Process Simulation in Chemical Engineering Design: A Potential Impediment to, Instead of Catalyst for, Meeting Course Objectives

Colin S. Howat
Kurata Thermodynamics Laboratory
Department of Chemical & Petroleum Engineering
University of Kansas
Lawrence, Kansas 66045-2223 USA
cshowat@ukans.edu

Capstone Design is creativity -- synthesis and evaluation.
It is focuses on developing the confidence to practice.
Any interference that detracts from this should be rooted out and discarded.

Abstract

Chemical engineering design course objectives must focus on process synthesis and evaluation, specification identification and evaluation, solution estimation and information ambiguities. These should be met while reviewing fundamentals and problem solving methodology. The effectiveness of the structure of the University of Kansas Capstone Design course is evident by the number of awards that students have won in the only long-term measure of design performance, the AIChE National Student Design Competition.

Process simulation software usage is a necessary tool in professional practice. While students should be exposed to this software, the myriad of options and the ethereal ease of use pose a Sirenic temptation to students. Student use is deceptively inefficient and unproductive despite the apparent proliferation of work product embodied in software output. This inefficiency increases the likelihood that the course objectives are not met.

The competing goals of meeting course objectives and using process simulation software can only be met if the course objectives remain paramount, the software takes its proper role as a mere tool and the students are taught to use it in this context. This paper provides a synergistic integration of software into chemical engineering capstone design. Recommended practice guidelines are proposed.

Introduction

ABET requires integration of computing across the curriculum, a reasonable requirement given the engineering environment. The explicit purpose is to improve the breadth of student skills and the implicit is to enhance their learning of chemical engineering. The proliferation of software presents a challenging obstacle to determining what should and shouldn't be included. Applications including word-processing, graphics, statistics, numerical methods, spreadsheets, data bases, programming, CAD and process simulation are some of the categories from which an instructor can choose. Deciding among alternatives in a specific application adds further complication. A coherent policy is as imperative as syllabi control is.

Consider process simulation software. Even with a policy established and software selected, students face a myriad of single application options having romantic appeal to faculty and curious appeal to students. Ease of use and a student reluctance to embrace manual calculation result in excursions from the task at hand and a loss of focus on the chemical engineering fundamentals. Restraints imposed by the instructor or self-imposed by the students may reduce student excursions, but it is difficult to determine *a priori* which might be seductive. Simulation software cannot be merely appended to capstone design without the expectation that the course objectives will not be met.

This paper discusses the evolution of process simulation applications in design starting from a stand-alone distillation program through limited option process simulation to a commercially available simulation package. When a commercial simulation package was introduced, the course structure had to change to refocus student effort on the objectives.

The paper presents a synergistic approach to the integration of simulation software and chemical engineering design. This approach has improved student performance, has kept them engaged in chemical engineering, has reduced student excursions and has reduced student workload. The approach increases productivity and success in meeting the course objectives.

Impediments to Effective Capstone Design

Howat[3] discusses the principal impediments to effective design instruction for those experienced in design applications. These are shown in Figure 1. Swift and Howat[4] discuss the student preparation arriving at design. Howat[2] discusses effective problem solving methodology in design instruction. Howat[3] discusses the effective tiered-approach to teaching design. This paper is a derivative of Howat[2] wherein he discusses computer simulation experiences.

Students come to design with poor problem solving skills. Without these, the practice of synthesis and evaluation and specification identification, selection and evaluation in the uncertain, ambiguous arena of design is problematic. The process simulator is merely a tool. If it becomes the principal aspect of design, student performance drops because of loss of focus. Effective design methodologies such as an evolutionary or tiered approach are required. Without this, students follow the Sirens of optimization without understanding process fundamentals and without recognizing the role of synthesis and evaluation in developing the design path.

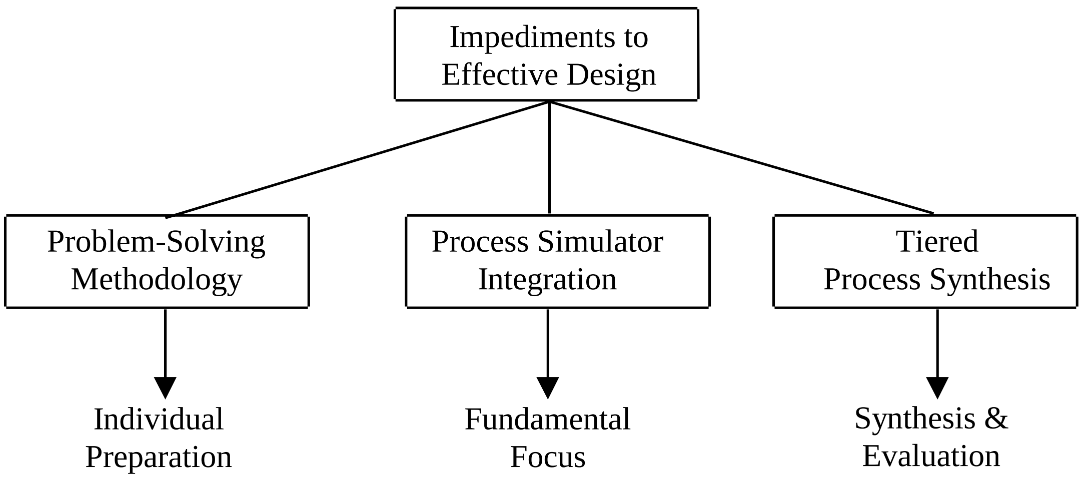

Figure 1: Principal Impediments to Effective Design Instruction

Qualifications

The only long-term national measure of student performance in design is the AIChE National Student Design Competition. Since 1984 when this instructor began teaching design at the University of Kansas, students from KU have won more national awards than students from any other institution have won. While this record is certainly a testimony to student talent and while this measure has been diluted recently because of AIChE actions, it is indicative of the effectiveness of the KU design experience. The history of KU performance is given in Table 1.

Objectives

Howat[1] discusses the principal chemical engineering design course objectives. They are listed in Table 2. Any modifications to design should be dedicated to enhancing the probability that students will meet the objectives. Any modifications, which detract from meeting these objectives, should be reconsidered.

Table 1
University of Kansas Performance
In the
AIChE National Student Design Contest

Student	Award	Year
Russ Berland	Second Place	1984
Richard Kuckleman	First Place	1985
Richard MacDonald	Third Place	1985
Diane Jobson	First Place	1986
Nancy Roberts	Honorable Mention	1986
Curtis Stubbings	Third Place	1989
Cathy Zartman	Second Place	1993
Jennifer Collins	Second Place	1995
Mark Stover	First Place	1996
Robert Babst	First Place	1997

Table 1
Principal Objectives of Chemical Engineering Design

1. *Students must experience the creation process of design and be able to apply it to synthesize and evaluate solutions to significant integrated problems.*
2. *Students must recognize the need for, select values for and evaluate the impact of the specifications inherent in a process subject to process and project constraints.*
3. *Students must develop the confidence to begin the creation of a solution to a problem even though the solution path is unknown and to use the discoveries along the path to continue the development.*
4. *Students must be able to develop solutions without extensive computational support.*
5. *Students must develop the confidence to work with the ambiguity of chemical engineering information and the uncertainty in their solutions.*
6. *Students must review the content of the chemical engineering curriculum reinforcing the foundation of their knowledge.*
7. *Students must recognize the need for, develop and practice problem-solution strategies that are appropriate for the practice of synthesis and evaluation in the context of chemical engineering design.*

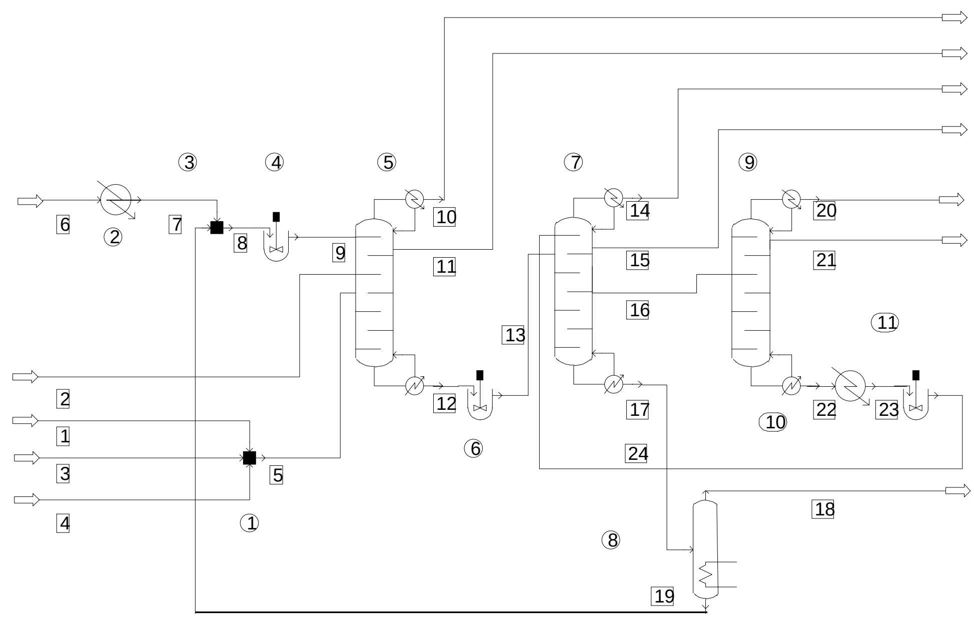

Figure 2: Sample Senior Design Flowsheet

Flowsheet Example

Figure 2 presents a sample flowsheet which students would be expected to synthesize, specify, evaluate and optimize. It consists principally of three distillation columns and three reactors. There are associated mixers, dividers and component separators, as well. While this flowsheet can be developed and completed by hand, effective use of the simulator can save students significant time -- if they focus on the engineering and not the simulation.

However, simulator use typically requires a significant increase in student time required to solve the problem. Improper use losses the potential advantages gained by being free from the distraction of redundant calculations. While it is important to recognize that students use the simulator improperly, it is more important to recognize that the instructor improperly integrated it into design when students deviate from good practice. Meeting course objectives requires that the instructor modify his/her approach to the use of the process simulator.

Horizons

The integration of process simulation software into design has the potential to improve the likelihood that objectives 1, 2 and 5 will be met. Synthesis and evaluation can be improved if some of the repetitive, less significant calculations are done automatically. Evaluation of the impact of specifications on other units in addition to the one under study is more easily accomplished if the simulation models of the equipment are integrated. Appreciating and evaluating the significance of the ambiguity of chemical engineering information is more easily accomplished if the information can be readily substituted into the design and calculation bases and the impact evaluated.

However, the use of the process simulator is Sirenic, precisely because of its ease of use.

- It takes significantly less mental effort to arbitrarily modify a specification and have the simulator perform the calculations than it does to:
  → Think about the engineering significance of why constraints are not met;
  → Anticipate the impact of each specification change on the constraint; and,
  → Do the simulation to confirm the above.

- It takes significantly less work to use the library database without evaluating the accuracy or precision of the parameters than it does to:
  → Go to the library to collect primary data;
  → Evaluate those data for suitability within the context of the design;
  → Develop a suitable database of parameters to describe those data; and,
  → Store the resultant data analysis in the simulator files.

- It takes significantly less effort to alter the database specifications until a design constraint closes than it does to:
  → Evaluate the potential database specification selections;
  → Select the one that most properly represents the system;
  → Evaluate the set of process specifications that causes nonclosure;
  → Choose the one that will have the greatest impact;
  → Simulate the unit again; and,
  → Develop an understanding of why the unit is deficient.

- It takes significantly less effort to continually press ↵ than it does to:
  → Make sound engineering estimates; and,
  → Simulate the unit once to confirm the estimate.

- It takes significantly less effort to follow poor habits developed earlier than it does to:
  → Develop sound engineering skills.

The significance of the downside is not fully understood even by those who profess that simulators must be included. For example, the 1996 AIChE Student Design Contest First Place Group Award was given to a group who used the default database in a well-known process simulator. While the topology of the simulated flowsheet was elegant, that database is incorrect, the subsequent design was incorrect and the process would not work had it been built. The 1997 First Place Group Award was another elegantly simulated process, but the group handled water improperly suggesting that it appeared in the bottoms instead of overhead, a significant error.

The allure of the significant process simulation work may have been more important than the integrity of the underlying design.

The potential reward for integrating a process simulator into the capstone design class is significant. But the downside is so alluring to students and faculty that extreme care and forethought are required before it is included in the curriculum.

Process Simulation Timeline

Design History

Process design was originally done by a select few. Any change in design would require review and approval by those individuals. Through extensive experience and appropriate self-developed rules-of-thumb, they had developed a mental ‘model’ of the process. Design control was in the hands of centralized experts.

Simulation History

Once computers became sufficiently powerful, software was developed to model parts of processes. The software was not robust and the computers were centralized. Consequently, the control was still in the hands of the expert designers.

Most simulators were written ‘in-house’. Few simulation packages were available. Simulation Sciences 100 was available but geared toward refinery operations. The time that was required to complete a simulation meant that few were run. An engineer had to ensure that he/she was right given the slow turnaround implying that the simulator was used to confirm the engineer’s estimated performance.

The energy crises spawned significant research in improving modeling. Coincident with the research developments was the substantial increase in computing power.

The era of centralized control and understanding came to end. Distributed computing, robust modeling and enhanced computing power combined together on the desktop. The number of individuals to whom process simulation was possible increased. These engineers were still trained in the era of estimation and confirmation. There was no great impact, at first, on the quality of the simulation work.

Now, engineers are trained using software from their engineering infancy. Estimation, failure and re-estimation are becoming a lost art form. The power of the computing and software tools available is such that what once took overnight now takes seconds. Aggressive marketing has made simulation software available to all. The impact is that designs are being proposed which will not work. Improper modeling of processes has resulted in improper control and operating decisions. Proper integration of simulation into the curriculum with specific emphasis in capstone design is required.

University of Kansas History

In 1983, KU did not have and could not afford a commercially available process simulator. The mainframe system was not compatible with FLOWTRAN without significant effort. An 'in-house' simulator was written and incorporated into the design class. This was a modular simulator including most of the principal process steps. The interpretative language allowed students to modify the code as necessary to meet their particular goals. Because it was modular, only those modules that were a benefit to the students were released. The organization of the class, experience gained by the students and the restricted software support melded into a successful learning experience.

Courses must evolve to use new tools, to try new teaching methods and to modify the syllabus. In 1990, the Department Chair mandated that a commercial process simulator was to be included into design. Through the initial generosity of two of our alumni and an attractive contract, KU could afford a simulator. Chemcad was selected because of its interface. The software was merely substituted into design for the 'in-house' simulator. Design performance plummeted.

This was unexpected and very troublesome. Clarity of thought became clouded. Students seemed to have lost insight as to the relationship between specifications and outcome. Computer usage substantially increased. The work product was poorer. While these observations may not have been entirely due to the inclusion of the simulator and to the failure to change other aspects of design to accommodate it, part of them were.

Perhaps the most telling effect of the use of the computer is the amount of time spent on the contest problem. Figure 3 presents a summary. The contest problem had been designed for 70-90 hours of student work. Those readers who remember the student presentations during the late 1970's and early 1980's will remember Max Peters questioning the students about their time commitment. Rarely did they meet this expectation. When the 'in-house' simulator was introduced, the number of hours spent on design appeared to increase. Students then began recording their time. The average approached 140 during the 30-day period. When AIChE required word-processed reports in 1989, the number of hours increased to 160. As students became more familiar with word processing, hours dropped. But, when the commercial simulator was introduced with its increased power and options, the number of hours increased to about 150 average. KU students won no awards. While the failure to win awards is visible, the decreased effectiveness and increased time were substantially more troubling.

After the introduction of the simulator and observed impact on student achievement, class performance was monitored and compared to previous classes. Design problems

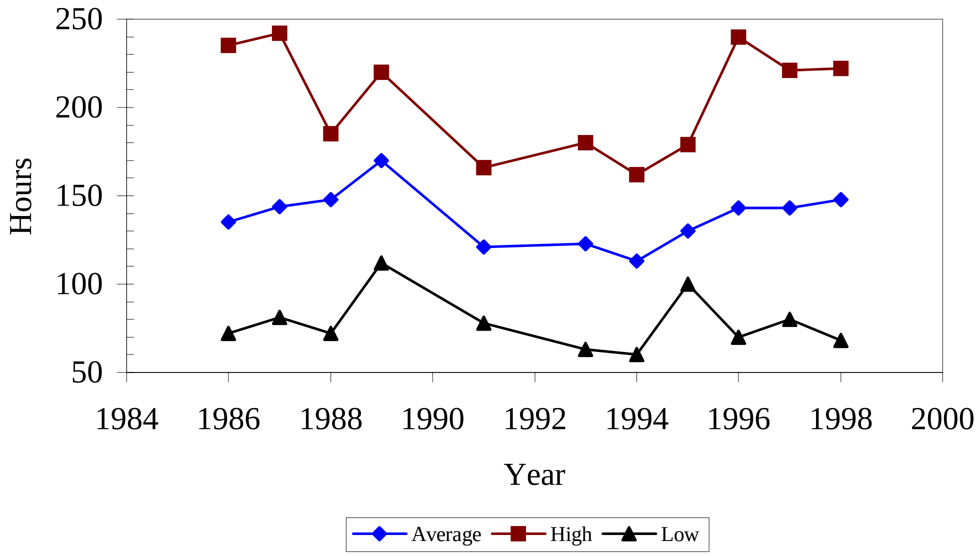

Figure 3: History of Effort Expended on AIChE Contest

and examinations from the early 1980's were used as the foundation. Extensive problem-by-problem records showed that performance was lower than earlier.

- Data base selections were haphazard.
- Specifications were poorly considered.
- Flowsheets were too complex.
- Data base errors caused all simulations to be incorrect.
- Excessive runs were made to search of desired performance.
- Problem-solving methodology skills were lost.

This is not entirely attributable to the introduction of the process simulator as discussed by Swift and Howat[4]. But the coincidence of this performance with the introduction was of sufficient concern to review course structure.

Given the mandate that a commercial simulator had to be used in design and that student quality had not dropped, the design approach had to be altered to integrate effectively the commercial simulator such that the potential that students would achieve the seven objectives would increase.

In recent years, student performance has improved as seen in Table 1. KU students are again winning national awards. Student performance on previous equivalent test problems has improved. Computer usage is still above expectations but it is dropping. The hours on the contest problem are still higher than expected but the increase has steadied. Student focus has improved. While this improvement cannot entirely be attributed to more effective integration, a portion of them is.

Guidelines for integration of powerful software are given below based on this thirteen-year experience.

Guidelines for Integration

Instructor Watchwords

- Recognize that this is merely a tool that the students do not know how to use.
- Recognize that just because students can set up complicated topology, it doesn't mean that they know how to effectively use a simulator.
- Recognize that the myriad of options and interesting graphics will lull students into believing that the answers that they get from the simulator are correct.
- Recognize that the ease of calculation will be an alluring substitution for thinking.
- Recognize the power that a simulator inherently has and that using this power should never be divorced from the process and project constraints.

These watchwords have lead to the guidelines below. These guidelines are all intended to steer students to effective usage without stifling creativity

Integration Guidelines

<u>Sensitize</u> *Convince students early that there are limitations to the software usage.*

- Assign example problems where the library parameters are incorrect. Have them compare the computed results against data.
  (This will take some effort since process simulator suppliers do not advertise which components have errors. Instructors can bypass this problem by establishing their own user defined components with slight errors and insist that the students use these.)

- Assign example problems where the selected option will lead to substantially different results.
  (The favorite examples are in phase equilibria where different solution models and equations of state will lead to substantially different estimates of the phase equilibria. Since thermodynamics is rarely the uniformly favorite subject, student comfort and understanding is low. Students will select the phase equilibria relation that gives them the answer that they want. Another example is to assign problems where there are no solution model parameters loaded. Students, undaunted, will use the selection.)

- Incorporate sensitivity analysis into the design sequence. Have students compare their computed data base to the data, perturb the data base in some manner consistent with the data uncertainties and evaluate the process again.
  (This should be included in any design activity since students inherently believe that the information, e.g. phase equilibria in mass transfer, is absolutely correct. The purpose of this exercise within the context of simulator integration is to have students recognize the importance of selecting the correct model and correct parameters.)

- Encourage use of the simulator in a responsible way emphasizing that overuse will lead to loss of performance and judgment.

<u>Develop</u> *Convince students to minimize acceptance of library databases.*

- Enforce the development of their own data base using primary data.
  (It is instructive for students to develop their own phase equilibria parameters. Do not allow use of library or literature values for these parameters. Have students do error analyses so that they recognize the uncertainty in their parameters.)

- Encourage evaluation of the underlying data to maintain their familiarity with fundamentals.
  (As part of the database development, have students identify acceptable data, e.g. thermodynamics consistency for phase equilibria.)

<u>Restrict</u> *Convince students to limit the types of specifications that they may make.*

- Restrict the specifications that you will allow them to use within any module.
  (An example is to restrict their specifications to distillate rate and reboiler duty in distillation towers. This may seem unnecessarily punitive. But during initial simulations, their projected equipment is far afield. Other, seemingly more pertinent specifications lead to unstable and unreasonable answers requiring excess student time as they follow false paths. These types of restrictions also help students to focus on material and energy balances as underpinnings to any chemical engineering solution.)

- Restrict material balance solutions to an external program or spreadsheet so that they must put their specifications into another program.
  (Process simulators have robust material balance solvers. But, if left to the simulators, the students never solve a material balance. The amount of numbers being printed by simulators is far too many to appreciate the subtleties of the process. Having students develop their own material balance helps them to develop the mental model of the process. Further, since these material balances are linear, they begin to appreciate the relationship between the simulator specifications and the process constraints.)

- Restrict total flowsheet simulation until near the completion of the base case. *(Simulating an entire flowsheet with all interconnected streams is particularly appealing to students. Starting with complex simulations insulates the students from the relation among design specifications and material balance performance. Limiting the size of the flowsheet that can be simulated at once and ensuring use of an external material balance solution helps to develop the relationships. Once the mental model is developed, they can move to more complex simulations.)*

<u>Estimate</u> *Convince students to develop a mental model of the process.*

- Have students estimate performance by hand.
  (Objective 6 in Table 2 is to reinforce student understanding of the fundamentals. This helps to establish the understanding that chemical engineering is not magic. By estimating performance, the fundamentals are strengthened in preparation for the following.)

- Have students perturb the process through estimation to project the effect of changes.
  (The students should write and justify their estimate of the impact of a specification on all aspects of the material balance before they run the simulator for any particular case.)

<u>Experiment</u> *Convince students to approach simulation as if it were a laboratory experiment.*

- Enforce experimental approach by having students write a plan for every set of simulation runs and every set of altered specifications explaining why they are changing a specific specification and what the expected impact on the constraint closure will be. *(Having students treat each simulation study as the equivalent of a laboratory experiment accomplishes two tasks. First, the requirement that they must write the explanation and justification of what they expect to accomplish focuses the simulation run. Second, writing the experimental plan eliminates unnecessary simulation studies and runs within a study.)*

- Enforce the development of a run log recording every run and elapsed personal times. *(Run logs are the equivalent of laboratory data sheets. Settings for all specifications that are varied during the run are recorded in the left most columns. Dependent results are recorded in the right most columns. After each run, an explicit identification of those constraints that failed, e.g. distillate composition, is stated. A statement is then written justifying the next set of specifications for the next run justifying why they will improve the likelihood of meeting the violated constraint(s). Have written explanations* *and justifications contribute to focusing the student effort. This guideline has been most effective in reducing student computer usage.)*

<u>Oversight</u> *Maintain contact with students by having them explain orally their approach.*

- Require meetings where students explain the basis of their simulations and defend their approach.
  (As stated above, it very easy to run the simulator. It is very difficult to think about the underlying meaning of the approach, the specification values, the expected results and the justification of the results. Requiring students to explain orally what they are doing and why forces them to slow to think about their work. It forces them into their preferred active learning mode.)

- Incorporate 'blue-sky' class discussions of simulation approach so that other students are aware of the diversity of views.
  (These discussions require that the professor is fully engaged in the project. Having discussions about various flowsheet configurations, the perturbing of specifications and the expected impact requires that the professor have an effective mental model. Students begin to hear about how others are approaching a problem and can evolve their own methods to become more effective.)

Afterword

The above guidelines are not all inclusive. They are not equally important. Some may be more effective than others in integrating the simulator into design from class to class. Nevertheless, they all have contributed to the improvement in student performance in chemical engineering design. Instructors must always be aware that student tendencies will be to follow the easiest and, as perceived by them, least time consuming path.

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Biographical Sketch

The author is the John E. & Winifred E. Sharp Professor, a professorship awarded for outstanding teaching. His teaching emphasis is process design and safety. He is also the Director of the Kurata Thermodynamics Laboratory. His research emphases include the phase equilibria of highly non-ideal systems, the development of plant performance analysis methodologies and the development of design reliability estimation methods.