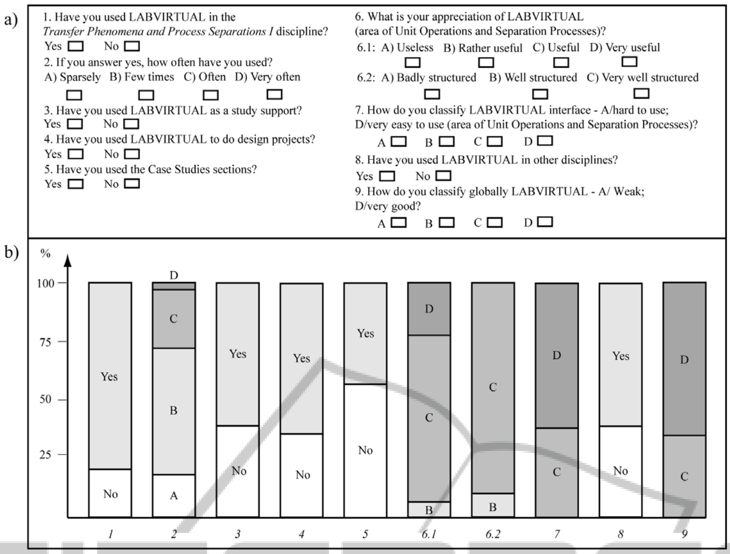
We have been monitoring the use of the portal by the students and collecting their opinions about the tools available, asking them to fill out an anonymous questionnaire in each course.

The questionnaire is very similar for the different courses. Figure 6 (a) presents the questionnaire which is being used in the course of “Separation Processes” of the Chemical Engineering Masters degree of the University of Coimbra. The questions addressed different aspects of the learning experience, students frequency and purpose of use, which facilities they had used, as well as their evaluation of the interface and of the structure of the portal. The results of the students’ responses to the questionnaire handled during the three last editions (since 2008), corresponding to a total of 78 respondents, are given in Figure 6 (b).The students’ response was, as a whole, very positive: 82% had used the platform in the Process Separations I discipline and about 91% had also used it in other subjects. Moreover, it was observed that the majority of the students had used LABVIRTUAL as a support to their study, with most of them using the platform several times. Another good point was that the vast majority of the students considered the Unit Operations and Separation Processes area of the platform as useful, very easy to use and very well structured. Globally, LABVIRTUAL had a very good rate among the students enquired.

## 4 END NOTES

Web tools are important complementary instruments for the teaching and learning process. They can be accessed with maximum flexibility, from any place at any time, and contribute to the students autonomy. In the case of the multi-functional web platform presented here, there are advantages from the combination, in a single platform, of several features: co-existence of teaching tools for a broad range of Chemical Processes, which motivates knowledge integration; diversity of approaches for a deeper insight of each chemical process, going from multimedia libraries, supplying the theoretical concepts, to simulators and case studies, used for the design of the different processes and, finally, virtual experiments. The student should be able to: understand and relate basic concepts and principles associated to each process; establish analogies between different processes; understand, apply and know the limitations of the modelling methodologies commonly used to interpret and troubleshooting industrial problems; have an idea of the impact of operational parameters on the equipment design, dimensioning and cost. This makes it easier to introduce the students to more practical and realistic approaches to Chemical Engineering problems.

The experience of using this multi-purpose platform, during three school years, has been evaluated very positively by the students.



a)

1. Have you used LABVIRTUAL in the *Transfer Phenomena and Process Separations I* discipline?
Yes ☐ No ☐
2. If you answer yes, how often have you used?
A) Sparsely ☐ B) Few times ☐ C) Often ☐ D) Very often ☐
3. Have you used LABVIRTUAL as a study support?
Yes ☐ No ☐
4. Have you used LABVIRTUAL to do design projects?
Yes ☐ No ☐
5. Have you used the Case Studies sections?
Yes ☐ No ☐
6. What is your appreciation of LABVIRTUAL (area of Unit Operations and Separation Processes)?
6.1: A) Useless ☐ B) Rather useful ☐ C) Useful ☐ D) Very useful ☐
6.2: A) Badly structured ☐ B) Well structured ☐ C) Very well structured ☐
7. How do you classify LABVIRTUAL interface - A/hard to use; D/very easy to use (area of Unit Operations and Separation Processes)?
A ☐ B ☐ C ☐ D ☐
8. Have you used LABVIRTUAL in other disciplines?
Yes ☐ No ☐
9. How do you classify globally LABVIRTUAL - A/ Weak; D/very good?
A ☐ B ☐ C ☐ D ☐

Figure 6: LABVIRTUAL assessment: a) enquiry; b) enquiry's results (A- bad, D- very good).

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## REFERENCES

Bell, J. T. and Fogler, H. S., 1998. The application of virtual reality to chemical engineering and education. In *Proc. AIChE Annual Meeting*, Miami, USA, session 170.

Edgar, T.F., 2006. Enhancing the undergraduate computing experience. *Chemical Engineering Education*, 40 (3) 231─238.

Felder, R.M., 2006. Teaching engineering in the 21st century with a 12th-century teaching model: how bright is that?. *Chemical Engineering Education*, 40 (2) 110─113.

Garcia-Herreros, P. and Gómez, J. M., 2010. Modeling and optimization of a crude distillation unit: a case study for undergraduate students. *Comp. Appl. Eng. Ed.*, DOI: 10.1002/cae.20469.

Granjo, J. F., Rasteiro, M. G., Gando-Ferreira, L. M., Bernardo, F. P., Carvalho, M. G., Ferreira, A. G., 2009. A virtual platform to teach separation Processes. *Computer Appl. in Eng. Ed.*, DOI 10.1002/cae.20383.

Hasna, A.M., 2010. E-competence in chemical engineering learning and teaching. In *Proc. ICETC 2010 - 2nd. Int. Conf. Ed. Tech. and Computers*, China, art. no. 5529669, V4330-V4336.

Henry, J., 2005. Real laboratories at a distance. In *Proc. AIChE annual meeting*, Cincinnati, USA, 3640.

Henry, J., Miletic, M., DiBiasio, D., Clark, W., 2008. Varieties of ways for learning about distillation. In *Proc. ASEE annual meeting*, Pittsburg, USA.

Poling, B. E., Prausnitz, J. M., O'Connell, J. P., 2001. Properties of Gases and Liquids. McGraw-Hill, N. Y., 5th edition.

Rasteiro, M. G., Ferreira, L. M., Teixeira, J. C., Bernardo, F. P., Carvalho, M. G., Ferreira, A. G., Ferreira, R. Q., Garcia, F. P., Baptista, C. G., Oliveira, N. M., Quina, M. M., Santos, L. O., Saraiva, P. A., Mendes, A. M., Magalhães, F. M., Almeida, A. S., Granjo, J. F. Ascenso, M., Bastos, R. M., Borges, R., 2009. LABVIRTUAL – a virtual platform to teach chemical processes. *Education for Chemical Engineers*, 4 (1) e9─19.

Seader, J. D. and Henley, E. J., 2006. Separation Process Principles. John Wiley & Sons, Hoboken, NJ, 2nd edition.

Shacham, M., Cutlip, M. Brauner, N., 2009. From numerical problem solving to model-based experimentation – incorporating computer based tools of various scales into the ChE curriculum, *Chem. Eng. Ed.*, 43 (4).

Streicher, S. J., West, K., Fraser, D. M., Case, J. M., Linder, C., 2005. Learning through simulation ─ student engagement, *Chem. Eng. Ed.*, 39 (4), 288─301.

Wankat, P. C., 2007. Separation Process Engineering. Prentice-Hall, Upper Saddle River, NJ, 2nd edition.