The Use of Commercial Simulators in the Engineering Teaching: A Naturally Stimulating Approach

MACIEL, M.R.W., MACIEL-FILHO, R. and VASCONCELOS, C.J.G.
Faculty of Chemical Engineering
State University of Campinas (UNICAMP)
CP 6066, CEP 13081-970, Campinas-SP,Brazil
Phone: (55-19)788-7840, Fax: (55-19) 2394717
E-mail: wolf@feq.unicamp.br

Introduction

Recently, many things have been discussed about new trends in the engineering education. Probably, the most important of them is the computer development. The increasing power and speed of the computers allow the calculation of complex multivariable problems. In Chemical Engineering it can be mentioned molecular simulation, neural networks, dynamic modeling, expert systems and others. In this way, the commercial simulators, each time using algorithms more robust and reliable, are becoming very important in the undergraduate course. Simulations help the student to develop the skills of analysis, synthesis and evaluation that are important to the engineers. Simulations in design projects bring sense of reality and students become more active and interested (Whiting, 1993).

For the actual generation of students, computers play a very important hole; they are sometimes their toys, or their communication means or, even, their sophisticated calculators. However, very little attention has been given to the use of computers together the commercial simulators as an effective way to teach engineering concepts. In fact, the exciting world of computers and the interactive way in which the good commercial simulators were developed, make an interesting combination that has to be added to the natural explorer feeling of the young people.

Besides the commercial simulators, another point, which comes out in the chemical engineering course, is the use of Internet as a mean of improving of communication and getting more information. The use of Internet grew very fast in the last five years and changed the communication means. Today, everybody uses the World Wide Web (WWW) to obtain information and email to communicate, both within and outside industries and universities.

The use of this tool promises to expand in the Chemical Engineering world. It has been created automated processes monitoring tools that can function like WWW (Koch, 1997). The engineer can monitor the plant performance by any Internet-connected computer. Of course, it must be adequately addressed to guarantee security.

In the Chemical engineering course, the use of Internet is increasing very fast, and it has potential to change the education. Navigating the WWW the student can obtain actual materials in a entertaining way (Bungay and Kuchinski, 1995).

On the other hand, the interaction between universities and industries has given to the students the opportunity to know the present market demand. In this manner, the availability of commercial simulators is important because they present a wide data bank, covering, in the best cases, the majority of substances and equipment of interest in the chemical industry, they have facilities for the interactive use and interactions with different unit operations, allowing to reproduce the whole plant efficiently. It is important to training the students to make deci-sions and evaluate economic aspects, what has been required by the industry (Buonopane, 1997). In this work, we will simulate the ethanol dehydration by distillation, taking into account strategies for optimization and waste minimization.

Commercial Simulators

The commercial simulators have been used both in industry and universities. In the chemical engineering field it has many options such as: HYSIM and HYSIS, by Hyprotech simulators, PRO/II, by simulation science, ASPEN PLUS, by Aspen Technology, Inc. and others. This kind of simulator possibilities to the chemical engineer to evaluate the operating conditions, new alternative of processes and of equipment and has a wide and robust data bank, avoiding the necessity of the users to procure in sources the necessary data.

The engineer that uses a commercial simulator must have knowledge of all system characteristics and the advantages and limitations of the method used to solve the problem. If it is being simulated a distillation column, he must know the algorithm that is used and its validation. For example, if it is an azeotropic column, the algorithm is different from that used for a conventional one. The commercial simulators are closed packages, but this kind of information can be obtained from the manual.

Another aspect that must be evaluated is the choice of the thermodynamic model to represent the system correctly. If it is an azeotropic mixture, it must be selected an activity model to represent the non-idealities of the liquid phase. If the user select an unapropriated method, the operation will not work properly. In a near future, in the simulations will be presented expert systems to help in these decisions.

Ethanol Dehydration Plant Simulation

The ethanol dehydration by distillation is an important process to obtain anhydrous ethanol, a renewable energy source.

Ethanol is produced in a fermentation tank with a mass composition of 10% ethanol and 90% water. The ethanol-water mixture forms an azeotrope with molar composition of 89% ethanol and 11% water. One available technique to obtain anhydrous ethanol is to concentrate the mixture that comes from a fermentation tank by conventional distillation until the azeotropic point and then, to apply an azeotropic or extractive distillation (or even others, like reactive distillation, electrolytic distillation, etc.) to separate the azeotrope, if it is not sensitive to the pressure. The azeotropic distillation is very difficult to converge. It is due to the presence of the two liquid phases in the stages on the top of the column.

Figure 1 represents the flowsheeting for the dehydration of ethanol by distillation. Feed enters to the column (a), water is removed as bottom product. The top product goes to the column (b) that concentrate the mixture in 87% ethanol and 13% water mole fractions. The entrainer (benzene) breaks the binary azeotrope and forms a ternary azeotrope with minimum boiling point. Ethanol is obtained at the bottom and the top product (ternary azeotrope) goes to a decanter (d) where it splits in two phases: an organic phase, rich in benzene, that returns to the azeotropic column and an aqueous phase, rich in water, that goes to the solvent recuperation column (e). At column (e) the entrainer and ethanol are recovered in the top product and returns to the azeotropic column (c). Water is removed as bottom product.

The specifications established for the products are: 1) mole fraction of ethanol at the bottom of the first tower equal to 0.9999, and 2) mole fraction of water at the bottom of the second tower with less than 50 ppb in benzene. All the organic phase separated in the decanter returns to the top of the azeotropic tower.

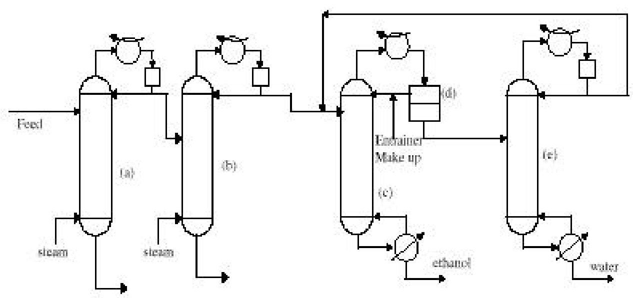

Figure 1 - Flowsheeting for the ethanol dehydration plant by distillation.

It is important to mention that we have got two important results for this problem. The first one is concerned with the high purity of the desired product (0.9999). The another one is the very few concentration of the entrainer, which is a substance extremely toxic (the maxi-mum permitted in the wastewater is 50 ppb; Cusack, 1996). To get these both concentrations, several steps had to be made, including optimization and formulation of new alternatives for configurations of the complete process, to get convergence.

Simulations were performed using the PRO/II Commercial simulator, by Simulation Science, inc. (1993). The thermodynamic model to represent the liquid phase was the NRTL. The algorithm selected to calculate the columns (a), (b) and (e) was the Inside-out and for the azeotropic column (C) it was selected the Naphtali-Sandhoom due to the necessity for representing the liquid-liquid-vapor-equilibrium (VLLE). In the top trays of the column (c) it was used a VLLE method and for the rest of the column it was used the VLE data, to save computational time.

It was desired to obtain the minimum energy consumption, then it was investigated four configurations to obtain the best one for the process. The best one is represented in Figure 1.

Figure 2 shows a configuration with one more column and Figure 3 shows a configuration with a different recycle position.

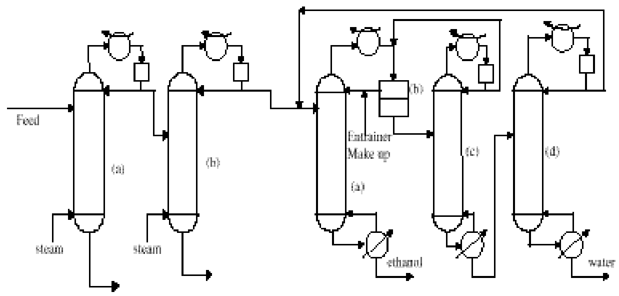

Figure 2 - Configuration 2: three columns sequence.

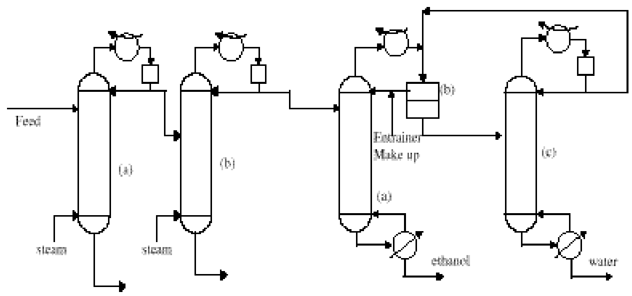

Figure 3 - Configuration 3: recycle position in the decanter, (Kovach e Seider, 1987 e Prokopakise Seider, 1983).

These configurations are always cited in the literature, but in this work, it was verified the best one in terms of energy consumption and in terms of avoiding the formation of two liquid phases in the internal trays of the azeotropic column. It is desired to avoid this due to the reduction on the efficiency of the stages.

This study would be impracticable without simulations using computers and the commercial simulator, because the process is very sensitive to changes in operating and design variables. Furthermore, is too complex and, so, impossible to be explored in pilot plant.

Conclusion

The simulation of a process allows the engineer to evaluate the influence of the variables in the process, to evaluate new configurations and make the optimization.

In the 21st century, the optimization of processes will be an obligatory task due to the economic factors and to the waste minimization, and, in this way, the simulation is a powerful tool.

In the undergraduate course, the introduction of simulation techniques are very important, and it was verified that in the classes where the students were proposed to work with simulation, they have got higher level of knowledge.

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