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Using professional simulation software for better integration in the chemical engineering undergraduate curriculum

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ABSTRACT: Computer simulation has become very user friendly and powerful for the simulation and design of various engineering processes. For example, in chemical engineering, computer simulation packages like *HYSYS*™ have been a very useful tool for different companies throughout the world. In order to produce students who are more proficient in the use of such software, it is proposed that a simulation package is introduced and integrated early in various fundamental chemical engineering courses at second and third year levels, rather than in the final year of study. Efforts are underway at Universiti Kebangsaan Malaysia, Selangor, Malaysia, to introduce and integrate *HYSYS* in fundamental courses. The article presents several case studies involving the use of *HYSYS* in understanding thermodynamics, distillation and heat integration. In using *HYSYS*, more time is spent exposing students to the complexities of a real processing environment, similar to that found in industry. This can be extended to other courses, such as thermodynamics, reactor design, heat transfer equipment and other separation processes. It is also possible to collaborate on a mini project to link up the reaction and separation phases of a chemical plant; this can then act as a prelude to a larger, more elaborate plant design in the final year.

INTRODUCTION

The chemical engineering curriculum at most universities around the world normally consists of courses in basic chemistry, transport phenomena, thermodynamics, unit operations, reactor systems, plant design and advanced chemical engineering. The fundamental and basic courses of transport phenomena, thermodynamics, unit operations and reactor systems are normally taught in the second and third years of a four-year degree programme. These courses are normally taught separately, while a plant design course usually appears only in the fourth year, wherein different aspects of chemical engineering are integrated.

Another feature in teaching these basic courses (and this can be found in many textbooks) is the use of simple systems, such as a binary component, in order to explain and describe the many fundamental principles of chemical engineering. This is undertaken simply because the equations involved are more comprehensible and easier to be solved for simple systems. In teaching the distillation process, for example, students have been taught to design a distillation column using the McCabe-Thiele graphical method, which was introduced almost 80 years ago. This method is quite effective in introducing the fundamentals of distillation design and thus this method is still the only method used in teaching introductory courses in distillation for second year or third year students [1]. However, for many real applications, chemical engineers will face a system that almost certainly includes more than two components.

Based on the authors' experiences at Universiti Kebangsaan Malaysia (UKM), Selangor, Malaysia, one of the shortcomings in the current approach is that students do not think laterally and, as a result, fail to grasp and appreciate the interdependence of these basic courses. This phenomenon was observed when students were undertaking the plant design project in their final year. Plant design is a course whereby students are expected to design a complete plant that produces specific chemicals at a specified production capacity. The design data and specifications were taken based on industrial production. At the same time (in the final year), students were introduced to a professional simulation package, such as *HYSYS*™. *HYSYS* simulation software (from Hyprotech Ltd, Canada) was developed as a complete package to design a chemical plant consisting of various unit operations. Students are able to simulate each unit's operation or combined unit operations, as well as a complete plant, using the *HYSYS* package.

However, this is where the problem lies. Since students have been introduced to a system that is not as simple as what has been taught in the basic courses, they find it difficult to comprehend the complexities of the system and its impact on their design. Furthermore, each sequence of production, ie from raw materials to the reaction system to the separation sequence is dependent on each other. Thus, even though *HYSYS* may be able to churn out a great deal of design numbers, students fail to at least understand qualitatively and appreciate the simulation result.

One of the ways in which it is planned to solve this shortcoming is by integrating the simulation package early on: during the basic courses rather than in the final year of study. Advancements in computer and information technology have enabled computer simulation packages like *HYSYS* to become very sophisticated and user-friendly. Therefore, introducing such a package to students early on should not be a problem. The use of *HYSYS* in an introductory distillation course has been reported previously [2].

In this article, several case studies on the use of *HYSYS* to aid in the learning of several single and combined unit operations

will be discussed. The first case study involves the use of thermodynamic packages in *HYSYS* in order to understand the different equations of state and activity coefficient models. The second case study shows the use of *HYSYS* so as to understand and optimise parameters in a distillation column. The third case study provides some understanding in integrating the heat that is produced within a simple chemical production plant.

In each case study, the authors will discuss how the *HYSYS* aspect can be integrated within the current basic courses. Various ways to incorporate similar simulation elements in other chemical engineering courses will also be discussed. Such incorporation will also enable students to integrate and better understand the various courses within the chemical engineering discipline.

HYSYS SIMULATION SOFTWARE

HYSYS simulation software was developed as a complete package in order to design chemical plants that consist of various unit operations. *HYSYS* uses object-oriented design, together with an event-driven graphical environment, in order to produce a complete interactive simulation environment.

The *HYSYS* environment consists of the basic environment and the simulation environment. The basic environment is used to select the chemical components that are involved in the simulation, as well as the thermodynamic property suitable for the components. If there is a reaction involved in the simulation, the reaction package can be invoked whereby the specific reaction or reactions can be defined.

The simulation environment consists of the worksheet and the Process Flow Diagram (PFD). The worksheet contains the information on every flow and heat stream involved in the simulation. Some of these streams require input while *HYSYS*, depending on the degree of freedom, will calculate the output streams. The PFD will graphically show exactly the unit's operation and the streams that are involved. Students are required only to provide the necessary information for the chosen unit operation in order to be able to design the unit automatically. As a process tool, *HYSYS* is very convenient and user-friendly and is thus very suitable as an introductory tool for students early in their studies.

CASE STUDIES

In the following sections, three case studies are presented to show the powerful features of *HYSYS* and how these can be used in undergraduate teachings.

Thermodynamics

The first case study involves the calculations of bubble and dew points pressures for acetone-chloroform mixture. An acetone-chloroform mixture is considered a far from ideal solution and, as such, the activity coefficients for the liquid phase need to be calculated. Among the activity coefficient models that can be used are the Van Laar model, the Margules model and the UNIQUAC or UNIFAC models. The Van Laar model is the easiest to use, while the UNIQUAC and UNIFAC models require several parameters in order to be used. These parameters are not easily available. Thus, for undergraduate teaching, the Van Laar and Margules models are frequently used (and this is for the binary component only!) [3].

HYSYS can be used to calculate the thermodynamic properties of any mixture of the components. The first step in using *HYSYS* is the selection of the thermodynamic property that accurately reflects the nature of the mixtures. There are eight activity models that can be selected. Once the model has been selected, the user can then select the components of the mixture available in the component page. Once this is done, the user can then enter the simulation environment in which the stream's information will be input.

In this case study, by varying the component fractions and vapour fraction at the selected temperature, *HYSYS* will automatically calculate the dew and bubble pressures. Figure 1 shows the result of the calculations using the Van Laar and UNIQUAC models, as compared to the available published experimental data. As shown in the figure, the UNIQUAC model yields a much better agreement with the experimental data. This is to be expected since the UNIQUAC model is a very sophisticated model that takes into account the physical and chemical nature of the molecules in the mixture.

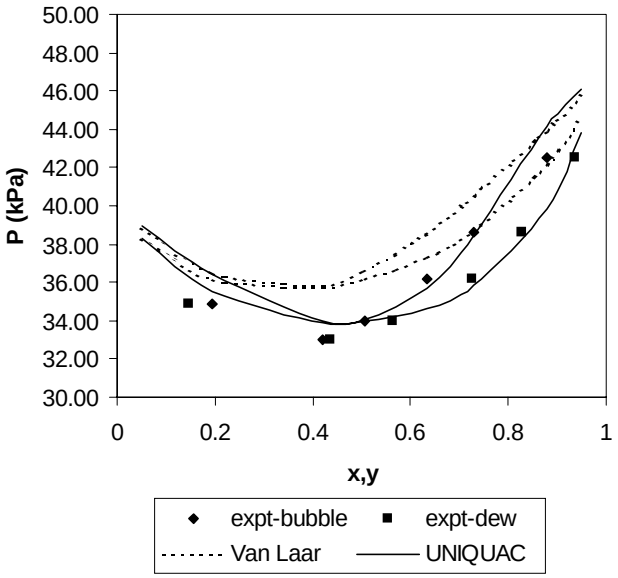

Figure 1: Calculated values of bubble and dew pressures compared to *HYSYS*.

Other various thermodynamic calculations can be undertaken using *HYSYS* for any chemical component and mixtures. What are required are case studies that should complement the abstract theories that are taught in the classroom.

Distillation

For this study, a problem in the textbook by Seader and Henley will be used as a case study in order to show how the *HYSYS* simulation software is used to enhance the understanding of the distillation operation. The problem involves separating methanol from water using a multi-staged distillation column; 100 kmol/h of a mixture of 60 mol% methanol in water at 30^{o}C is to be separated by distillation at the same pressure into a liquid distillate that contains 98 mol% methanol and a bottoms liquid product that contains 96 mol% water. The design problem would be to determine the number of equilibrium stages that are required in order to achieve the separation and to determine the outgoing flow rates, as well as the reboiler and condenser duties.

In order to solve this problem using the McCabe-Thiele method, provided that the reflux ratio has been specified, the equilibrium data has to be plotted and then the top, bottom and feed operating lines can be drawn. The reboiler and condenser heat duties can then be determined using enthalpy data. For the methanol-water system, the enthalpy data are available in many textbooks. However, for many other systems, the enthalpy data are quite difficult to obtain. Now with *HYSYS*, the design solution can be enhanced, for example, by looking at the effect of different reflux ratios.

In distillation, the reflux ratio plays an important role in determining the optimum operation for the distillation column. A minimum reflux can be obtained when the operating lines intersect the equilibrium line, thereby creating a pinch zone. However, at this minimum reflux, the number of stages required to achieve the desired separation is infinite. As the ratio is increased, the number of stages decreases, the column diameter increases and the reboiler steam and condenser cooling water requirements increase. There is an optimal reflux ratio that will minimise the total annualised cost. In the following study using *HYSYS*, students will able to see the interplay of these parameters for simple distillation.

Table 1 shows the simulation result as provided by *HYSYS*. In this simulation, the number of stages has been fixed at 11, with only the distillate composition fixed at 98% methanol. *HYSYS* has been used to determine the reboiler duty (Q_R) and condenser duty (Q_c) as functions of reflux ratio (R). The outgoing flow rates (D and B) and bottom compositions were calculated as well. If one were to do this type of calculation using the McCabe-Thiele method, there would be too many repetitive graphical solutions and calculations required.

As shown in Table 1, as the reflux ratio increases, the heat requirement for the reboiler and condenser also increase. It has been reported that the annual cost of steam for the reboiler is almost eight times that of the cost of condenser cooling water [4]. Thus, the large increase in reboiler duty is not highly recommended. Furthermore, the bottoms compositions are too small (specified 10 mol% methanol), which is really over-specified. This is due to the fixed number of stages used in the simulation.

Table 1: Simulation results for a fixed number of stages using *HYSYS* (N=11).

R	D (kmol/h)	B (kmol/h)	$Q_c x10^{-6}$ (kJ/h)	$Q_R x10^{-6}$ (kJ/h)	x_B (mol%)
1	60.71	39.29	-4.3	+4.75	1.283
1.5	61.21	38.79	-5.42	+5.88	0.037
3	61.22	38.78	-8.68	+9.13	0.011
5	61.22	38.78	-13.0	+13.5	0.011
9	61.22	38.78	-21.7	+22.1	0.011

Students can then investigate whether it is possible to reduce the heat duty and also achieve the necessary separation specification. Simulating the separation in a diverse number of stages can achieve this. Various other operations can be instituted and students should be able to learn the complexities involved in operating a distillation column interactively.

Heat Integration

The last case study involves the simulation of a simple plant for the production of toluene from n-heptane by dehydrogenation over a Cr_2O_3 catalyst. Figure 2 shows the process flow diagram (PFD) of the simulated process. The feed stream is heated up to 800^oF using a super-heater before entering the reactor. The reaction has to take place at 800^oF. The effluent coming out of the reactor is cooled down to 65^oF again by using a heat exchanger before entering the separator.

Based on the simulation, it was found that the heating and cooling duties required by the super-heater and heat exchanger (C-1) was comparable. As such, it was possible to integrate the heat coming out of the reactor to pre-heat the feed stream before entering the super-heater. In this way, the heat load required for the super-heater is reduced and thus minimises the utility costs. Figure 3 shows the PFD of the plant after undertaking the heat integration. The features of *HYSYS* facilitate the changes and variations of the PFD in a very user-friendly manner.

DISCUSSION

All of the three case studies presented above show that *HYSYS* is indeed a powerful and useful software package, which should be utilised early on during students' undergraduate education in order to enhance their learning experience. Problems and case studies should be developed within each course so as to complement the theories that are taught in the classroom.

Based on the authors' experience, the current methods utilised for calculations in chemical engineering courses rely heavily on graphical techniques and shortcut methods, yet these do not represent a real system very well. Most of these methods take some time to solve and, as such, there is not much of a problem variation that can be given within the limited time available.

However, if case studies are developed carefully, *HYSYS* can be used to show and simulate various conditions that represent a *real system*. Lecturers can also introduced Problem-Based Learning (PBL) wherein students can use *HYSYS* to discover the complex nature of what is being taught in the classroom. In this way, students will be more inquisitive and should be able to find out answers to a many questions that may not be covered in textbooks or lecture notes.

Mini Project

Once the case studies are developed for all of the related courses (ie thermodynamics, separation processes, reaction engineering, heat transfer and equipment, etc), it will then be possible for each lecturer to collaborate in order to produce a mini project that will link up the reaction phase and the separation phase of a chemical plant.

It is envisaged that this mini project will be a prelude to a larger and more elaborate plant design course in the final year. In this way, students will be able to integrate the different subjects that are being taught at the introductory level and, hopefully, they will be able to see the relevance of each subject to the working environment of a chemical engineer. To expect students to do this type of integrated project based on the graphical and short cut methods of calculation currently in use is simply impractical in this computer age.

CONCLUSIONS

It has been shown in this article how professional simulation software can and should be introduced to students early in their education process. This will enable them to appreciate many other factors that are involved in the design and operation of a chemical process. Hopefully, with such early exposure, students will be able to appreciate the complexities involved in the real working environment as chemical engineers. Other chemical engineering courses should also incorporate the professional simulation element; then students will be able to integrate other various subjects involved. This will lead to a better understanding of the chemical engineering profession.

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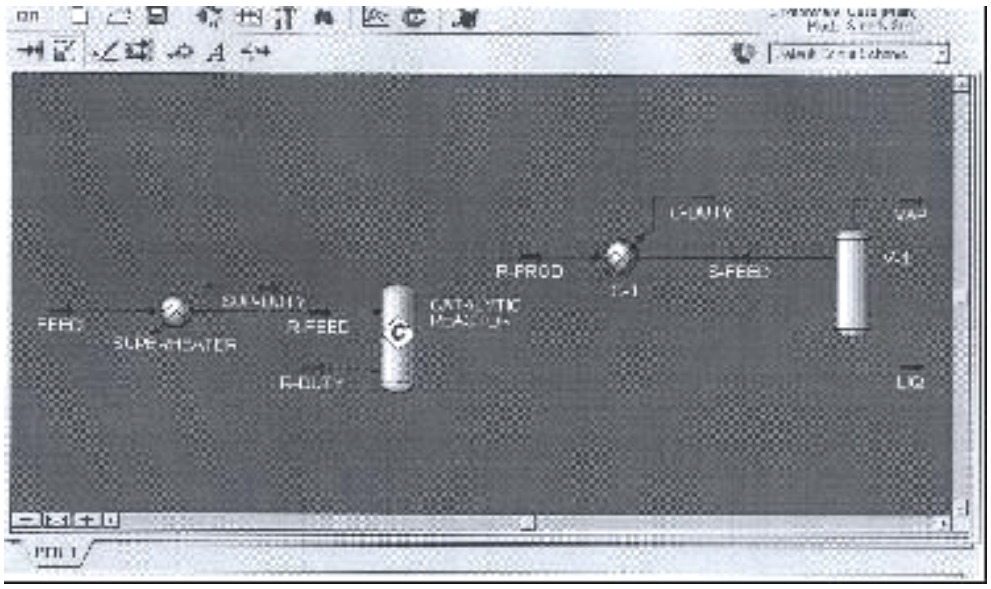

Figure 2: Process flow diagram before heat integration.

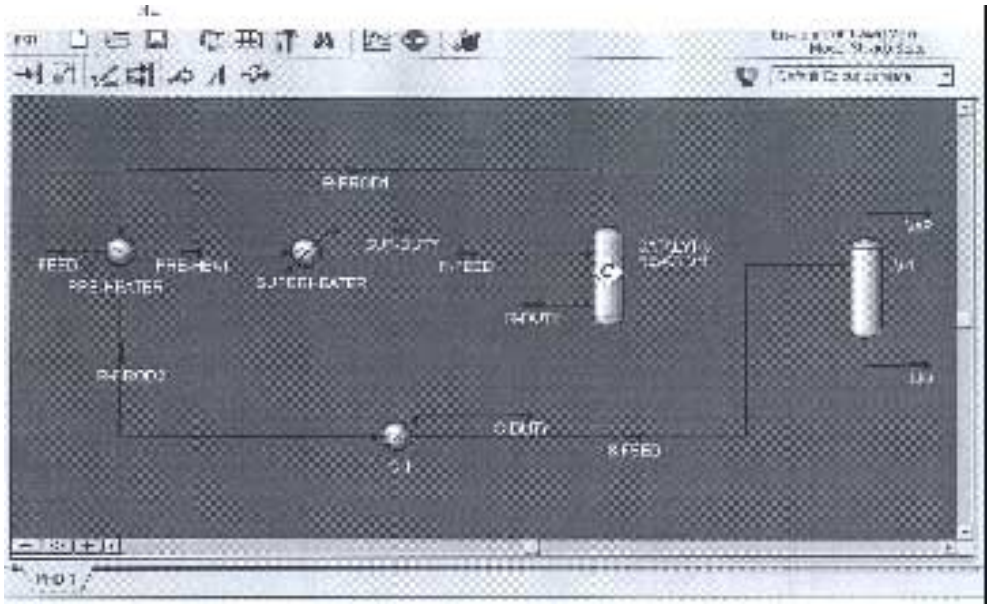

Figure 3: Process flow diagram after heat integration.