A Virtual Platform to Teach Chemical Processes

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***Abstract* - This paper presents a virtual platform to teach chemical processes aiming to support a more autonomous learning and providing a practical approach to the subjects, parallel to the scientific background. The platform is organized in five sections: Separations and Unit Operations, Reaction Engineering, Process Systems Engineering, Biological Processes and Virtual Experiments. The first four sections deal with the chemical/biochemical processes and include simulators, applications and case studies aimed at leading the students to understand those processes. The fifth section, Virtual Experiments, deals both with the laboratory visualization of the basic phenomena related to the processes in the other four sections, and with the remote monitoring of laboratory experiments. Moreover, this platform will allow discussion forums and is aimed at sharing experiences with other schools. This paper describes the different applications included in the web platform, as well as the simulation strategies and web methodologies used for its construction, presenting also examples of application in the classroom.**

***Key Words*- Chemical Processes, E-learning, Virtual Laboratories, Web Platform.**

INTRODUCTION

Teaching methodologies have been changing all over the world, namely in Engineering Education. On the one hand educators want their students to develop capacities of autonomous and critical thinking. However, they face, quite often, difficulties resulting from the strategies adopted at the basic education level, and also from the diversity of backgrounds that students have when they enroll a university degree. On the other hand, engineering educators also feel that it is absolutely necessary to develop in engineering students a practical approach to the subjects addressed, parallel to the scientific background.

These facts have been acting as a driving-force to motivate engineering educators to develop new teaching methodologies. Furthermore, the Bologna Process, that suggests a reduction of formal lecture hours and stresses the importance of autonomous work of the students, is also contributing to motivate the development of new teaching strategies.

The Chemical Engineering Departments of both the Universities of Coimbra and Porto, have been experimenting, on their own, for quite sometime, new teaching methodologies [1,2], taking into consideration the concerns referred above, and also taking advantage of the information technologies skills showed by the new students' population.

Recently, these departments got engaged in a broader project, involving a large group of academics (13 Chemical Engineering Faculty members and 5 research students) with complimentary competencies. This project is aimed at developing a virtual platform with a wide scope, directed to the learning of Chemical Processes.

The platform is organized in five different sections: Separations and Unit Operations; Reaction Engineering; Process Systems Engineering; Biological Processes and Virtual Experiments, as shown in Figure 1.

The first four sections deal with the chemical/biochemical processes and will present applications and case studies aimed at leading the students to understand, for instance, how different operating conditions result in different process designs, or which are the alternatives available for a certain process, etc. Moreover, in each section there will be a sub-section of fundaments and, whenever possible, process integration and intensification will also be addressed.

The fifth section, Virtual Experiments, deals both with the laboratory visualization of the basic phenomena related to the processes in the other four sections, and also with the remote monitoring of laboratory experiments. Additionally, these visualizations will also be used to help students to better prepare their lab classes, in order to take a maximum profit from them.

Some of the modules mentioned above are already in use in Chemical Engineering undergraduate classes. The whole web application is expected to be ready by the end of 2007.

Additionally, the platform foresees also an area more directed to the school outreach, where students from the basic education levels interested in chemical and chemical engineering subjects can obtain information of high scientific quality. This platform is intended to be a dynamic Web Portal open to share experiences with other schools and educators.

In this paper we will explain, briefly, the objectives of the different modules which make up the virtual platform, giving notice of some of the applications already in use in the classroom. In addition, a brief explanation of the simulation strategies and web methodologies adopted in the development of the platform will be presented. To finalize, some examples of using the platform in the classroom, to teach Chemical Processes, will also be shown.

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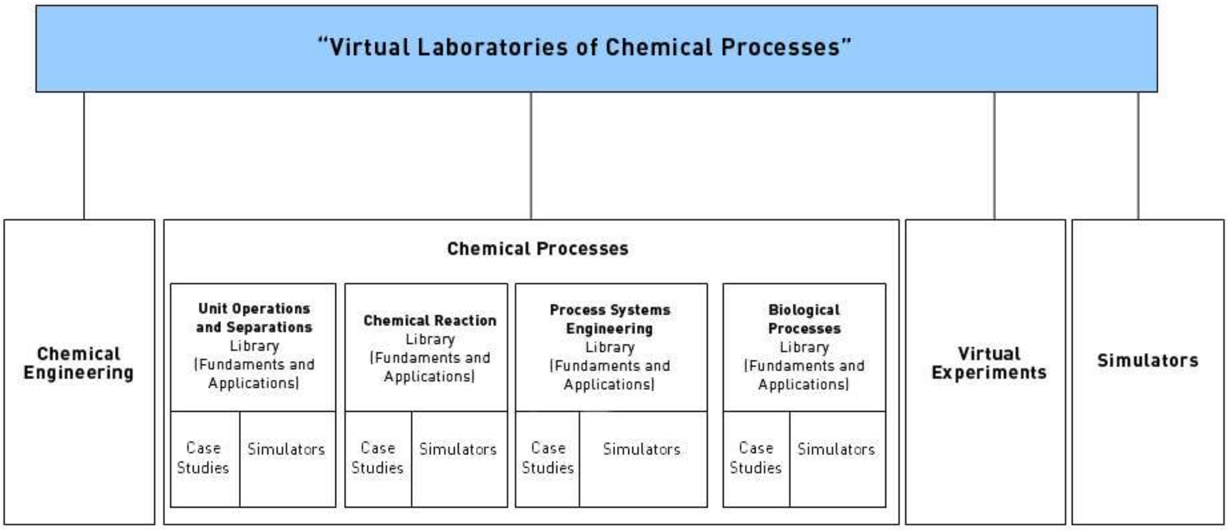


FIGURE 1
SCHEME OF THE PLATFORM

CONSTRUCTION OF THE VIRTUAL PLATFORM

I. Simulation Strategy

One of the key components of the web platform is process simulation. The study of the different chemical processes is supported by interactive simulation modules, covering both fundamental topics as well as more practical and complex applications. Figure 2 depicts the basic architecture of the simulation system, comprehending two main blocks: the *web interface*, which helps the user in entering the data required for simulation and supports the visualization of the corresponding results, and the *computational platform*, where the mathematical model of the chemical process is solved. The exchange of information between these two levels is mediated by a simulation gateway, designed in agreement with the CGI (Common Gateway Interface) standard. The input data set, collected in a simulation form, supports numerical values as well as discrete options (chemicals to be processed, type of model to be used or different modes of simulation). The simulation output may include graphics and in some cases several sets of results for different input conditions and also dynamic profiles draw in real time.

Matlab was chosen as the preferential computational platform, although other tools are also being used, such as Octave and Fortran, namely because of previously developed codes. Matlab is a well recognised general-purpose platform combining numerical, symbolic and graphical capabilities and has available an extensive library of add-on packages [3]. It is widely used in engineering teaching, research and practice, and is part of the chemical engineering curriculum at our universities. In addition, it is affordable and easy to integrate with other applications.

Regarding the mathematical process models embedded in the simulators, the level of detail, complexity and generality varies from application to application. They may be sets of algebraic and/or differential equations, depending on whether the process operation is batch or continuous and on whether the model has or has not variables distributed on space. These sets of equations are solved using standard numerical methods and in some more complex problems a decomposition strategy and/or iterative procedure may also be needed. These tools are in most cases recognizable by the students who are thus prepared to explore the codes, understand details and adapt or extend them for some particular homework or project.

In some modules, a database of physico-chemical properties for a short set of chemicals is available and simulations can be performed for different feed mixtures. Also, modularity is explored in some cases, with a given process simulator being composed of several more fundamental modules. For instance, there is an autonomous module of vapor-liquid equilibrium to perform calculations such as the boiling point of a liquid mixture, which is also invoked within the distillation module, where a large scale equipment to separate a liquid mixture is simulated. It should be noted, however, that our concern is not to develop a professional platform with large databases and a sophisticated structure of interconnected modules, but instead build a pedagogical tool. In this regard, the set of modules so far developed represents a great value and in the future we intend to extend it with more illustrative processes and applications.

II. Web Methodologies

The Virtual Laboratories of Chemical Processes Platform will be an information platform based on free software, e.g. software under the GPL license. This approach allows similar functionalities provided by other commercial software, with the flexibility to better adapt software code to the specific needs of this Portal. Therefore, the choice of the software to be used in the portal's development was carefully assumed to satisfy the project expectations.

Since one of the Portal goals is the support to the initial and the life-long learning processes, the use of a Learning Management System was one possible natural option. However, and despite of the pedagogical perspective of the

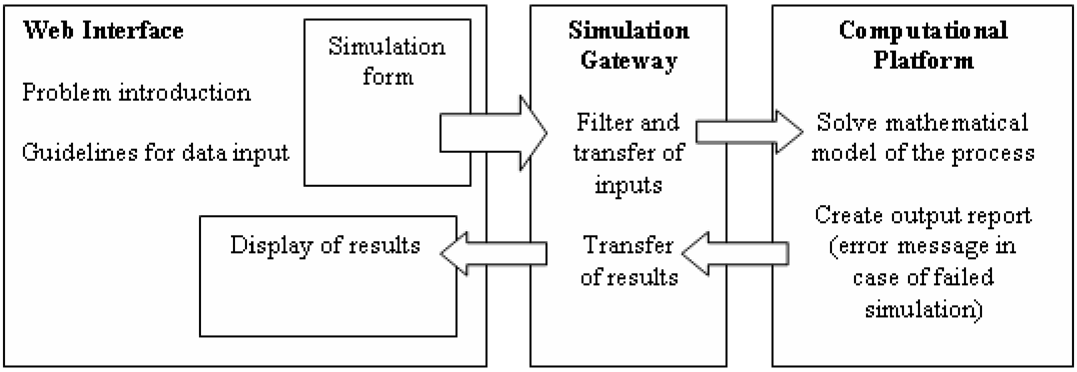


FIGURE 2
FLOWCHART WITH THE SIMULATION COMPONENTS.

portal, we decided to use a Content Management System (CMS) for flexibility and because some specific functionalities of an e-learning platform such as exercises, wikis, etc are not required. Therefore, to provide a clear presentation of the theoretical principles of chemical processes and link them to case studies and simulators, the use of Joomla!, one of the most well known CMS , is well adapted. This option allows an easy edition of all content, based on predefined templates for presentation, and the adequate management of several kind of information.

A relevant social aspect related with the development of information systems is the inclusion of all potential users. Nowadays, the Web presentation of information has to follow rules related with accessibility of people with disabilities, including the visual disabilities. The present platform is being developed according to those rules.

From the functional point of view, the portal is organized in four main areas: Chemical Engineering, Chemical Processes, Virtual Laboratories and Simulators (Figure 1). The Chemical Processes area is then also organized in four other blocks as explained previously.

The integration of simulators with the information platform is a critical point. Since the CMS used allows the construction of customized templates for information presentation, this integration shall be made by developing forms for the insertion of parameters used by the simulators, to run calculations and present the results to the users. These forms are developed using Perl, through Perl scripts, acting as the Simulation Gateway (Figure 2), appealing to a system call that should run a simulation and return graphics and numerical results to be later shown on the page.

In addition to these functionalities, the use of Joomla! is well suited to support other functionalities of the portal such as discussion forums, search box, downloads, etc.

THE PLATFORM TOPICS

Next, in this section, we will present the main features of the different blocks in the Chemical Processes area. Each block, as shown in Figure 1, includes a library of fundaments and applications, simulators and case studies to lead the students through the study of the processes. Quite often, there are also links to applications in other web sites.

I. Unit Operations and Separation Processes

This section is directed to the study of Unit Operations, especially Separation Processes applied to Chemical Processes. Four different separation processes have been considered so far: 1. Distillation; 2. Liquid/liquid extraction; 3. Absorption; 4. Adsorption and ionic-exchange.

The motive for this choice was to address both equilibrium and rate based processes. In the future other processes will be considered, namely processes involving a disperse phase and unit operations dealing with heat transfer. It must be stressed that the processes selected, so far, for inclusion in the web platform, are quite typical of Chemical Processes and also equally important for Bioprocesses.

Due to its great importance to all the processes, Thermodynamics was considered as an autonomous module and has been developed, as well, in this section, preceding the Separation Processes modules. In this module both vapor/liquid and liquid/liquid equilibrium are addressed. The student is guided from the easier (ideal gas and ideal liquid) to the more complex approaches (real gas described through the Virial equation and real liquid making use of the UNIFAC method). The module includes several case studies, where the calculated results are compared with experimental data, so that the student understands the validity of the different models for the specific system analyzed. Moreover, in this section there are links for other web sites making use of other approaches for vapor/liquid equilibrium, namely, those based on state equations and molecular simulation.

Referring to the different separation processes, in each module there is always a section on fundaments, followed by another section describing the models used in the simulation and in the design program which can be assessed through the platform.

Moreover, for each separation process, different case studies have been prepared, which will help the students to understand different aspects of the process itself, namely the influence of operating conditions on the design and performance of the separation equipment.

So far, both the Distillation and Liquid/Liquid Extraction modules are finalized and can be used in the classroom. For the design of distillation equipment both short-cut and the rigorous Wang-Henke method [4] have been implemented. As for the design of liquid/liquid extraction equipment a

McCabe-Thiele type method [4] has been implemented, which is only valid when both solvents can be considered immiscible. The design of tray absorption towers is also being based on the McCabe-Thiele method for the determination of the theoretical number of trays, for concentrated solutions, and on the Kremser-Brown-Sonders equation for diluted solutions.

The rate based processes, Liquid/Gas Absorption in packed towers, Adsorption and Ion-exchange in solid/liquid systems, are still in the development stage. Referring to the separation by Ion-exchange, this application will be closely related to the Virtual Experiments section, since there is an experiment to study the uptake of an electrolyte in a column packed with a cation-exchange resin in this last section. So, in this case, the students will be able to connect equipment design and performance analysis through simulation, with the visualization, in the laboratory, of the phenomena studied. All these features are accessible, through the web, without needing to be physically in the laboratory.

II. Chemical Reaction Processes

The industrial chemical processes transform raw materials in valuable products for the market, being the reactor often considered as the "heart" of the process. In fact, selection and design of the reaction units are primordial for the economic success of a chemical industry, imposing final yields and conversions in line with the expected commercial profits. The Chemical Reaction Engineering is then a branch of the Chemical Engineering with a relevant role intrinsically associated to Separation Engineering, which involves the purification units before and after the reactors. The global performance of the overall process will be then dictated by the optimisation of the total assembly of units.

At the Chemical Reaction Engineering level our main goal focus on the development of e-learning tools in the domain of kinetic studies and design and operation of reactors able to be used in homogeneous and heterogeneous processes. In what regards kinetics, modelling analysis will be associated to experimental tests to determine kinetic parameters, reaction orders and activation energies integrated in the Arrhenius expression, in order to obtain mathematical expressions that will reflect the effect of temperature and reactants composition in the reaction rates. In the context of reactor analysis this section of the platform addresses firstly the chemical reactors with ideal behaviour, stirred tanks under continuous, batch and semi-batch operation as well as the plug flow reactors. Afterwards, catalytic reactional systems will be analysed with particular emphasis in fixed-bed reactors that are largely used in industry. In this domain, several mathematical models were developed including pseudo-homogeneous and heterogeneous models in steady state and transient regimes, which required different numerical techniques for computer simulation of the resulting ordinary differential equations, ODEs, and partial differential equations, PDES, which are solved using various commercial Fortran codes, namely, GEAR, PDECOL, FORSIM, DDASAC. The illustration of the behaviour of such systems is proposed through two case studies involving the synthesis of phthalic anhydride and formaldehyde through partial oxidation of ortho-xylene and methanol, respectively. In particular, the operation of these gas-solid systems highlights the importance of the thermal instabilities that are possible to occur in such highly exothermic processes, such as temperature runaway and wrong way behaviour, very important in relation with safety concerns.

Studies in the context of reactors networks will also be included in this module aiming the optimization of the economical balances and desired yields of chemical processes, through the selection of adequate reactor types, as well as convenient unit configurations, in series and/or parallel. Moreover, studies in the frame of the Residence Time Distribution, RTD, will be addressed in order to identify non-ideal behaviours and propose mathematical models for the operation of real systems.

III. Process Systems Engineering

Process System Engineering (PSE) deals with the performance of various engineering decisions using mathematical tools and algorithms. The main engineering systems activities that are involved in these decisions include the following topics: modeling, simulation, integration, optimization, instrumentation and control, data reconciliation and product and design process. The objective of the present project in the PSE domain is to develop simulators supported in real industrial processes with different characteristics in terms of chemical related products (pharmaceuticals, novel material, commodities and specialties) and operating modes (batch and continuous). For that purpose, interactive teaching modules will be developed in some of the areas identified above.

One module of the virtual platform will include a set of examples covering key concepts in the domain of instrumentation and process control. Through these examples, chemical engineering students can experience an introduction to process control virtual simulation to learn the concepts of feedback and feedforward control. The simulation modules allow to interact with a few examples (hydraulic tank system, continuous stirred tank reactor-CSTR, distillation column, etc) to analyze the process open and closed-loop responses. Here, the students can exploit the main features of the PID control law by interactively adjusting and tuning the PID parameters. Also, examples of advanced control techniques such as model predictive control will be available to illustrate their advantages to control multivariable processes.

The instrumentation, including sensors and valves to measure and influence the process conditions, respectively, is essential in the study of automatic control applied to industrial processes. The static and dynamic characteristics of the sensors will be illustrated by linking to a multimedia library prepared to assist the chemical engineering students to learn industrial instrumentation used in most of the chemical processes. Moreover, a data acquisition system is being implemented to monitor indoor and outdoor air quality (SO_2, NO_2 and CO_2 emissions, temperature and relative humidity), in real time, using electrochemical sensors.

Finally, a module with an illustrative example involving process optimization and energy integration concepts will also be included in the virtual laboratories platform. The importance of such PSE tools to the development of sustainable and environmental friendly processes will be emphasized along this module.

IV. Biological Processes

Day after day the chemical engineers get more and more involved in non traditional areas forcing the education in chemical engineering to evolve in order to correspond to the new needs and new opportunities of the profession. Biochemical engineering is closely related to chemical engineering in applying physical principles to the resolution of biological processes. Sharing a common language with biological scientists is necessary for an understanding of each others in an interdisciplinary cooperation. Modelling biological processes using theory, empirical correlations and mathematical tools contributes to the understanding of biological phenomena, to determine process parameters, to predict the performance of the equipment under different working conditions, etc., always considering the properties of the biological entities. The predictive capacity of the mathematical models is particularly useful for training and education, facilitating the demonstration of phenomena in virtual experiments that otherwise would be expensive and take long time in the lab. Such an approach will be used to the quantitative analysis of biological kinetic data, to evaluate simple or more complex fermentations as affected by process conditions such as cell density and growth rate, substrate concentration, air flow rate, dissolved oxygen concentration, stirrer speed, etc. Enzyme catalysis will also be demonstrated and the dynamics of enzyme reactors will be covered.

The recovery of bioactive products is more constrained in comparison with the unit operations that are more traditional in chemical engineering, in order to avoid loss of activity and contamination by other products. At this stage only the basic principles of membrane and chromatographic processes will be covered. The simulation of the ultrafiltration process, in batch or continuous mode, will be tested as an example for illustrating the potentialities of the membrane technology in separating macromolecules. Regarding the chromatography, the partition of two components between a mobile and a stationary phase (adsorbent) will be simulated by using the technique of the elution chromatography, in which the sample is injected into the column as a pulse. The students, in both cases, have the opportunity of testing key concepts involved in these operations and evaluating different operating approaches to achieve the best separation efficiency.

V. Virtual Experiments

The site, as already mentioned, will also have a section named "Virtual Experiments". This is meant to be an independent section, with links to other relevant areas of the site, as reaction, separation, biologic systems and process control. In this way different approaches for facilitating the learning and teaching processes in Chemical Engineering laboratories, will be coupled.

Four experiments are included here: Determination of the Kinetic Constant and Activation Energy for the Liquid Phase Homogeneous Reaction between Ethyl Acetate and Sodium Hydroxide; Flow Pattern Characterisation in a Tubular Reactor Packed with Glass Beads; Study of the Sucrose Inversion and Study of a Cation-Exchange Resin. In addition to the description of the experimental setups and procedures and the theoretical background for each work, multimedia support is provided in the form of a video, illustrating each setup's components and the major steps in the operation procedures and experimental occurrences. The experimental results collected and their treatment are also illustrated. Finally, a template model for a short report of each work is provided.

In the section of process control, the students may carry out remotely one feedback control experiment, which setup is located at the Chemical Engineering Department of the Faculty of Engineering of the University of Porto. Using the webserver capabilities of LabVIEW, the experiment interface can be accessed via a web browser and one Webcam placed in the laboratory captures live images of the experiment. This way the students will be able to experiment and contact with the basic concepts of PID processes control.

At a later point of the project, a lab report management and verification tool will be developed. This will include, among other features, e-mail report delivery management, validation of lab results, computation of parameters from reported data, comparison to the expected parameters and the reported ones.

USING THE VIRTUAL PLATFORM IN THE TEACHING OF CHEMICAL PROCESSES

The platform just described is mainly oriented to teaching Chemical Processes, in the aforementioned fields, at the graduation level (both 1^{st} and 2^{nd} cycles according to the Bologna scheme), though other features are foreseen for the portal. In fact, there will also be applications directed to long life learning and to the lower school levels outreach. In this section of the paper we will discuss only the use of the platform in the teaching at the graduation level.

According to the philosophy behind the construction of the platform, the site can be used in the classroom to illustrate the design and operation of process equipment, as for instance to show the influence of operating conditions, feed characteristics, etc. on the design outcome, or still to evaluate the validity of different models to do the design.

After this first contact with the facilities of the platform in a certain course, the student can go on using the site on her/his own, taking advantage of the case studies there included, in relation with the phenomena described in the fundamentals section, as well as to solve new problems. Furthermore, the student can use this tool to solve other assignments (design problems) or, even, at a later stage, to use modules of the simulators to build more complex programs required to work out complex design problems, like for instance in project work.

A first prototype of the platform has already been in use, over the last two school years, for the teaching of Distillation in the Chemical Engineering curriculum from the University of Coimbra [1]. In this paper we will next describe another example of the use of the platform either in a Chemical Thermodynamics course or in a Process Separations course.

The portal comprises a vapor/liquid equilibrium (VLE) module. In this module the user can perform different calculations: flash point, bubble point or dew point calculations (at constant pressure or temperature); or, still, build the Txy, Pxy or just the yx, vapor/liquid equilibrium diagrams. The module comprises a thermodynamic data base of 20 common components, which is accessible to the students, and allows a wide range of simulations. The user can try different thermodynamic models to describe the vapor and/or the liquid phases (ideality of both phases; real liquid and ideal vapor; real liquid and real vapor). The models used to simulate the real liquid and real gas are, respectively, the UNIFAC method and the Virial equation. Moreover, for the case studies, the student can compare the simulated results (Txy, Pxy or yx diagrams) with experimental data. Table 1 summarizes the input variables the student is asked to introduce in the VLE module.

One of the case studies in the module is the construction of the equilibrium diagrams (Txy, Pxy and yx) for an ethanol/water mixture. We know this is a non-ideal mixture, thus, the student is led to understand that if he considers both phases as ideal he can not reproduce the experimental data. On the other hand, if he chooses to use a non-ideal model for the liquid phase or for both phases, fitting of the simulated results to the experimental ones is much better.

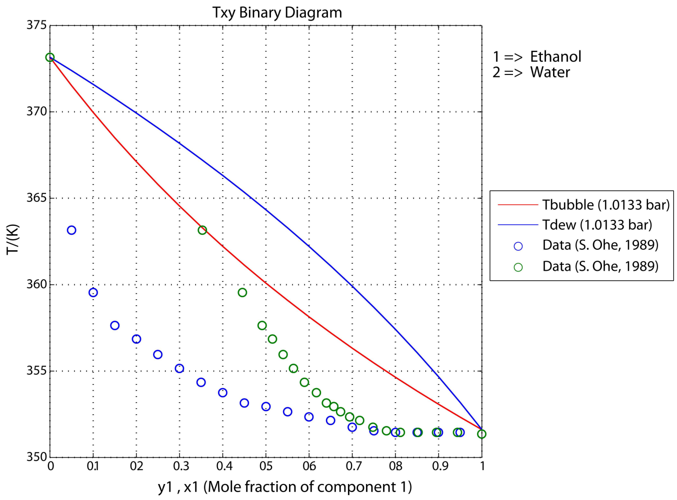
TABLE I
INPUTS FOR THE VLE MODULE

Variables Description
Type of calculation (varies from 0 to 6)
Component indices
Molar composition of the feed
Pressure or Temperature for the calculations (respectively for bubble/dew temperature or bubble/dew pressure)
Choice of thermodynamic model (liquid and/or vapor)

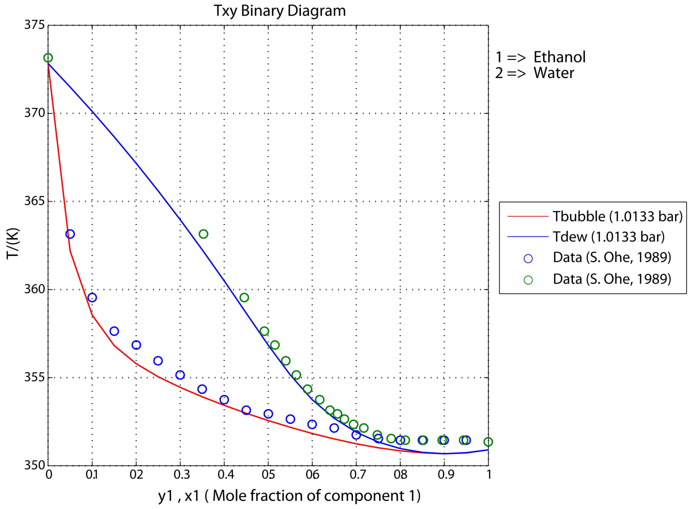
Figure 3 shows the outputs obtained at one atmosphere (Txy diagram) for the case where both phases are considered ideal (Figure 3a) and for the case where both phases are considered real (Figure 3b). It is evident that in the first case it is impossible to predict the azeotrope. The experimental data has been taken from S. Ohe [5].

In addition, the user can also get an output text file with the tabular data from the simulation. The text file does also show the input variables and the average deviations between calculated/experimental values for both vapor compositions and bubble temperatures. This example clearly illustrates some of the teaching capabilities of the VLE module

To finalize, it must be stressed that the authors face the use of this type of tools as a complement to other teaching approaches. It is the opinion of the authors that web tools should not substitute, entirely, laboratory classes, which are essential for the education of Chemical Engineers. Nevertheless, web applications can overcome physical or economic restrictions, enabling access to experiments that would be impossible to set up in the laboratory, due to its complexity, cost or safety problems. They can also be used to help students in preparing laboratory classes. Nevertheless, the main advantage of these tools comes from supporting the student's autonomy.



(a)



(b)

FIGURE 3
VLE MODULE OUTPUTS: EQUILIBRIUM DIAGRAMS (Txy) FOR THE ETHANOL/WATER MIXTURE - (a) IDEAL; (b) REAL

ACKNOWLEDGMENT

We want to acknowledge the receipt of a sponsorship from POSC, Portugal, contract 743/4.2/C/REG, which is enabling the development of the platform described in this paper.

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