IS PROCESS SIMULATION USED EFFECTIVELY IN ChE COURSES?

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Process simulators are becoming basic tools in chemical engineering programs. Senior-level design projects typically involve the use of either a commercial simulator or an academic simulator such as ASPENPLUS, ChemCAD, ChemShare, FLOWTRAN, HYSYS, and ProII w/PROVISION. Many design textbooks now include exercises specifically prepared for a particular simulator. For example, the text by Seider, Seader, and Lewin[1] has examples written for use with ASPENPLUS, HYSYS, GAMS,[2] and DYNAPLUS.[3] Professor Lewin has prepared a new CD-ROM version of this courseware giving interactive self-paced tutorials on the use of HYSYS and ASPEN PLUS throughout the curriculum.[4,5]

This paper will analyze how effective it is to include computing (particularly process simulation) in the chemical engineering curriculum. Among the topics of interest will be vertical integration of process simulation vs. traditional use in the senior design courses, the role of computer programming in the age of sophisticated software packages, and the real pedagogical value of these tools based on industry needs and future technology trends. A course-by-course analysis will present examples of specific methods of effective use of these tools in chemical engineering courses, both from the literature and from the authors' experience.

DISCUSSION

In the past, most chemical engineering programs viewed process simulation as a tool to be taught and used solely in senior design courses. Lately, however, the chemical engineering community has seen a strong movement toward vertical integration of design throughout the curriculum.[6-9] Some of these initiatives are driven by the new ABET criteria.[10] This integration could be highly enhanced by early introduction to process simulation.

Process simulation can also be used in lower-level courses as a pedagogical aid. The thermodynamics and separations areas have a lot to gain from simulation packages. One of the advantages of process simulation software is that it enables the instructor to present information in an inductive manner. For example, in a course on equilibrium staged operations, one concept a student must learn is the optimum feed location. Standard texts such as Wankat[11] present these concepts in a deductive manner. The inductive presentation used at Rowan University is outlined below in the section on equilibrium staged separations.

Some courses in chemical engineering, such as process dynamics and control and process optimization, are computer intensive and can benefit from dynamic process simulators and other software packages. Henson and Zhang[12] present an example problem in which HYSYS.Plant (a commercial dynamic simulator) is used in the process control course. The process features the production of ethylene glycol in a CSTR and purification of the product through distillation. The authors use this simple process to illustrate concepts such as feedback control and open-loop dynamics. Clough[13] presents a good overview of the use of dynamic simulation in teaching plantwide control strategies.

A potential pedagogical drawback to simulation packages such as HYSYS and ASPEN is that it is possible for students to successfully construct and use models without really understanding the physical phenomena within each unit operation. Clough emphasizes the difference between "students using vs. students creating simulations." Care must be taken to insure that simulation enhances student understanding, rather than simply providing a crutch that allows them to solve

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problems with only a surface understanding of the processes they are modeling. This concern about process simulators motivated development of the phenomenological modeling package ModelLA.[14] This package allows the user to declare what physical and chemical phenomena are operative in a process or part of a process. Examples include choosing a specific model for the finite rate of interphase transport or the species behavior of multiphase equilibrium situations. One uses engineering science in a user-selected hierarchical sequence of modeling decisions. The focus is on physical and chemical phenomena, and equations are derived by the software.

Despite these concerns, the survey results discussed in the next section indicate that HYSYS, ASPEN, and ProII remain the primary simulation packages currently in use.

SURVEY: COMPUTER USE IN CHEMICAL PROCESS SIMULATION

In 1996, CACHE conducted a study discussing the role of computers in chemical engineering education and practice. The study surveyed both faculty members and practicing engineers, but little emphasis was placed on the specific use of process simulation. To fill this gap and obtain up-to-date results, a survey on computer use in the chemical engineering curriculum was distributed to U.S. chemical engineering department heads in the spring of 2001. It addressed how extensively simulation software is used in the curriculum, as well as motivation for its use. The use of mathematical software and computer programming was also examined. A total of 84 responses was received, making the response rate approximately 48%. Tables 1-7 summarize the results. The wording of questions and responses in the tables is taken verbatim from the survey. The survey also provided a space for written comments and some of these are presented throughout this paper.

In a 1996 publication that discussed the results of the CACHE survey, Kantor and Edgar[15] observed that computing was generally accepted as an integral component of teaching design, but that it had not significantly permeated the rest of the curriculum. The survey results suggest that this perception is outdated. Table 1 shows that only 20% of departments reported that process simulation software is used exclusively in the design course, and Tables 2 and 3 show that it is particularly prevalent in the teaching of equilibrium staged separations, process control, and thermodynamics. It must be noted, however, that the survey did not ask respondents to quantify the extent of use; a "yes" response could indicate as little as a single exercise conducted using a simulator.

Table 1 also indicates that over one-fourth of the responding departments felt that their faculty have "an overall, uniformly applied strategy for teaching simulation to their students that starts early in the program and continues in subsequent courses." Many other respondents acknowledged the merit of such a plan but cited interpersonal obstacles, with comments such as

> *With each faculty member having their own pet piece of software, it's tough to come to a consensus.*
>
> *Not many faculty use ASPEN in their courses because they haven't learned it, think it will take too much time to learn, and aren't motivated to do so.*
>
> *I would like to see the use of flowsheet simulators expanded to other courses in our curriculum but haven't been able to talk anybody else into it yet.*

At Rowan University, the incorporation of mini-modules (described further in the next section) into sophomore-and-junior-level courses has proved to be an effective solution to this problem. They require only limited knowledge of the simulation package on the part of the instructor because they employ models that contain only a single unit operation.

Table 4 (next page) summarizes the responses to a question on motivation for using simulation software. Four options were given, and the respondent was asked to check all that apply. The most common choice was "It's a tool that graduating chemical engineers should be familiar with, and is thus taught for its own sake." A total of 83% of the respondents selected this option, and in 15% of the responses it was the *only* one chosen.

TABLE 1
Responses to:
"Which of these best describes your department's use of process simulation software?"

Response	*% Yes*
☐ The faculty has an overall, uniformly applied strategy for teaching simulation to their students that starts early in the program and continues in subsequent courses.	27%
☐ There is some coordination between individual faculty members, but the department as a whole has not adopted a curriculum-wide strategy.	35%
☐ Several instructors use it at their discretion, but there is little or no coordination.	18%
☐ Only the design instructor requires the use of chemical process simulation software.	20%
☐ No professor currently requires simulation in undergraduate courses.	1%

TABLE 2
Responses to:
"Please indicate the courses in which professors require the use of steady-state chemical process simulation programs."

Course	*% Yes*
☐ Design I and/or II	94%
☐ Process Safety	4%
☐ Process Dynamics and Control	10%
☐ Unit Operations	31%
☐ Equilibrium Staged Separations	57%
☐ Chemical Reaction Engineering	19%
☐ ChE Thermodynamics	36%
☐ Fluid Mechanics	7%
☐ Heat Transfer	13%
☐ Chemical Principles	29%

TABLE 3
Responses to:
"Please indicate the courses in which professors require the use of dynamic chemical process simulation programs."

Course	*% Yes*
☐ Design I and/or II	12%
☐ Process Dynamics and Control	52%

In their 1996 study of computer skills in chemical engineering, Kantor and Edgar[14] analyzed survey results from both faculty and practicing engineers, finding that faculty tended to drastically underestimate time spent at the computer by practicing engineers in industry. The main software tools they used, however, did not include simulators; they were spreadsheets (74%), graphics presentation packages (80%), database systems (70%), and electronic communications (89%). Indeed, many engineers will not even have access to process simulators.

Our department collaborates with many small companies and has found that they use self-made Excel macros to solve problems that are readily solved with commercial simulators, simply because they cannot afford the software. These observations certainly do not invalidate the opinion that process simulation software is "a tool that graduating chemical engineers should be familiar with." They do, however, suggest that a department would do well to examine how much time it is spending on activities designed to familiarize the student with simulation software while serving no other purpose.

Another finding presented in the 1996 study by Kantor and Edgar was that computer programming (in languages such as FORTRAN, C, or PASCAL) is not a vital skill for chemical engineers in industry. Indeed, "many companies explicitly tell their engineers *not* to write software because of the difficulty of maintaining such programs written by individuals." Courses on computer programming appear to remain a staple of undergraduate programs. Table 5 shows that 83% of the respondents require a computer-programming course (taught by either computer science or engineering faculty) and 45% require programming in "several" subsequent courses. There is a shift away from teaching traditional computer programming, however. A total of 17% of the respondents indicated that their curriculum no longer contains computer programming at all, with a number of them mentioning that programming had been recently phased out. Many other respondents indicated that the programming present in their curriculum does not employ traditional languages such as C or FORTRAN, but instead uses higher-level programming environments such as Maple. Example comments are

> *Our situation is that we teach a course that introduces students to Excel and Maple. Maple is the programming tool. They are not required to program thereafter, but many of them choose to do so in later courses.*
>
> *We dropped our programming course last year, because simulation packages (as well as general equation solvers, spreadsheets, etc.) were becoming so powerful that it was becoming much less important to know how to program and more important to know how to configure/use existing packages.*
>
> *Our undergraduate students no longer take a computer programming course, per se. Instead, they learn and make extensive use of packaged software (*e.g., *Matlab) in an integrated freshman sequence on engineering analysis. Subsequent classes draw upon this experience.*

This is a trend that may well continue to grow. The CACHE survey indicates that 5% of respondents said it "is not important" to teach computer programming to undergrads, and 57% thought it was "becoming less important." In addition, the current ABET Chemical Engineering criteria[16] requires that graduates have a knowledge of "appropriate modern experimental and computing techniques" but does not specifically mention programming as it did in the past.

Two respondents identify one potential drawback to this shift away from traditional computer programming. They emphasize the importance of the logic and problem-solving skills that programming experience stimulates, even if the ability to program in itself is unnecessary for chemical engineers. The specific comments were

> *We dropped our programming course a number of years ago as the capabilities of the various software packages increased to the point where programming input from the user became insignificant. We're now seeing a drop in the logical approach to problem solving in our students that we feel is related to this lack of exposure to programming. As the software becomes more powerful, however, hit-or-miss or brute-force techniques work so is there really a need for a more reasoned approach to problem solving?*
>
> *Although programming languages (FORTRAN) are in some disfavor at present and probably will pass from the scene, I find that students develop an increased ability for the logic of solutions and of thinking about problems when they learn a language... I find that students can use programs such as POLYMATH, etc. with a great deal more understanding and efficiency once they have learned a language.*

The chemical engineering community thus may have a use for teaching tools and techniques that challenge students to think logically and develop algorithms without necessarily taking the time to learn a full programming language. One option is template-based programming as developed by Silverstein.[17]

TABLE 4

Responses to:

"Which of the following best describes your motivation to use simulation packages? Please check all that apply."

Response	*% Yes*
☐ It helps to illustrate essential chemical engineering concepts.	64%
☐ It makes numerical computations less time consuming.	70%
☐ The modernity is good for attracting and retaining students.	30%
☐ It's a tool that graduating chemical engineers should be familiar with, and is thus taught for its own sake.	83%

TABLE 5

Responses to:

"Which of the following best describes your department's use of computer programming languages?"

Response	*% Yes*
☐ One required course taught by computer science and no programming required in subsequent chemical engineering courses.	13%
☐ One required course taught by chemical engineering and no programming required in subsequent chemical engineering courses.	11%
☐ After students take the required programming course, they are required to program in one subsequent ChE course.	7%
☐ After students take the required programming course, they are required to program in several subsequent ChE courses.	45%
☐ Students are required to program in upper level chemical engineering courses without having taken a formal programming course.	8%
☐ None of the above selected.	16%

EXAMPLES OF CHEMICAL PROCESS SIMULATORS IN CHEMICAL ENGINEERING

In this section of the paper we give some practical ideas on how to effectively implement chemical process simulators into courses other than the capstone design course.

Freshman Engineering

At Rowan University, an inductive approach has been used to introduce freshmen and sophomores to chemical process simulators. The methodology used was

- Show the students a heat exchanger. This can be either a laboratory unit or part of a cogeneration plant.[18] The students are asked to record their observations of fluid flowrate and temperatures.
- Next, have the students start a process simulator and put these experimental results into a simple heat-exchange unit operation of a process simulator to determine the heat duty.
- Finally, have the students conduct an energy balance by hand on the system. In this manner the students have first seen the equipment and then modeled it using a simulator on hand calculations. This helps to familiarize them with what a simulator actually does and what sort of problem can be tackled with simulation.

Chemical Principles or Stoichiometry

In many programs with vertical integration of design throughout the curriculum, the design project starts in this typically sophomore-level course. Many project examples can be found in the literature. Bailie, *et al.*, [19] proposed a design experience for the sophomore and junior years. In the first semester of the sophomore year, the students are given a single chemical design project, and they focus on material balances and simple economic evaluations such as raw material cost and the products' selling prices. Throughout the sequence, the students must apply newly acquired knowledge to improve and optimize the process. The ultimate goal is to produce a fully sized and optimized design, including the analysis of the capital and operating costs by the end of the junior year. This approach is comparable to problem-based learning.[20] There have been other contributions to this vertical approach.[21-23] In the above work it is unclear how process simulators are being used and it is not mentioned if the simulators are used in the early stages of integration. Process simulators certainly can be used for such problems, however, since they provide an efficient way to evaluate many variations on a single design concept.

TABLE 6

Responses to:

"Indicate the mathematical applications software required of chemical engineering undergraduates. Check all that apply."

Response	*% Yes*
☐ POLYMATH[40]	37%
☐ MATLAB	65%
☐ Maple	24%
☐ MathCAD	37%
☐ EZ-Solve	5%
☐ Spreadsheets	82%
☐ Mathematica	13%
☐ Other	15%

TABLE 7

Responses to:

"Please indicate all applicable steady-state Chemical Process Simulation programs currently being used in your department's undergraduate courses. Check all that apply."

Response	*% Yes*
☐ ProII/Provision	12%
☐ HYSYS or Hysim	32%
☐ Aspen Plus	45%
☐ ChemCAD	32%
☐ Other	13%

Chemical Principles—Energy Balances

In Felder and Rousseau[24] (a standard text for this course), the chapter on multiphase systems introduces the concepts of bubble and dew points. An inductive method of teaching these concepts is to start with an experiment on a binary system, using a 1L distillation unit or an interactive computer module[25] with a visual examination of the bubble and dewpoint. These methods result in the students examing their data by using a binary T-x-y diagram. The next step is to use the process simulator to predict bubble and dewpoints for binary and multicomponent systems. In using HYSYS, the dewpoint temperature is automatically calculated after specifying the vapor fraction as 1.0 (dewpoint), the compositions, and pressure in a single stream. The calculations for multicomponent systems are usually reserved for an equilibrium staged operations course.

In new editions of many textbooks for the chemical process principles course there are chapters on process simulation.[24-26] They give examples with solutions done by calculators, Excel spreadsheets, and FORTRAN. This gives the students an excellent reference on how a system of equations is used by chemical process simulators. In section 10.4 of Felder & Rousseau, commercial process-simulation packages are discussed, but no examples are given. The last problem in the chapter suggests, however, that any of the other fourteen homework problems could be solved by a chemical process simulator. This could be another starting point for introducing commercial process simulators in this course.

Equilibrium Staged Operations

In teaching distillation, the standard modeling approach is to use the McCabe-Thiele graphical method. This is an excellent tool for introducing students to binary distillation problems. Before extensive use of the computer became feasible, the next step was to add the energy balance and use the Ponchon-Savarit method. Many professors no longer teach this method, using the simulator instead. This decreasing use of Ponchon-Savarit has been promoted by Wankat, *et al.*,[27] and recently published textbook descriptions of the method have been shortened.[28]

Using simulators throughout the curriculum requires that faculty have knowledge of the simulator that the students are using. In the discussion of the survey results, there were concerns about the faculty time and motivation required to be come proficient in using a simulator. One possible solution is to implement mini-modules of the type used at Rowan University. In equilibrium staged operations, a student must learn the optimum feed location and the improved separation resulting from increasing reflux ratio for a given number of stages; in an approach that has been used at Rowan University

- *The instructor prepares a complete HYSYS model of a distillation column and distributes it to the class.*
- *The class receives a brief (less than five minutes) tutorial on modeling columns with HYSYS—just enough to tell them how to change specific parameters such as the reflux ratio and where to locate the resulting stream compositions and other output parameters of interest.*
- *The students take a column through a series of configurations, varying the reflux ratio, number of stages, and feed stage location, and then answers a series of questions about the results. The students are thus introduced to concepts in an inductive manner.*
- *Subsequent classroom instruction further examines the "whys" of the results. This is used as a starting point in deductive derivation of the McCabe-Thiele model.*

Mini-modules analogous to this have been integrated throughout the course, as well as in thermodynamics and principles of chemical processes. The primary purpose of the modules is that the HYSIS model provides a time-efficient and effective way for students to examine the cause-effect relationships among column operational parameters. The modules also serve a curricular purpose in that they begin to introduce process simulation. This is accomplished with a minimal requirement of faculty time. It is not necessary for professors to learn all aspects of the simulation package; they merely need to learn how to model one particular unit operation.

Other forms of mini-modules have been proposed where students learn the process simulator in self-paced tutorials.[1,4] The proposal is that these modules be given to the students—the professor does not need to prepare time-consuming tutorials and may not need to learn how to use the simulator. Another paper by Chittur[29] discusses preparing tutorials for ASPEN Plus simulators using HTML. Finally, the University of Florida maintains a web site for ASPEN where tutorials are available.[30]

Chemical Engineering Thermodynamics

Judging from the survey results, it seems that process simulators are now widely used in thermodynamics (see Table 2). This is fertile ground for a pedagogical use of the process simulators, and the first thing a new user of a simulator faces is the variety of thermodynamics packages that are available. The new user will quickly learn that an incorrect choice of a thermodynamic model will yield meaningless results regardless of the convergence of the simulation case. Unfortunately, there are so many thermodynamics models in commercial simulators that it is impossible to educate our students in each one of them. Elliott and Lira[31] present a decision tree for the proper selection of the thermodynamic model.

Traditionally, students are taught how to perform equilibrium and properties calculations by hand or, in the best scenario, with the aid of custom-made software programs for hand calculators or computers. The increasing influence of process simulators opens up a completely new spectrum of possibilities. Since simulation results are only as good as the thermodynamic package chosen, there is value in teaching the fundamental aspects that will permit students to pick the right thermodynamic package for a system. Simulators also offer the advantages of combining thermodynamic models in the same simulation and picking different models for certain properties within the overall process model; PRO II with Provision is very versatile in this respect. For instance, an equation of state such as Soave-Redlich-Kwong (SRK) is chosen as the overall simulation package, but it is modified so liquid density is calculated using the American Petroleum Institute (API) equation.

In many cases, professors have been taught thermodynamics using earlier versions of Sandler[32] and Smith and Van Ness,[33] which did not emphasize predictions of thermodynamic properties based on an equation of state. More recent versions of both texts and new texts such as Elliott and Lira now contain at least one chapter devoted to predicting thermodynamic properties from other equations of state. One of the fundamental aspects of a modern chemical thermodynamics course is not only to teach students how to use these equations, but also which equation of state they should select for a particular problem. An example of the prediction of the enthalpy of a single component where values of the correlating parameters of a=f(T) and b are from the Peng-Robinson equation of state is

$$\frac{\left(H - H^{ig}\right)}{RT} = Z - 1 - \ell n\left[\frac{Z + \left(1 + \sqrt{2}\right)B}{Z + \left(1 - \sqrt{2}\right)B}\right]\frac{A}{B\sqrt{8}}\left[1 + \frac{\kappa\sqrt{T_r}}{\sqrt{\alpha}}\right]$$

where $B \equiv bP/RT$ and $A \equiv aP/(RT)^2$

From the above equations it is easily seen how complicated these predictions can become compared to a table or a graph in a standard handbook.[34,35] Many recent thermodynamic textbooks have included computer programs that allow the reader to use various equations of state to solve homework problems. The drawback of these programs is that a student will only use them for the thermodynamics course. Instead of using these textbook computer programs, a professor can encourage use of the thermodynamic packages contained in the chemical process simulators. In this manner, the students can become familiar with the available options in the various simulators.

Chemical Reaction Engineering

In the current chemical reaction engineering course, most students are familiar with ODE solvers found in POLYMATH or MatLab. The philosophy given by Fogler[36] is to have the students use the mole, momentum, and energy balances appropriate for a given reactor type. In this manner a fairly detailed model of industrial reactors can be developed for design projects.[37] By using POLYMATH or MatLab, a student can easily see the equations used to model the reactor. In modern process simulators there are several reactors that can be used. For example, in HYSYS 2.2 there are the two ideal reactor models of a CSTR and a PFR. The CSTR model is a standard algebraic model that has been in simulation packages for a number of years. The ODE's of the PFR are a recent addition to simulation packages and are solved by dividing the volume into small segments and then finding a sequential solution for each volume element. In these more recent models, the reactors not only include energy balances, but pressure drop calculations are also a standard feature for packed-bed reactors.

With the above set of reactions, chemical reaction engineering courses can easily use the process simulator. Simulation can be integrated throughout the course and used in parallel with the textbook, or it can be introduced in the latter stages of the course, after the students have developed proficiency in modeling these processes by hand. As mentioned in the discussion section, the primary dilemma is how to insure that the simulator is used to help teach the material rather than simply giving students a way to complete the assignment without learning the material. Taking care that assignments require synthesis, analysis, and evaluation in addition to simple reporting of numerical results will help in this regard. Requiring that students do calculations by hand will ensure that they understand what the simulator is actually doing. The professor can select chemical compounds that are not in the simulator database to ensure that these are done by hand.

Rate-Based Separations

An example of an integrated approach to teaching rate-based separations with design is given by Lewin, Seider, and Seader (1998).[38] In this paper the authors state that while design courses fully use advances in modern computing through the process simulators, many other courses in the curriculum still use methods employed over sixty years ago. Many modern computing methods are visual and are thus very useful in teaching chemical engineering concepts. The authors suggest that professors who teach junior course(s) in separations, equilibrium-stage operations, rate-based operations, and/or mass transfer consider including

- *Approximate methods (Fenske-Underwood-Gililand and Kremser algebraic method)*
- *Rigorous multicomponent*
- *Enhanced distillation using triangular diagrams*
- *Rate-based methods contained in the ChemLSep program and the RATEFRAC program of Aspen Plus*
- *Adsorption, ion exchange, chromatography*
- *Membrane separations*

which are similar to Chapters 9 through 12 in the new Seader and Henley text.[28]

One major drawback in current process simulators is a lack of standard unit operations for membrane and other novel separators. This can be partially addressed by importing programs into the process simulators. For example, on the HYSYS web site, an extension program can be downloaded for a membrane separator and other operations.[39] As simulators develop, we believe that more unit operations will become available.

CONCLUSIONS

Chemical process simulation is currently underused in the chemical engineering curriculum at many schools. According to survey results, process simulators are used in essentially all design courses and are also heavily used in equilibrium stage operations, primarily with respect to multicomponent distillation. But many respondents acknowledge that the role of simulators could be beneficially expanded in their curriculum. Process-simulation designers can make their products more valuable to chemical engineering educators by adding new and innovative unit operations while they continue to improve their thermodynamic models.

TABLE 8

Reaction Type	***Description***
Conversion	$F_i = F_{i0} - F_{A0} X_A$
Equilibrium	$K_{eq} = f(T)$; equilibrium-based on reaction stoichiometry; K_{eq} predicted or specified.
Gibbs	minimization of Gibbs free energy of all components
Kinetic	$r_A = -k_f C_A^\alpha C_B^\beta + k_{rev} C_R^\phi C_S^\gamma$ where the reverse rate parameters must be thermodynamically consistent and rate constants are given by $k = AT^n \exp(-E / RT)$
Heterogeneous Catalytic	Yang and Hougen form, which includes Langmuir-Hinshelwood, Eley-Rideal and Mars-van Krevelen, etc. $-r_A = \dfrac{k\left(C_A^a C_B^b - \dfrac{C_R^r C_S^s}{K}\right)}{1 + \sum K_i C_i^{y_i}}$
Simple Rate	$r_A = -k_f \left(C_A^\alpha C_B^\beta - \dfrac{C_R^\phi C_S^\gamma}{K_{eq}}\right)$ in which K_{eq} is predicted from equilibrium data

This paper contains practical suggestions and references for implementing a unified strategy for teaching simulation to their students, starting early in the program and continuing in subsequent courses. We believe that simulation packages are a fundamental tool for the future chemical engineer.

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