



C. Stewart Slater

... of Rowan University



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Author Guidelines for the LABORATORY Feature

The laboratory experience in chemical engineering education has long been an integral part of our curricula. CEE encourages the submission of manuscripts describing innovations in the laboratory ranging from large-scale unit operations experiments to demonstrations appropriate for the classroom. The following guidelines are offered to assist authors in the preparation of manuscripts that are informative to our readership. These are only suggestions, based on the comments of previous reviewers; authors should use their own judgment in presenting their experiences. A set of general guidelines and advice to the author can be found at our Web site: <<http://che.ufl.edu/~cee/>>.

- c Manuscripts should describe the results of original and laboratory-tested ideas. The ideas should be broadly applicable and described in sufficient detail to allow and motivate others to adapt the ideas to their own curricula. It is noted that the readership of CEE is largely faculty and instructors. Manuscripts must contain an abstract and often include an Introduction, Laboratory Description, Data Analysis, Summary of Experiences, Conclusions, and References.
 - An Introduction should establish the context of the laboratory experience (e.g., relation to curriculum, review of literature), state the learning objectives, and describe the rationale and approach.
 - The Laboratory Description section should describe the experiment in sufficient detail to allow the reader to judge the scope of effort required to implement a similar experiment on his or her campus. Schematic diagrams or photos, cost information, and references to previous publications and Web sites, etc., are usually of benefit. Issues related to safety should be addressed as well as any special operating procedures.
 - If appropriate, a Data Analysis section should be included that concisely describes the method of data analysis. Recognizing that the audience is primarily faculty, the description of the underlying theory should be referenced or brief. The purpose of this section is to communicate to the reader specific student-learning opportunities (e.g., treatment of reaction-rate data in a temperature range that includes two mechanisms).
 - The purpose of the Summary of Experiences section is to convey the results of laboratory or classroom testing. The section can enumerate, for example, best practices, pitfalls, student survey results, or anecdotal material.
 - A concise statement of the Conclusions (as opposed to a summary) of your experiences should be the last section of the paper prior to listing References.

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C. Stewart Slater



*of Rowan
University*

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JAMES H. TRACEY
*(Founding Dean Emeritus,
Rowan University)*

*Above: Stew in the atrium of Rowan Hall, home of the Chemical Engineering Department.
Below: Stew's students compete on his hand-held reverse osmosis experiment.*



It is always an exciting time seeing chemical engineering students in the classroom working vigorously on an experiment. Teams of students are at a station that has a hand pump connected to a cylinder, a tank of blue salt water, and a second tank with a small amount of clear fluid. Next to these students there is a professor who is vigorously encouraging these students to “Pump it up!” He has gotten

them so excited that they are competing to see how quickly they can fill a 1-L graduated cylinder with pure water. Then you remember that C. Stewart Slater (Stew) is teaching reverse osmosis membrane separations today! Next you hear Stew commenting, “Now you can physically understand the applied pressure necessary to overcome the osmotic pressure of the salt solution.”

Stew exhibits this high level of enthusiasm whether teaching students, faculty at workshops, or board of trustees members of the university. Based on his accomplishments, Stew has received many accolades for his teaching, research, and service activities.

But Stew considers his most significant achievement to be the job he did as founding chair of the Chemical Engineering Department at New Jersey’s Rowan University, a school that he’s proud to say has provided the opportunity for students from the part of his home state locals call South Jersey to receive a first-rate chemical engineering education. Supporting that belief: The program he created has been ranked by *U.S. News & World Report* as one of the country’s best

undergraduate chemical engineering programs for seven consecutive years (2003-2009).

GROWING UP AT THE JERSEY SHORE

Stew grew up in Ventnor, N.J., a small resort town on the South Jersey shore. He was the youngest child in a family of professional educators. His father was a department head at Atlantic City High School and his two older sisters are both teachers, Susan in elementary education and Elizabeth in high school mathematics. The Jersey shore was a great laboratory for a young scientist. Digging in the sand for crabs and observing the dynamics of tides and beach erosion were nearby introductions to natural phenomena that fascinated him. Even today, Stew usually spends his weekends at the Jersey shore with his sisters and mother who still live in Ventnor. He comments that although the region has changed a lot in the last several decades, it is always comforting to come back to the place where you grew up.

Stew excelled in elementary and middle school; he always loved math, science, and history topics. Stew went to Atlantic City High School, where he followed a college-prep track with emphasis on science and mathematics. He took A.P. chemistry in his senior year and says that the intense laboratory experience and project work made the class



fun. His math experience was equally engaging, advancing to A.P. Calculus in his senior year and winning a school award for excellence in mathematics. His teachers encouraged him to consider an engineering career.

During high school, Stew worked part-time for the various conventions held in Atlantic City hotels and the convention center. One of these would have a pivotal impact on his life. In 1971, he worked as a session aide for the AIChE 70th National Meeting in Atlantic City. At this meeting, Stew got the chance to hear various talks from the sessions he aided. One session focused on pilot plants, which really excited Stew because of the concept of how processes are scaled up.

ON THE BANKS OF THE RARITAN

When Stew made the decision to go to college to study engineering, he looked at many colleges and attended the open house at Rutgers University in New Brunswick, N.J.. He was most impressed with the chemical and biochemical engineering department's equipment demonstrations, and became convinced that this program was the best choice for him.

Stew excelled at Rutgers, earning straight A's in his first Spring term. Sadly, his father died of cancer in the summer after his freshman year, but Stew's strong faith and family helped him through this difficult time. Stew says he was always encouraged in his career that he was following in his father's footsteps.

While at Rutgers, Stew joined AIChE as a student member and in his senior year was elected student chapter treasurer. Stew helped the chapter with a fund-raising campaign to support student activities such as a Thanksgiving party with turkeys and cider, and numerous social events. He especially enjoyed the camaraderie with fellow engineering students. Before teamwork was as popularized as it is today, Stew was a member of a study group that he recalls as being key to helping him succeed; the benefit students gain from working with other team members on various assignments was something he learned to appreciate first-hand.



Left, Stew playing and learning on the Jersey shore. Right, Stew with sisters Elizabeth and Susan (l to r).

Stew with his college friends and study group at Rutgers: (l to r) Stew, John Jacquin, George Swier, John Nikityn.



When Stew graduated in 1979, he interviewed with many of the companies that visited campus. He was intrigued with non-traditional aspects of chemical engineering, so a presentation by Procter & Gamble on chemical engineering in product development excited him. Stew accepted a job offer in Product Development for their Personal Products Division, located in Cincinnati, Ohio. He worked in dentifrice (toothpaste) process development on a gel-based product to complement the Crest® line. He met senior scientists and engineers from the Research Division, and soon realized that a career path in research would require an advanced degree. He was also told that his presentations were quite good and that he should consider being a professor since he was able to explain difficult concepts equally well to technicians and to non-chemical engineers.

When Stew decided to return to graduate school, he talked to his former professors at Rutgers, who strongly encouraged him to come back. At that time, Robert Ahlert had secured a major grant from the U.S. Environmental Protection Agency to examine the treatment of hazardous wastes from landfill leachates. Stew signed on to Ahlert's group at Rutgers and worked on the use of membrane processes, such as ultrafiltration and reverse osmosis, in the treatment of the leachates from a New Jersey Superfund site. One of the aspects Stew liked best was when he got the chance to involve undergraduate students in his research. This provided a meaningful mentorship opportunity for these students as well as giving Stew the chance to learn how to effectively supervise students. He also enjoyed his teaching duties when he was asked to fill in for a

faculty member going to a conference or to help undergraduates with class projects and grade homework assignments.

IN THE BIG APPLE

While completing his dissertation, Stew pondered his future plans and decided to enter the academic ranks, once again honoring his father's influence. He wanted to work for an institution that valued teaching while allowing him to continue developing his expertise in membrane processes.

In September 1983, he accepted a tenure-track position at Manhattan College. There, Stew immersed himself in the triad of teaching, scholarship, and service, and rose through the ranks, reaching full professor in 1992. During his time at Manhattan, he was very active in developing new laboratories for advanced separation processes and biochemical engineering with financial support from the National Science Foundation and from industry.

Stew says that he was influenced by numerous faculty members during his time at Manhattan College, including Br. Conrad Timothy Burris and Helen (Connie) Hollein. Br. Burris, who was Stew's first department chair, provided the support and encouragement necessary for faculty development and initiated Stew's involvement in ASEE. Connie was hired the year before Stew and they shared many of the growing pains of new faculty. They also worked together in the areas of educational development and bioseparations research. Stew earned high marks for his teaching, research, and service, and was recognized by his peers with the ASEE New Engineering Educator Excellence Award, the Dow Outstanding New

Faculty Award, and ASEE's Fluke Corporation Award for Excellence in Laboratory Instruction.

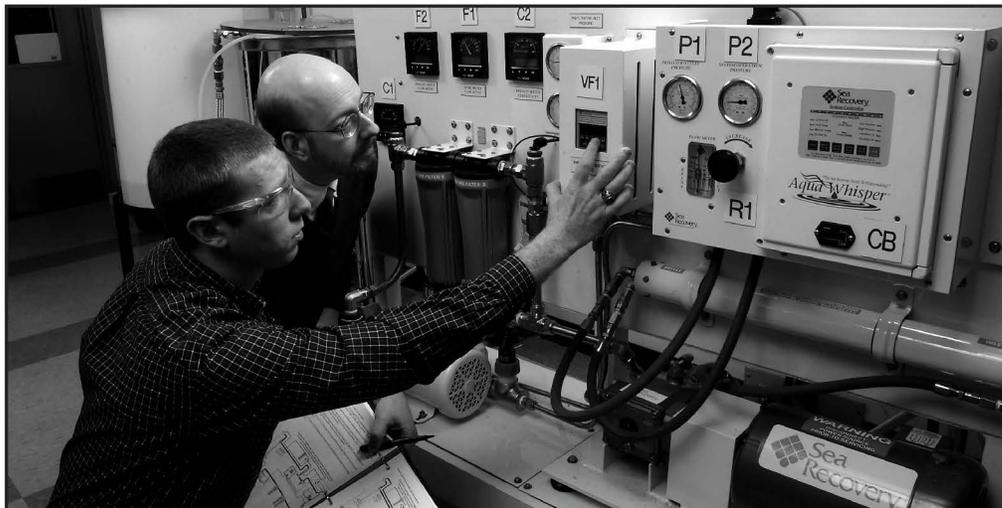
Stew continued to expand his research and teaching interest in membrane technology, developing new courses at both the senior and master's level. He analyzed what was taught in separations courses and found that new separations, such as membranes, were underserved. As a result he developed methods to incorporate membrane processes. He developed new courseware and experiments for membrane processes that are still used in Manhattan College's undergraduate laboratories (as well as in other universities across the country). His work resulted in many pedagogical publications and in new approaches that would later earn him the prestigious Chester Carlson award from ASEE. It also left a positive impact on the many whose lives he has touched. Stew embraced the LaSallian tradition of excellence in teaching.

As A Teacher

Br. Christopher Dardis, who served for many years as director of Manhattan's Center for Teaching & Learning, remembers Stew fondly as a faculty member who came to him for help to improve his teaching—help he clearly did not need, as Br. Christopher calls Stew one of the best teachers that he has ever seen. Br. Christopher cited Stew's demonstrations with "cut-away" membrane modules as an ingenious and highly effective teaching method.

Connie Hollein, who served as Chemical Engineering Department Chair after Br. Burris retired, recalls Stew's winning style in the classroom. "He was one of the most organized faculty members I've known, with step-by-step detailed notes and the reputation as a tough but fair teacher." But in balance with that serious side, Connie notes, "His jokes and funny stories kept the students engaged even at the end of a long day."

She recalls one story in particular: "When he showed a cut-away hollow fiber membrane permeator to the students, he would tell them that last year's class took one of the cut-away permeators and he didn't know where it went. He went on to claim that at the end of that semester, he got a present from the class and it was the hollow fiber permeator—with the fibers removed and cut up into a hair piece for him! Then, he takes a cut-up bundle of fibers and places it on his head. The *whole class* erupts in laughter!"



Above, Stew with a student in the Unit Operations lab; below, working with a student on a membrane laboratory experiment he developed.



As a Mentor

Supplementing his natural gifts in the classroom, Stew was mentored by Br. Burris in how to obtain industrial funding from industry for his research activities. His research focused on: reverse osmosis for industrial waste minimization, modeling and simulation, and water recovery and reuse; ultra/microfiltration for protein separation; and pervaporation for separation of various organic-water mixtures. He became well known for his work in organophilic pervaporation, which provided him an opportunity to attend numerous international conferences and seminars. These projects were supported by various companies including Air Products & Chemicals, ExxonMobil, Pfizer, Joseph E. Seagram & Sons, and United Technologies. In all of these projects Stew passed along the gift of mentoring, involving undergraduate and master's students, many of whom went on to obtain advanced degrees and



related positions in industry, academia, and government.

Kevin Devine, who has risen to the current job title Group Leader at Kraft Foods, Inc., says, “Dr. Slater was a demanding research advisor but did it in a way that encouraged us to succeed with our pervaporation projects. His mentorship taught me numerous things from experimental design and effective time management to presentation techniques, all of which have helped me advance in my professional career.”

Stew is deservedly proud of the successful careers of his research students and of the fact that four of his pervaporation research students won Manhattan’s campuswide Sigma Xi medal for research, and three won awards when they presented research papers at International Pervaporation Conferences.

Another former student, John Paccione—currently with the New York State Department of Health and on the faculty of State University of New York at Albany—was an undergraduate who worked with Stew during his early years. “Stew taught me how to design, develop, and operate state-of-the-art reverse osmosis systems. This work provided my colleagues and me with a greater view of opportunities in chemical engineering and an introduction into the activities of research. One of Stew’s greatest abilities was to inspire students to work to higher levels of achievement, which in my case included earning a Ph.D. at Rensselaer Polytechnic Institute. One of the greatest attributes of an educator is the ability to inspire his students and to provide visions of the possibilities beyond the classroom.”

Marco Castaldi (now on the faculty at Columbia University) is another former student. He remembers Stew for his genuine interest helping Marco during unit operations laboratory. Marco comments, “Unlike most professors in charge of student laboratory courses, Stew took the time to read my preliminary report and suggest improvements and changes that enabled me to see the important aspects of the labs. This directly translated to my abilities to develop excellent laboratory skills and techniques that have served me well during my graduate studies and subsequent industrial and academic career. In the classroom, he showed another side. One in which he could present complex, new material in a way that left you feeling confident you could understand and use it in real-life applications.”

As a Peer

Early in his career, Stew became quite active in professional societies and attended AIChE, ACS, and ASEE conferences to present papers and network with colleagues. One of the professors that he met at ASEE meetings, Angelo (Angie) Perna of New Jersey Institute of Technology, encouraged him to get more involved in that society. Stew began to rise through the ranks of leadership in ASEE, first in the Division for Experimentation and Laboratory-Oriented Studies (DELOS) and then in the Chemical Engineering Division, rising to Division Chair in each. Stew currently serves as vice-chair of the publications board of *Chemical Engineering Education*.



*Facing page, Stew teaches other teachers at an NSF workshop.
Left, Stew at the ASEE 2003 Annual Conference along with Rowan Chemical Engineering faculty Stephanie Farrell (far right) and Robert Hesketh (second from left), who are flanking ASEE President Jerry Jakubowski.*

SOUTH JERSEY HOMECOMING

In 1992 Henry and Betty Rowan gave a gift of \$100 million to start a new engineering school at Glassboro State College, which was renamed Rowan University in their honor. When the enviable position of founding chair of Chemical Engineering at the university was being created in 1995, Stew was a finalist for the job. Dean James Tracey recounted that Stew was very excited about this opportunity since it was a rare chance to create a new way of teaching engineering. Stew was additionally eager to return to his roots in southern New Jersey, where his family still lived. In pursuing the post, Stew's showman skills stood out. Jim Tracey comments, "Stew insisted on doing a membrane demonstration during his interview that really impressed me; I had never had a candidate insist on doing a demonstration before. But, Stew firmly believed in 'hands-on education,' and knew that this would be a critical component of our program." Stew got the job.

He spent his first year at Rowan multitasking—splitting time between curriculum development, facilities/lab development, student recruitment, and faculty recruitment, each of which had its challenges. Jim Tracey challenged the founding chairs to create an innovative program that would produce a 21st Century engineer. The resulting curricula was designed to produce graduates who could communicate effectively, have knowledge of business/entrepreneurship, work in multidisciplinary teams, and have a hands-on, minds-on approach to problem solving.

During Stew's initial year at Rowan he spent many hours working on plans for an innovative engineering building. Stew, who is well known for his detailed planning, devoted many hours to ensuring that the engineering labs were suited for chemical work. The end result is that every room in Rowan Hall has the capability of being easily converted to a chemical laboratory. Stew worked tirelessly on making sure

that the fresh-air exchange, hoods, point exhausts, and the like were sufficient to support chemical work. Of course, water sources and drains were placed in every lab, but Stew made sure that a pressurized water system was installed in the building so that no experiment would have a shortage of water flow in high demand times. Similarly, pressurized air, vacuum, and steam lines were placed in the building. Again, to get the steam lines Stew had to work with the architectural firm to install a special heat exchanger on the fourth floor. Most notably in this building, Stew had to defend the need for high bay laboratories that at first got removed from the plans as a cost-cutting measure, and then were reinstated only after his defense of these as absolutely necessary for a hands-on, minds-on curriculum.

Stew instilled the quote "Tell me and I forget, show me and I may remember, but involve me and I understand," that he attributes to Benjamin Franklin, as a fundamental philosophy for the engineering college. For example, one of the essential jobs of the first chairs and dean was to recruit a new set of students to a new program—without an engineering building! This tall task involved many trips and visits to high schools and college fairs alongside admissions office staff. As Jim Tracey recalls, Stew's unique slant on this activity was to bring his trademark hand-held reverse osmosis demo to allow high school students to get involved and run an actual chemical engineering process. Stew was able to convince students that Rowan would not be a place where you only sat in class and took notes; instead Rowan would be the place where you would become actively engaged in the learning process. Stew also convinced the University Board of Trustees that engineering at Rowan would be unique by having *them* perform this same experiment.

In working with the other founding chairs, Stew contributed to developing a program in which students are involved in the learning process from the first day of the program,

through multidisciplinary engineering clinics. These clinics are similar to the medical school approach to teaching (first used in engineering by Harvey Mudd College) in which students work in teams on actual engineering problems each semester. Each section of the engineering clinic sequence involves students from all four of the engineering disciplines, and many of the clinic projects are funded by industry and faculty-research grants. The Rowan program was one of the first in the country to have a one-year freshman experience with engineering experimentation, multidisciplinary teamwork, and communication skills. In the Fall semester, students start by conducting guided experiments, and then finish the semester with an open-ended project.

In 1996 the first engineering clinic was housed in an old cafeteria, which especially pleased Stew because he had water and what appeared to be drains. After doing some plumbing, these freshman students worked with pressure and flow measurement devices using newly purchased 40-gallon tanks. The students also learned some on-the-job training in trouble shooting: They found that the cafeteria drains had been plugged from previous use, and they observed that water will always take the path of least resistance!

In the Spring semester the freshman engineers worked on a reverse engineering project that focused on the coffee machine—a perfect match for a food-grade cafeteria lab.

By the time the first class graduated in May 2000, eight faculty had been hired and the labs were full of equipment and advanced instrumentation for teaching and project work. Based on his educational innovation and leadership, Stew was awarded the George Westinghouse Award from ASEE in 1996. Several years later, in 2000, ASEE recognized him with the Chester Carlson Award for his innovations in developing laboratory experiments and course materials on membrane technology. Stew excelled in teaching future educators at ASEE Summer Schools, EPA workshops, and NATO Advanced Study Institutes. He has conducted six NSF-sponsored workshops on novel process science and engineering, membrane technology, and advanced separation processes.

Stew's experience gained from some of his initial faculty workshops was very useful in inspiring new experiments for use in the Rowan courses. Stew helped faculty to obtain funding for these new teaching methods by introducing them to the NSF funding opportunities in laboratory development as well as in presenting national workshops. Through his leadership, faculty started out as co-PI's on these grants and then were mentored by him and became the lead on new education grants. Stew recalls one of the best things about Rowan is this willingness of faculty to work collaboratively. Whether it is team teaching a class or partnering in supervising a clinic project, the enthusiasm of faculty to work in teams has provided rewarding learning experiences for both students and faculty. Stew has worked alongside every member of the department—Kevin Dahm, Stephanie Farrell, Zenaida Ge-

phardt, Robert Hesketh, Brian Lefebvre, James Newell, and Mariano Savelski—on educational and research projects.

As chair, Stew encouraged Rowan's talented young faculty to develop and publish their educational innovations. Kevin Dahm points out, "Stew served as an outstanding mentor and passionate and effective advocate for his faculty. His support and encouragement led to numerous national awards garnered by members of the department." Once again, Stew's detailed planning paid off. He had even listed in advance who would be nominated for regional and national awards.

Rowan's Junior and Senior engineering clinics are primarily sponsored by industry. Getting these sponsors requires a tremendous amount of energy and skill. Not surprisingly, Stew was a very effective pitchman in obtaining sponsors; his tremendous enthusiasm and ideas are very convincing. He was the lead presenter to nearly all of the sponsors of engineering clinic projects during his tenure as chair, and faculty who have presented with him have observed the effectiveness of these presentations to industry.

Stew acknowledges that industrial clinic projects have been the most interesting to him, especially those with either food or pharmaceutical companies. His involvement in most of these projects has been in his area of interest of membrane separations, but recently Stew has "gotten green." He has been involved in EPA projects on the development of educational modules in green engineering for the undergraduate curriculum. In the last several years he has collaborated with Mariano Savelski on green engineering research in pharmaceutical manufacture focusing on organic solvent metrics, solvent reduction/recovery, and life cycle assessment, funded by EPA, Bristol-Myers Squibb, and Pfizer.

Mariano says, "Working with Stew has been a wonderful experience for me; he is one of the best-organized people I have ever worked with. His attention to detail, his perseverance, patience, and organizational skills are beyond description. In our projects, he helps guide students by giving them clear objectives for their work. As they present the results of their work he gives detailed feedback to the students both in meetings with students as well as on their written work."

Mariano is also impressed with Stew's planning, "He never misses a deadline! In fact, Stew always has everything ready days, if not weeks, in advance."

Stew's attention to detail was essential for starting a new department. He is always prepared for every meeting whether it is with an individual faculty member or the entire college of engineering. Based on either his agenda or an agenda he has been given, Stew carefully considers each point listed and makes extensive notes on his yellow legal pad. During the meeting he continues to take notes on important aspects so that they can be relayed to faculty. Stew's careful pre-planning was very useful for keeping discussions focused on accomplishing the required tasks on the agenda. One example of his attention to detail was in planning and

“One of Stew’s greatest abilities was to inspire students to work to higher levels of achievement, which in my case included earning a Ph.D. at Rensselaer Polytechnic Institute. One of the greatest attributes of an educator is the ability to inspire his students and to provide visions of the possibilities beyond the classroom.”

— A former student

preparing an NSF-sponsored workshop. In addition to all that is required in developing new experiments, preparing lecture and lab sessions, printing handouts, and recruiting participants and speakers, Stew paid attention to even the incidental details—pillows, for example. He personally visited every dorm room that the faculty would be staying in to make sure that it was suitable; when he discovered bed pillows were in short supply, it was Stew who went out and purchased them.

Stew also makes extensive use of this aptitude for planning in his lectures and presentations. His lecture notes are filled with comments directing students to conduct active-learning exercises as well as notes on some of his famous jokes. Class after class of students have been amused and bemused by Stew’s sometimes corny take on the subject matter.

In a lecture on thermal conductivity for building materials Stew tossed students a curve by asking them to look up, “What is the value for steel? For plywood?...*For the natural log?*”

Stew loves to stretch the truth and turn things around—“Did you know the origin of membrane terminology can be found in the Bible? Moses was a breach birth so when he was born they exclaimed ‘Reverse Moses’ (Reverse Osmosis).”

Brian Lefebvre, who co-teaches the separation course with Stew, remembered the lecture on ion exchange membranes. Stew first shows the class two similar-looking polymer sheets and asks which one is the cation and anion exchange membrane? After the students give a variety of answers, Stew then holds one of the sheets close to a student’s ear and obliquely makes a “meow” sound. (He uses this example to illustrate the importance of doing experiments.)

Stew says that the success of the Rowan chemical engineering department is based on the great faculty that he is blessed to be working with. He views his role of founding chair to go beyond the “bricks and mortar” of a start-up program. Jim Newell comments, “Stew built a department that ran

like a family. He mentored a generation of faculty members with concern, humor, and a genuine commitment to helping each one of us develop to our fullest potential. Stew always said that his job was to hire people that could become even more successful than him and then to help them achieve that potential.” Stephanie Farrell adds, “Stew is thoughtful, considerate, loyal, and a natural leader. As a friend and colleague he consistently puts others before himself. His work ethic and dedication to education are well known; during his time as department chair he was admired for his fairness, preparedness, and dedication, all while remaining friendly, pleasant, and easygoing.”

In 2004, Stew decided to return to a faculty position to allow other chemical engineering faculty to gain experience in leadership positions. Through his career he has amassed an impressive record for someone who has taught at primarily undergraduate institutions. He is principal author or co-author (with his students and faculty colleagues) of more than 50 journal articles, 75 conference proceedings, 140 conference presentations, and nine book chapters. He has served as a principal investigator or co-investigator on more than \$3 million in projects from industry and government. He is a Fellow of the American Society for Engineering Education (ASEE) and has received many awards from professional societies. Over the years, he has been asked at times to consider industrial and government positions, but always responds to such queries that “teaching is in my blood.” Stew loves it when a former student visits years after graduation and he can see the impact he has had on that person’s professional career.

Stew reminds seniors preparing for graduation that they are the future of chemical engineering and the ambassadors of the profession. He knows that these graduating seniors may not remember all the chemical engineering concepts they learned or all the jokes he has told. More importantly, Stew wants them to remember two things: to help others, and to use their chemical engineering know-how to serve and improve society. □

AN INNOVATIVE METHOD FOR INTEGRATING A DIVERSITY WORKSHOP *in a Chemical Engineering Course*

AYUMU YOKOYAMA

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As chemical engineering students graduate and enter industries or graduate schools, they will most likely be working in a diverse work environment where some of their colleagues, managers, and customers have cultural backgrounds different from their own. Thus, it is crucial for engineers to be able to work effectively with people from different backgrounds. In fact, in many multinational companies, it is becoming essential for employees to have successful international assignments as a prerequisite for moving up the corporate ladder.

Given this context in the corporate world, engineering students should be exposed to diversity in their undergraduate education. Diversity education usually takes place outside of core engineering programs, and it can be difficult for engineering students to see the relevance of diversity education to their engineering curriculum. To demonstrate to students the importance of diversity for engineering professions, we integrated a short diversity workshop as part of a chemical engineering course for undergraduate seniors (about 40 students) at the University of Michigan, entitled “Problem Solving, Troubleshooting, and Making the Transition to the Workplace.” (<See <http://www.engin.umich.edu/scps/>> for the course syllabus).^[1] This course, taught by Professor H. Scott Fogler, includes other topics such as critical and creative thinking skills, negotiation skills, teamwork skills, problem

solving skills, financial planning, technical communications, and trouble-shooting to prepare senior engineering students for real-world challenges when they make the transition to the workplace. Thus, we thought that a diversity workshop would fit in this course where students can learn how to deal with diversity in the workplace.

The author, who has a background in corporate diversity training and consulting at DuPont, designed a short diversity workshop for this course. The diversity workshop is 1.5 hours long and focuses on awareness-building of different communication styles. The workshop includes various exercises so that students can experience different communication styles and cultures through participation. Throughout the workshop, lecturing is minimized to enhance interaction among students.



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Asian culture is chosen to highlight and contrast with the U.S. majority culture. We chose Asian culture because it is the native background of the author, and it is quite different from the U.S. majority communication style.^[2] Since most students in the class represent the majority culture, this emphasis gives students more awareness of their own communication styles by contrast. Also, understanding Asian communication style is important for engineers in light of increasing business ties between U.S. and Asian companies.

DIVERSITY WORKSHOP CONTENT

To make engineering students interested in the subject of cross-cultural communication, this workshop uses various exercises and examples that have relevance for students. The following sections describe the framework of the workshop.

Ice-breaking Exercise.

Cross-Cultural Communication Simulation

The goal of this ice-breaker is to create an interactive class environment by having students experience cross-cultural communication in pairs. For this, the following simulation^[3] is used.

1. First, students are paired (Student A and Student B).
2. Then, in each pair, one student (Student A) is shown the slide with the communication styles he/she needs to present:
 - a. Ask about B's personal matters.
 - b. Minimize eye contact.
 - c. Minimize body language (hand movement).
 - d. Try to keep distance (2.5 feet or more) from Student B while talking.
3. The other student in the pair (Student B) is then shown the slide with the different communication styles he/she needs to present:
 - a. First, answer Student A's question.
 - b. While talking, use excessive body language.
 - c. Keep eye contact with Student A.
 - d. Stay close to Student A (1.5 feet or less).
 - e. After answering Student A's question, ask about Student A's view on the war in Iraq (or any sensitive political issue).
4. The pairs then start a cross-cultural conversation for a few minutes.

This situation simulates communication between individuals with different styles in use of eye contact, body language, and physical proximity. This exercise will give students a flavor of cross-cultural communication and its potential issues. Although the exercise is done with the same language (English), students can see how different communication styles

can negatively impact effectiveness in communication and the building of trust in relationships needed in the workplace.

The exercise also serves as a good icebreaker since most students find it enjoyable because of the acting involved. For example, since Student A in each pair is trying to keep their distance while Student B is trying to stay close, the result can be conversation constantly interrupted by physical movement.

Learning the Difference Between Generalizing and Stereotyping

One danger in any diversity workshop is reinforcing stereotypes. To avoid this and to let students know that in this workshop, generalization is used instead of stereotyping, two graphs are shown using a format familiar to chemical engineering students (Figure 1), in which generalization is shown as two normal distribution curves, whereas stereotyping is shown as two δ -functions. Students can easily understand that generalization allows some exceptions (for example, although most Americans behave in a certain way different from Asians, some Americans do behave in an Asian way); on the other hand, stereotyping does not allow any exceptions, and thus needs to be avoided.

Common questions raised during this part are “Are all stereotypes bad? Are there any good stereotypes? How about ‘Asians are good in math,’ which seems like a positive stereotype?” From sociology, we learn that stereotypes are always harmful because they encourage “myth-making” and curb the wants and desires of individuals and ultimately negatively affect societal attitudes towards groups.^[4] For example, for an Asian-American whose strength is art and design, the math-aptitude stereotype raises false expectations by others or by self—or worse, funnels individuals into narrow categories.

Understanding Common Asian Cultural Mores

Common Asian cultural norms are presented in the forms of the following exercises. The purpose of these exercises is not necessarily to make students understand Asian cultural mores but rather to make them aware that some cultures are quite different from their own. Thus, cultures other than Asian can

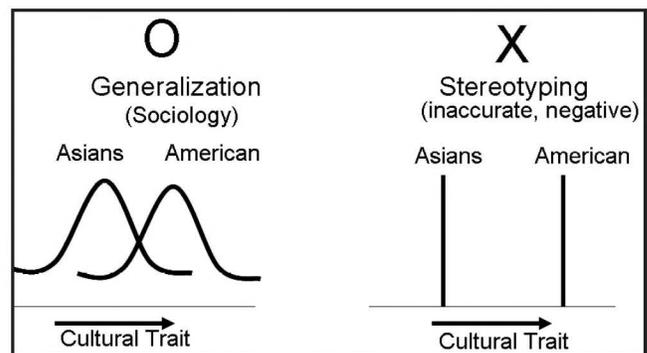


Figure 1. Difference between generalization and stereotyping.

be used here if the instructor is familiar with them.

It is also important in these exercises to urge as many students as possible to share their interpretation, so that students can see how diverse the interpretations can be depending on their upbringing.

Exercise 1.

Japanese Poem for Understanding Group Orientation

The goal of this exercise is to make students realize how differently people react to a similar situation depending on whether their culture is based on group orientation or individual orientation (Asians are more group-oriented than the U.S. majority group). The students are first asked to read the following Japanese poem entitled “Sunset.”^[5]

*The train was crowded as usual.
A young woman was sitting down, and an old man was standing in front of her.
The young woman stood up and gave her seat to the old man.
The old man got off at the next station.
The young woman sat down again.*

*Then, another old man was pushed by the crowd and ended up standing in front of her.
She stood up again and gave her seat to the old man.
The old man got off at the next station.*

*Another old man happened to be standing in front of her.
But, this time, the young woman did not stand up.
The train passed the next station.... and then the next station with the young woman looking down and ashamed.
I got off the train. I wonder how long she could endure the pain.*

The students are then asked to interpret why she was ashamed. It is important here to tell students that there are no right or wrong answers so that they feel at ease in giving their own interpretation.

Non-Asian students in the class typically will say, “The young woman was ashamed because she was not using good manners (younger people should give seating to elderly),” or “She was ashamed because she gave in to her desire to sit down.”

On the other hand, Asian students will say “The young woman has been struggling to balance good manners against the pain of sticking out in the crowd (Asians tend to have group orientation and avoid being singled out even when they are doing the right thing),” or “She did not want to get attention from other passengers.”

These different interpretations along with the different proverbs and pictures in Figure 2 can be used to talk about group orientation (“The nail that sticks out gets hammered down” is a Japanese proverb) vs. individual orientation (“The squeaky wheel gets the oil,” a U.S. saying).

This exercise will give students a real opportunity for finding various reactions among participants based on their various upbringings, especially when the class is diverse.

Exercise 2.

Short Vignette from a Japanese Movie for Understanding “Saving Face” Concept

The goal of this exercise is to teach students the importance of saving face in other cultures. Saving face means maintaining credibility, honor, the demonstration of kindness, or status in society or on the job. Saving face is practiced in western cultures as well, but saving face is especially important in Asian cultures in public situations or in the eyes of others.^[6] The following example illustrates this when “face” relates to maintaining credibility as a kind person.

A short vignette from a Japanese comedy movie^[7] is shown in the class. The vignette was chosen because it is full of actions and is funny and does not need translation. The vignette shows a crowded train, where a younger man finds a boy sitting while an elderly man is standing. This younger man then forcefully removes the boy from his seat and then tells the elderly man to sit down. But, the elderly man declines to sit down. Then the younger man becomes very *angry* with the elderly man.

After viewing the vignette, students are asked why the younger man got angry. Non-Asian students in the class typically say, “The younger man got angry because the elderly man did not thank him,” or “He got angry because the elderly man did not sit down.”

Asians’ interpretation is that the younger man got angry because he lost face. In Asian culture, face (in this case kindness shown by the younger man) must be acknowledged by other

people present in the situation (in the eyes of others). Since the young man’s face (kindness) was not appreciated by the elderly man in public, he lost his face in front of other people and got humiliated and angry. In Asian culture, saving face

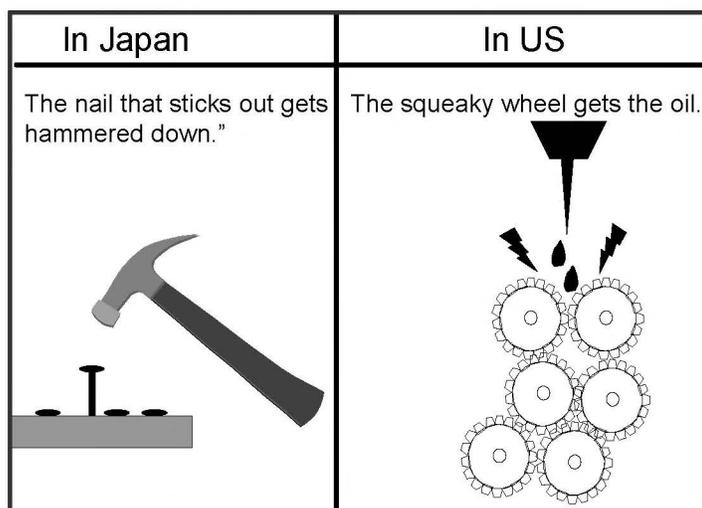


Figure 2. Group-oriented vs. individual-oriented culture.

is much more important in public situations than in private situations. If other people were not present in this situation, the younger man would not have been angry.

This exercise will teach students the reason why Asians often prefer to have private and one-to-one meetings to avoid losing face in public before discussing or negotiating important or sensitive issues in a large group.

Exercise 3.

Saving Face in the Global Workplace

The goal of this exercise is to show students how saving face (discussed in Exercise 2) adds complexity to the real workplace. In this example, “face” relates to credibility and status/rank on the job. The exercise uses a situation involving Japanese automotive transplant engineers and an engineer from their company’s supplier. In this situation (shown in Figure 3), both a Japanese process engineer, Ayumu, and a Japanese materials engineer, Yoko, are at an equally higher status than an American manufacturing engineer, Joe (Ayumu and Yoko give directions to Joe).

One day, the Japanese process engineer Ayumu tells the American manufacturing engineer Joe to use a new material. Then, this new material’s supplier, Akira (also Japanese), finds out that the Japanese material engineer Yoko is against the use of the new material (Ayumu and Yoko are both Japanese but have poor communication with each other because Ayumu is located in the United States while Yoko is located in Japan).

If the supplier’s representative Akira had not told Ayumu that his coworker Yoko might not agree on the use of the new material, then Ayumu would have had to change his directions to the American engineer Joe—and would have lost face in the eyes of others (Engineer Yoko and Engineer Joe). In this case, face refers to the higher status (giving directions) or credibility. Since Ayumu holds a higher status or rank than Joe, he would lose face if his directions are later changed by others’ decisions.

To prevent this loss of face, supplier Akira had to tell Japanese engineer Ayumu that the Japanese engineer Yoko was against the use of the new material. This way, Ayumu and Yoko could negotiate in private without involving the American engineer Joe, and Ayumu’s direction would not be denied completely in the eyes of Yoko and Joe.

This real situation shows the importance of saving face in the workplace and the complexity in dealing with different cultures.

Exercise 4.

High-context vs. Low-Context Communication Styles

The goal of this exercise is to teach students that it is critical to know the communication style (high- or low-context) for effective communication. Whereas the U.S. majority communication style is called low-context (the meaning of a statement is in the words spoken), Asian communication style is called high-context (meaning is unspoken but interpreted indirectly from the context, the history of relationship, or general social rules).^[8] The high-context style is:

- *Subtle, often nonverbal cues used to convey meaning (body language, facial expressions, silence, tilting head).*
- *Does not say a lot, but expects you to know a lot.*
- *Described well with the Chinese proverb, “He who knows does not speak, he who speaks does not know” (Lao-tsu, Chinese sage, 6th century B.C.).*

To illustrate this difference and the confusion caused by it, a few examples are given in the workshop in order for students to think about possible interpretations for high-context communicators with low-context statements or questions. For example:

- *A low-context question “Are you hungry?” can be interpreted by a high-context communicator to be that the person asking this question may be actually hungry and suggesting that they should go to eat together now, or the person may be suggesting that they should take a break from this intense negotiation.*
- *A low-context statement “I’d like that report as soon as you can get to it” can be interpreted by a high-context communicator to be “Drop the current project you’re working on and finish that report today.”*
- *A low-context statement “We need to tighten our budget”*

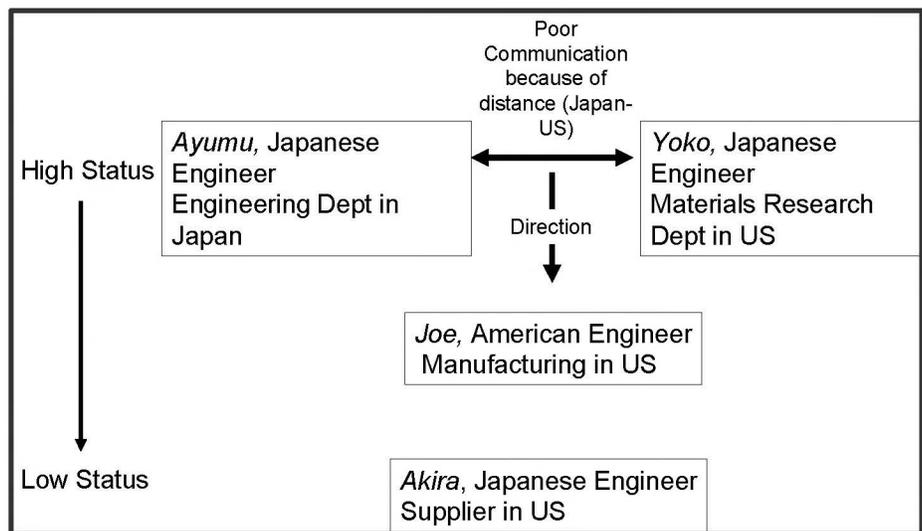


Figure 3. An example of saving face at Japanese plant in the United States.

can be interpreted by a high-context communicator to be “We should not spend at all,” or even “My position might be eliminated.”

Through these examples, students can see negative consequences of not understanding high-context communication style and can understand why it is so important to know which communication style is in use for other speakers.

Nonverbal Communications

Nonverbal communications are discussed around use of silence, use of eye-contact and use of gestures, and emotional expressions. For example, silence is considered negative in the U.S. majority culture, whereas silence has many positive aspects in Asian culture, such as showing respect to superiors. One of the negative consequences of not knowing this difference would be that people uncomfortable with an Asian person’s silence tend to disclose too much information during negotiation.

Homework Assignment

A homework assignment is given to reinforce the main points. The students need to find a person who grew up in a culture different from the majority culture and find out the following:

1. *What are/were some difficulties in communicating with Americans or with persons from the majority culture?*
2. *Ask how he/she communicates with elders, teachers, or supervisors in their native country.*
3. *Ask if their native communication style is more indirect than American communication style. Is what they say in a native culture what they really mean?*
4. *What can Americans do differently to make the person who grew up in a different country feel more comfortable in communication in the United States?*

This assignment can make students become aware of the reality that people with cultures different from the U.S. majority culture feel they always have to adjust their communication styles for majority members. It can also lead majority students to think about better ways of communicating with those from other cultures.

OUTCOMES

The goal of this workshop is to give students awareness of different cultures playing out in the real workplace, in a nonthreatening way. In general, neither defensive reactions nor guilty feelings were expressed in the class. This probably results from the use of Asian culture, which is mostly unknown and nonthreatening for a largely European-American audience. Feedback from students suggests that they were surprised to know how different cultures impact communication and that they did not know that their U.S. mainstream culture is so different from other cultures such as Asian culture. Also, we found that students with backgrounds different from the

U.S. majority culture could help the class understand diverse cultures when they were encouraged to share their experiences during the class.

CONCLUSIONS

The diversity workshop can be integrated into a chemical engineering course so that students can see the relevance of diversity education for engineering professions, where engineers from various backgrounds need to work together effectively. By having a diversity workshop as part of a course for senior undergraduate students, we can show the importance of diversity in the engineering profession and provide strong motivation to learn diversity for students who will be joining a diverse workplace shortly.

Generally, universities offer some type of diversity education as part of the general education requirements for undergraduates. This may be in many possible forms—courses with cross-cultural themes, courses that raise awareness about racism, or courses that promote a global perspective. Often, these courses are taken in the first two years of study. The exercises described here provide an extension of this foundation of diversity education during the upper-level portion of the undergraduate curriculum.

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Random Thoughts . . .

THE 10 WORST TEACHING MISTAKES II. Mistakes 1–4

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In our last column^[1], we presented the bottom six of our top 10 list of the worst mistakes college teachers commonly make. Here are the top four, with #4 being particularly applicable to engineering instructors.

Mistake #4. Give tests that are too long

Engineering professors routinely give exams that are too long for most of their students. The exams may include problems that involve a lot of time-consuming mathematical analysis and/or calculations, or problems with unfamiliar twists that may take a long time to figure out, or just too many problems. The few students who work fast enough to finish may make careless mistakes but can still do well thanks to partial credit, while those who never get to some problems or who can't quickly figure out the tricks get failing grades. After several such experiences, many students switch to other curricula, one factor among several that cause engineering enrollments to decrease by 40% or more in the first two years of the curriculum. When concerns are raised about the impact of this attrition on the engineering pipeline, the instructors argue that the dropouts are all incompetent or lazy and unqualified to be engineers.

The instructors are wrong. Studies that have attempted to correlate grades of graduates with subsequent career success (as measured by promotions, salary increases, and employer evaluations) have found that the correlations are negligible^[2]; students who drop out of engineering have the same academic profile as those who stay^[3]; and no one has ever demonstrated that students who can solve a quantitative problem in 20 minutes will do any better as engineers than students who need 35 minutes. In fact, students who are careful and methodical but slow may be better engineers than students who are quick but careless. Consider which type you would rather have designing the bridges you drive across or the planes you fly in.

If you want to evaluate your students' potential to be successful professionals, test their mastery of the knowledge and skills you are teaching, not their problem-solving speed. After you make up a test and think it's perfect, take it and time yourself, and make sure you give the students at least three times longer to take it than you needed (since you made it up, you don't have to stop and think about it)—and if a test is particularly challenging or involves a lot of derivations or calculations, the ratio should be four or five to one for the test to be fair.^[4]

Mistake #3. Get stuck in a rut

Some instructors teach a course two or three times, feel satisfied with their lecture notes and PowerPoint slides and

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assignments, and don't change a thing for the rest of their careers except maybe to update a couple of references. Such courses often become mechanical for the instructors, boring for the students, and after a while, hopelessly antiquated.

Things are always happening that provide incentives and opportunities for improving courses. New developments in course subject areas are presented in research journals; changes in the global economy call on programs to equip their graduates with new skills; improved teaching techniques are described in conference presentations and papers; and new instructional resources are made available in digital libraries such as SMETE (<www.smete.org>), Merlot (<www.merlot.org/merlot/index.htm>), and the MIT Open Courseware site (<<http://ocw.mit.edu>>).

This is not to say that you have to make major revisions in your course every time you give it—you probably don't have time to do that, and there's no reason to. Rather, just keep your eyes open for possible improvements you might make in the time available to you. Go to some education sessions at professional conferences; read articles in educational journals in your discipline; visit one or two of those digital libraries to see what tutorials, demonstrations, and simulations they've got for your course; and commit to making one or two changes in the course whenever you teach it. If you do that, the course won't get stale, and neither will you.

Mistake #2. Teach without clear learning objectives

The traditional approach to teaching is to design lectures and assignments that cover topics listed in the syllabus, give exams on those topics, and move on. The first time most instructors think seriously about what they want students to *do* with the course material is when they write the exams, by which time it may be too late to provide sufficient practice in the skills required to solve the exam problems. It is pointless—and arguably unethical—to test students on skills you haven't really taught.

A key to making courses coherent and tests fair is to write *learning objectives*—explicit statements of what students should be able to do if they have learned what the instructor wants them to learn—and to use the objectives as the basis for designing lessons, assignments, and exams.^[5] The objectives should all specify observable actions (*e.g., define, explain, calculate, solve, model, critique, and design*), avoiding vague and unobservable terms such as *know, learn, understand, and appreciate*. Besides using the objectives to design your instruction, consider sharing them with the students as study guides for exams. The clearer you are about your expectations (especially high-level ones that involve deep analysis and conceptual understanding, critical thinking, and creative thinking), the more

likely the students will be to meet them, and nothing clarifies expectations like good learning objectives.

Mistake #1. Disrespect students

How much students learn in a course depends to a great extent on the instructor's attitude. Two different instructors could teach the same material to the same group of students using the same methods, give identical exams, and get dramatically different results. Under one teacher, the students might get good grades and give high ratings to the course and instructor; under the other teacher, the grades could be low, the ratings could be abysmal, and if the course is a gateway to the curriculum, many of the students might not be there next semester. The difference between the students' performance in the two classes could easily stem from the instructors' attitudes. If Instructor A conveys respect for the students and a sense that he/she cares about their learning and Instructor B appears indifferent and/or disrespectful, the differences in exam grades and ratings should come as no surprise.

Even if you genuinely respect and care about your students, you can unintentionally give them the opposite sense. Here are several ways to do it: (1) Make sarcastic remarks in class about their skills, intelligence, and work ethics; (2) disparage their questions or their responses to your questions; (3) give the impression that you are in front of them because it's your job, not because you like the subject and enjoy teaching it; (4) frequently come to class unprepared, run overtime, and cancel classes; (5) don't show up for office hours, or show up but act annoyed when students come in with questions. If you've slipped into any of those practices, try to drop them. If you give students a sense that you don't respect them, the class will probably be a bad experience for everyone no matter what else you do, while if you clearly convey respect and caring, it will cover a multitude of pedagogical sins you might commit.

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MULTIPLE COMPARISONS OF OBSERVATION MEANS— ARE THE MEANS SIGNIFICANTLY DIFFERENT?

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Several currently popular methods of ascertaining which treatment (population) means are different, via random samples obtained under each treatment, are briefly described and illustrated by evaluating catalyst performance in a chemical reactor.

In a routine undergraduate classroom application of one-way ANOVA (analysis of variance), the null hypothesis

$$H_0 : \mu_1 = \mu_2 = \dots = \mu_k \quad (1)$$

is tested against the alternative hypothesis that at least two population means are different, given sample means $\bar{x}_1, \bar{x}_2, \dots, \bar{x}_k$ computed from n_1, n_2, \dots, n_k random observations. If H_0 is rejected, it is not always *a-priori* obvious which of the two or more means differ; multiple comparison tests help to provide the answer. We are especially interested in the “fate” of H_0 when the individual treatment/population variances $\sigma_1^2, \sigma_2^2, \dots, \sigma_k^2$ are considered to be equal, because if they are not equal, wide dispersion in the data is most likely the primary cause, and further testing may not be required.

Commonly, the rejection of H_0 is made at a 95%, or at a 99% level of confidence. In the first case, under H_0 , the error probability of falsely rejecting H_0 is (at most) 5%, in the second case, it is 1%. This, so-called Type I error is also known as the level of significance: $\alpha = 0.05$ (significant), and $\alpha = 0.01$ (highly significant), respectively. An H_0 maybe rejected at the significant level, but not necessarily at the highly significant level. Consequently, failure to reject H_0 at $\alpha = 0.05$ automatically implies no rejection at $\alpha = 0.01$, as well. The P- value is defined as the smallest level of significance (*i.e.*, the smallest value of α) that would lead to a rejection of H_0 . The 5% and 1% levels do not have a privileged position, because the real-life significance of the magnitude of the Type I error is left to the tester’s judgment. In the sequel, we shall adhere to the two traditional levels inasmuch as certain statistical tables include only critical values pertaining to $\alpha = 0.05$ and $\alpha = 0.01$ (F- and T- tables are, however, notable exceptions).

MOTIVATION: A CHEMICAL REACTOR WITH DIFFERENT CATALYSTS

In the chemical engineering classroom, we could explore, for instance, the hydrogenation of nitrobenzene^[1] in a

tubular reactor, using three different Ni-based catalysts. Under identical experimental conditions, conversion data shown in Table 1 (page 19) are assumed to be available for testing H_0 : the three mean conversions are the same. The alternative hypothesis, H_a , is that at least two catalysts render different mean conversions. If H_a is upheld, the next question to ask is which catalysts are significantly different, by testing whether $(\mu_3 - \mu_2)$; $(\mu_1 - \mu_3)$; $(\mu_1 - \mu_2)$ differ significantly from zero. This is the goal of multiple comparison tests, following a standard ANOVA applied to H_0 in Eq. (1).

Three fundamental assumptions are now made: (1) the three catalysts act independently of one another; (2) the observed conversions belong to a normal (Gaussian) population, at least approximately; and (3) the three observation sets are homogeneous, *i.e.*, the conversion-population variances are not significantly different. Since, as demonstrated in Appendix 1, the third assumption is not rejected, we expect that ANOVA will be sufficiently robust, even if the conversion data are only approximately normal.

We shall look at two variations of the theme. The first one involves equal observation sizes $n_1 = n_2 = n_3 = 8$. In the second one we stipulate that four of the observations are absent, *i.e.*, $n_1 = 8$; $n_2 = 6$; $n_3 = 6$. The multiple comparison tests are not the same, as seen in the sequel.

Details of ANOVA can be found in undergraduate statistics textbooks, and are omitted here. Table 1 indicates that rejection of H_0 in Eq. (1) carries only a 0.2%, and a 0.1% Type I error, respectively; we can say that H_0 is soundly defeated. Our inferences about the three catalyst populations (*i.e.*, very large number of observations) are data-specific, of course. With dif-



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ferent sets of observation, the numerical values of the F – statistic and our inferences may well be different.

We now proceed to find out how many of the three catalysts can be expected to behave differently from the others via multiple comparison tests.

MULTIPLE COMPARISONS: EQUAL-SIZE OBSERVATIONS

a. The Bonferroni method^[2-4]

This method is based on the concept of the simultaneous level of confidence (SLC), which guarantees that each individual difference in means carries a level of significance α_B as given below:

$$\alpha_B = \frac{\alpha}{k(k-1)} \quad (2)$$

The degrees of freedom for error are $\sum_{i=1}^k n_i - k$.

In our reactor, $n_1 + n_2 + n_3 - k = 6$, hence $\alpha_B = 0.0083$ for $\alpha = 0.05$, and $\alpha_B = 0.0017$ for $\alpha = 0.01$. The confidence interval may be written as

$$(x_i - x_j) - t[\alpha_B; k(n-1)]\sqrt{2(MSE)/n} < (\mu_i - \mu_j) < (x_i - x_j) + t[\alpha_B; k(n-1)]\sqrt{2(MSE)/n} \quad (3)$$

for the difference between two arbitrary population means. The degree of freedom of the T – statistic is $k(n-1)$. We find in T – distribution tables, e.g.,^[5] the values: $t(0.01;21) = 2.518$; $t(0.005;21) = 2.831$; $t(0.001;21) = 3.527$. By linear extrapolation we obtain $t(0.0083;21) = 2.623$ and $t(0.0017;21) = 3.406$. With $MSE = 7.786$, the confidence intervals in Table 2 are obtained.

What can we conclude from the results? Since $(\mu_3 - \mu_2) = 0$ is included in BCI_{32} , we cannot assert that the two means are significantly different. BCI_{12} and BCI_{13} , however, exclude zero—meaning that μ_1 appears to be significantly different from μ_2 and μ_3 . This conclusion is supported even at the highly significant level. In other words, the *mean* performance of Catalyst 1 appears to be different from (in fact, better than) the performance of the other two catalysts, but the *mean* performance of Catalyst 2 does not appear to be significantly different from the performance of Catalyst 3.

b. The Tukey method^[6,7]

In this method the statistic Q belongs to the *studentized range distribution*, where the degrees of freedom are $DF_1 = k$ and $DF_2 = k(n-1)$. Critical values of $Q[\alpha; k, k(n-1)]$ are tabulated at $\alpha = 0.05$ and $\alpha = 0.01$,^[8-10] but the Q-tables are not widely available in the textbook literature. We need linear interpolation based on the tabulated values $q[0.05;3,20] = 3.58$; $q[0.05;3,24] = 3.53$; $q[0.01;3,20] = 4.64$; $q[0.01;3,24] = 4.55$, yielding $q[0.05;3,21] = 3.57$ and $q[0.01;3,21] = 4.62$. The confidence intervals given by the expression

$$(x_i - x_j) - Q[\alpha; k, k(n-1)]\sqrt{MST/n} < (\mu_i - \mu_j) < (x_i - x_j) + Q[\alpha; k, k(n-1)]\sqrt{MST/n} \quad (4)$$

are given in Table 2. Agreement with the Bonferroni method is not the same for $(\mu_1 - \mu_3)$, inasmuch as the null hypothesis of no difference between them can be rejected only at the significant, but not at the highly significant, level (if the lower bound of the interval is set to zero, linear interpolation between the two critical values would indicate a P – value of about 0.023).

c. The Scheffé method^[11,12]

In establishing the confidence intervals, the Snedecor-Fischer F – distribution provides values of the critical statistic, when two individual means are compared:

$$(x_i - x_j) - \Phi(\alpha; k, n) < (\mu_i - \mu_j) < (x_i - x_j) + \Phi(\alpha; k, n) \\ \Phi(\alpha; k, n) \equiv \sqrt{2(k-1)(MSE)F[\alpha; k-1, n-k]/n} \quad (5)$$

and, specifically in our case,

$$(x_i - x_j) - 0.5\sqrt{(MSE)F[\alpha; 2, 21]} < (\mu_i - \mu_j) < (x_i - x_j) + 0.5\sqrt{(MSE)F[\alpha; 2, 21]} \quad (6)$$

The significant and highly significant critical F – values are $f[0.05;2,21] = 3.47$, and $f[0.01;2,21] = 5.78$.

The confidence intervals in Table 2 indicate complete qualitative agreement with the Bonferroni method, and nearly complete agreement with the Tukey method.

d. The Duncan method^[13,14]

In this approach, differences in the sample means are compared to a statistical parameter to ascertain significance; there are no confidence intervals to deal with. Only equal-size observations can be considered for the test. We have seen that in our case $x_1 > x_3 > x_2$, hence we have two single ranges ($p = 2$) and one double range ($p = 3$) of sample mean differences. If any difference exceeds the numerical value of the Duncan parameter

$$R_p = r_p \sqrt{(MSE)/n} = 0.9865r_p; p = 2, 3 \quad (7)$$

then that difference is at least significant, or even highly significant. The quantity r_p , called the *least significant studentized range*, depends on α and the degree of freedom of $MSE = 7.786$, i.e., $DF = 21$. Critical tables of r_p are provided in various textbooks, e.g.,^[15-17] for $\alpha = 0.05$ and $\alpha = 0.01$. In our case, $r_2 = 2.950$ ($\alpha = 0.05$) and 4.024 ($\alpha = 0.01$), and $r_3 = 3.097$ ($\alpha = 0.05$) and 4.197 ($\alpha = 0.01$) at $DF = 20$. The next set of critical values given for $DF = 24$ differing but slightly from the $DF = 20$ values, interpolation may be bypassed and we accept $R_2 = 2.910$ and $R_3 = 3.055$ at $\alpha = 0.05$, and $R_2 = 3.970$; $R_3 = 4.140$ at $\alpha = 0.01$. The conclusion drawn from this test is that $(\mu_1 - \mu_3)$ and $(\mu_1 - \mu_2)$ are different from zero even at a highly significant level, but $H_0: (\mu_3 - \mu_2) = 0$ is acceptable at a significant (and, of course, at a highly significant) level.

MULTIPLE COMPARISONS: UNEQUAL-SIZE OBSERVATIONS

We now proceed to postulate that the last two conversion measurements with Catalysts 2 and 3, i.e., the entries 81 and 83%, and 80 and 84%, respectively, are unknown. In this instance, the mean conversions are $\bar{x}_1 = 84\%$; $\bar{x}_2 = 77\%$; $\bar{x}_3 = 79\%$, and on account of the computed F – statistic of 15.45, H_0 in Eq. (1) is rejected very strongly, with a Type I error less than 0.1%. We are now ready to investigate the differences in conversion means.

For the establishment of the confidence intervals, there are essentially two modifications with respect to the equal-size observations case. The MSE multiplier for the confidence intervals becomes $(n_1^{-1} + n_2^{-1} + \dots + n_k^{-1})$, and the second degree of freedom is smaller due to the smaller number of observations. In our case $MSE = 5.988$, and the MSE-multipliers are $7/24$ and $1/3$. For the Bonferroni method, the critical T – statistics are $t[0.00833; 17] = 2.678$ ($\alpha = 0.05$) and $t[0.00167; 17] = 3.521$ ($\alpha = 0.01$). In the Scheffé method, $f[0.05; 2; 17] =$

TABLE 1
Exit conversions in a tubular reactor using three different catalysts. The observations are hypothetical under identical experimental conditions.

Catalyst 1	Catalyst 2	Catalyst 3		
82	74	79		
86	82	79		
79	78	77		
83	75	78		
85	76	82		
84	77	79		
86	81	80		
87	83	84		
Means:	84	78.25	79.75	
ANOVA (equal – size)				
Source	SS	DF	Mean SS	F
Treatments	142.34	2	71.17	9.14
Error	163.50	21	7.786	
Total	305.84	23		
Critical values of the F – statistic: 3.47 ($\alpha = 0.05$); 5.78 ($\alpha = 0.01$); 9.77 ($\alpha = 0.001$); P – value: ≈ 0.002				
ANOVA (unequal – size) (Last two entries in column 2 and 3 above are removed)				
Source	SS	DF	Mean SS	F
Treatments	185.0	2	92.5	15.45
Error	101.80	17	5.988	
Total	286.80	19		
Critical values of the F – statistic: 3.59 ($\alpha = 0.05$); 6.11 ($\alpha = 0.01$); 10.66 ($\alpha = 0.001$); P – value: < 0.001				

TABLE 2
Lower (LB) and upper (UB) bounds of the confidence intervals for mean conversions with equal-size observations
B: Bonferroni; T: Tukey; S: Scheffé
 $\alpha = 0.05$ $\alpha = 0.01$

Difference	Bound	B	T	S	B	T	S
$\mu_1 - \mu_2$	LB	2.091	2.228	4.401	0.998	1.192	3.646
	UB	9.409	9.272	9.599	10.502	10.308	10.354
$\mu_1 - \mu_3$	LB	0.591	0.728	2.401	0.502	- 0.308	1.646
	UB	7.909	7.772	7.599	9.002	8.808	8.354
$\mu_3 - \mu_2$	LB	- 2.159	- 2.022	- 0.599	- 3.252	- 3.058	- 1.354
	UB	5.159	5.022	4.599	6.252	6.058	5.354

3.59, and $f[0.01;2;17] = 6.11$. The corresponding confidence intervals in Table 2 indicate complete qualitative agreement among the three methods.

DISCUSSION

What are the relative merits of the three methods? In accordance with pertinent literature, the following statements can be made. (A) The Bonferroni method is “very effective” for small-size comparisons, and if the observation-set sizes are equal, Tukey’s method is “optimal” in the sense of yielding the shortest confidence interval.^[18] (B) If the product of the two degrees of freedom of the test statistics is large, the smaller of the Bonferroni and Scheffé intervals are to be taken.^[19] Tables 1 and 2 are in compliance with (A), excepting the Tukey interval for $(\mu_1 - \mu_3)$ at $\alpha = 0.01$, but this result is not surprising in view of the usually higher power of the Bonferroni method for small k .

One advantage of dealing with confidence intervals with only positive bounds resides in the rejection of the null hypothesis that a difference in the related two population means is not significant. The shorter the confidence interval, the less likely that the lower bound will be negative, therefore $H_0: (\mu_i - \mu_j) = 0$ will be rejected. This is the desired outcome, since rejection of a null hypothesis is a statistically stronger result than failure to reject it.

It follows from what we have already stated at the outset that we would be hesitant about preferring Catalyst 1 if the population variances were shown to be unequal (the case of heteroscedasticity), especially at a very high degree of confidence. Data transformation techniques, *e.g.*,^[20] for the removal of heteroscedasticity are known, but they are beyond the objective of this paper.

Multiple comparison methods can readily be extended to contrasts, where arbitrary linear combinations of population means can be treated. A short description is given in Appendix 2.

Finally, we may be interested in comparing our mean conversions with the mean conversion obtained with, for instance, a Ni-free metal oxide catalyst. This exercise would fall into the “treatment comparison with control” test category. In so

doing, the hypotheses^[21]

$$\begin{aligned} H_0: \mu_0 &= \mu_i; i = 1, \dots, k \\ H_1: \mu_0 &\neq \mu_i; i = 1, \dots, k \end{aligned} \quad (8)$$

are tested by the Dunnett parameter^[22,23]

$$D_1 = \frac{x_i - x_0}{\sqrt{2(\text{MSE})/n}} \quad (9)$$

where the 0 subscript denotes control. If the absolute value of d_1 exceeds the critical value $d[(\alpha/2);k,DF_2]$ with first degree of freedom k , and DF_2 , the second degree of freedom of MSE, which includes the control observations, then H_0 in Eq. (8) is rejected at a chosen α . Critical Dunnett parameter values are tabulated for two sided tests, *e.g.*, in Reference 24.

For our reactor, if we assume a control conversion set of 73,80,76,82,77,75,79,83%, we obtain $SSE = 247.88$ and $MSE = 247.88/[4(8-1)] = 8.8528$. The values $d_1 = 3.949$; $d_2 = 0.084$; $d_3 = 1.0925$ are computed from Eq. (9). Since at $\alpha = 0.05$, $d[0.025;3,24] = 2.51$ and $d[0.025;3,30] = 2.47$, and at $\alpha = 0.01$, $d[0.005;3,24] = 3.22$, and $d[0.005;3,30] = 3.15$, only the mean of Catalyst 1 appears to be significantly different from μ_0 .

CLASSROOM EXPERIENCE

Respecting the necessity of numerous other topics that also have to be covered in the introductory probability and statistics course taught to second year undergraduate ChE students, this author could go beyond Duncan’s multiple-range method only to a rather limited extent in dealing with the subject matter. Class reaction was (not unexpectedly) mixed, depending on the degree of willingness to accept the statistical way of reasoning. Students exposed to statistical techniques during their work terms (the co-op structure of engineering programs at Waterloo alternates in-house lecture terms and practice-based work terms) generally showed more appreciation, if not enthusiasm, than their fellow classmates with different work-term orientation. The author’s quest for a course devoted solely to the analysis of variance including multiple comparisons is motivated not only by personal experience arising from the introductory course, but also by the steadily increasing importance of probability-based thinking in all walks of life.

TABLE 3
Lower (LB) and upper (UB) bounds of the confidence intervals for mean conversions with unequal – size observations.

B: Bonferroni; T&: Tukey; S: Scheffé
 $\alpha = 0.05$ $\alpha = 0.01$

Difference	Bound	B	T	S	B	T	S
$\mu_1 - \mu_2$	LB	3.461	3.607	3.459	2.346	2.570	2.380
	UB	10.539	10.393	10.541	11.654	11.430	11.619
$\mu_1 - \mu_3$	LB	1.461	1.607	1.217	0.346	0.570	0.064
	UB	8.539	8.393	8.783	9.654	9.430	9.936
$\mu_3 - \mu_2$	LB	- 1.783	- 1.627	- 1.541	- 2.975	- 2.736	- 2.619
	UB	5.783	5.627	5.541	6.975	6.736	6.619

&modified for unequal-size observation sets [Devore, J.,L., loc.cit., (2004), p.434.]

FINAL REMARKS

Because the statistically informed chemical engineer is especially valuable to industry, education of our students in statistical techniques is highly desirable in today's world. Multiple comparisons make up an integral part of this education in demonstrating the utility of statistical approaches, and the importance of applying proper judgment to test results.

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NOMENCLATURE

B_1, B_2	Bartlett-parameters in Equations (A.4;A.7)
BCI_{ij}	Bonferroni confidence interval for $(\mu_i - \mu_j)$
C	Bartlett-parameter in Equation (A.6)
c_i	contrast coefficient [Eq. (11)]
DF	degree of freedom
d	two-sided Dunnett's critical parameter [Eq. (13)], at level of significance α
F	critical parameter of the Fischer-Snedecor F-distribution, at level of significance α
f	numerical value of an F-statistic
G	Cochran statistic in Eq. (A.2)
H_a	hypothesis alternative to null hypothesis H_0
H_0	Null hypothesis
k	number of treatments (observation sets)
LB	lower bound of a confidence interval
M	Bartlett-parameter in Eq. (A.5)
MSE	mean square of experimental errors
MS	mean sum of squares
N	total number of observations
n	number of observations in each equally sized treatment
n_i	number of observations in the i - th treatment
Q	Tukey - statistic in Eq. (4)
q	numerical value of a Q - statistic
r_p	least significant studentized range in Duncan's test in Eq. (5)
R_p	least significant range of means in Duncan's test in Eq. (5)
S^2	sample variance
SCI	Scheffé confidence interval
SS	sum of squares
T	Student's T - statistic
t	numerical value of a T - statistic
UB	upper bound of a confidence interval
x_i	mean value of x_i observations in the i -th treatment

GREEK SYMBOLS

α	level of significance (Type I error, i.e. the maximum value of the probability of rejecting H_0 when H_0 is true)
α_B	simultaneous level of significance (Bonferroni method)
μ_i	the (true) population mean of observations due to the i - th treatment

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APPENDIX 1. TESTING THE HYPOTHESIS OF EQUAL-POPULATION VARIANCES

The null hypothesis

$$H_0: \sigma_1^2 = \sigma_2^2 = \dots = \sigma_k^2 \quad (\text{A.1})$$

is a statement of homoscedasticity, or homogeneity of variances, against the alternative hypothesis H_a : at least two variances are unequal.

(i) Equal-size observations

The Cochran test^[27-31] compares the numerical value of the G – statistic

$$G = \frac{\max_{(i)} S_i^2}{\sum_{i=1}^k S_i^2} \quad (\text{A.2})$$

composed of the sample variances, to critical values of $g(\alpha; k, n)$ tabulated for $\alpha = 0.05$ and 0.01 ; H_0 in Eq. (A.1) is rejected if $G > g(\alpha; k, n)$. In our case $g = 11.857 / (6.857 + 11.357 + 5.0714) = 0.4877$ being less than $g(0.05; 3, 8) = 0.6530$,^[27-32] we fail to reject the assumption of variance homogeneity among the three sets of conversion.

(ii) Unequal-size observations

Two versions of the Bartlett test for Eq. (A.1) are given in the literature. In the earlier version^[33,34] of the test a pooled variance estimate

$$S_p^2 = \frac{\sum_{i=1}^k (n_i - 1) S_i^2}{N - k} \quad (\text{A.3})$$

is used to compute the Bartlett – statistic

$$B_1 = \frac{M}{C} \ln(10) \quad (\text{A.4})$$

where

$$M = (N - k) \log_{10}(S_p^2) - \sum_{i=1}^k (n_i - 1) \log_{10}(S_i^2) \quad (\text{A.5})$$

and

$$C = 1 + \frac{1}{3(k-1)} \left(\sum_{i=1}^k \frac{1}{n_i - k} - \frac{1}{N - k} \right) \quad (\text{A.6})$$

The B_1 – statistic is approximately chi – square distributed with $(k - 1)$ degrees of freedom.

In the more recent version,^[35] the pooled variance computed via Eq. (A.3) is used to obtain the B_2 – statistic defined as

$$B_2 = \frac{\left[\prod_{i=1}^k (S_i^2)^{n_i - 1} \right]^{1/(N-k)}}{S_p^2} \quad (\text{A.7})$$

belonging to the Bartlett – distribution. It has the curious, if not confusing, distinction that H_0 is rejected if B_2 has a numerical value less than the composite critical value

$$b_k(\alpha; n_1, n_2, \dots, n_k) = \frac{\sum_{i=1}^k n_i b_k(\alpha; n_i)}{N} \quad (\text{A.8})$$

For our catalysts, $S_1^2 = 6.857$; $S_2^2 = 8$; $S_3^2 = 2.8$, hence $S_p^2 = 6$; $M = 0.62441$; $C = 1.0777$, and $b_1 = 1.334$. At $\alpha = 0.05$, the critical chi – square value at $DF = 2$ is 5.991 (found in any statistics textbook or tables), and we fail to reject H_0 in Eq. (A.1). In the second version, B_2 has the numerical value of 0.919 from Eq. (A.7). The critical value at $\alpha = 0.05$ is computed^[36,37] as $b_3(0.05; 8, 6, 6) = [8(0.7387) + 2(6)(0.6483)] / 20 = 0.6845$ via Eq. (A.8). Since (*careful!*) 0.919 is *larger* than 0.6845, we fail to reject the null hypothesis of equal population variances (at $\alpha = 0.01$, the critical value, $[8(0.6282) + 2(6)(0.5149)] / 20 = 0.5602$ is expectedly lower).

APPENDIX 2. ELEMENTARY CONCEPTS OF CONTRAST THEORY

Suppose we have tested a larger number – say, five – catalysts in our reactor and have at our disposal five observation means $\bar{x}_1, \bar{x}_2, \dots, \bar{x}_5$. We may want to test more involved null hypotheses, e.g., $H_0: (\mu_1 - \mu_2) - (\mu_3 - \mu_4) = 0$; $H_0: (\mu_1 - \mu_3) - (\mu_2 - \mu_5) = 0$, etc. for some reason. These combinations are called contrasts. In general, a contrast is $c_1\mu_1 + c_2\mu_2 + \dots + c_m\mu_m$ where the c_i coefficients can be positive, negative, or zero. The confidence intervals are accordingly more complicated than for the ones shown in the text. For example, if we employ the Scheffé method, the expression

$$\sum_{i=1}^m c_i x_i - \left[\sum_{i=1}^m \frac{c_i^2}{n_i} \right]^{1/2} \Psi(\alpha; n, m) < \sum_{i=1}^m c_i \mu_i < \sum_{i=1}^m c_i x_i + \left[\sum_{i=1}^m \frac{c_i^2}{n_i} \right]^{1/2} \Psi(\alpha; n, m)$$

$$\Psi(\alpha; n, m) \equiv \sqrt{(n-1)(\text{MSE})F(\alpha; n-1, (n-m))} \quad (\text{A.9})$$

provides the α -level confidence interval in the case of unequal-size observation sets. If $m = 2$, Eq. (5) is regained.

For the sake of illustration, we assume that four catalysts with observation set sizes $n_1 = 10$; $n_2 = 8$; $n_3 = 7$; $n_4 = 9$ yield mean conversions 72; 75; 80; 82%, respectively, and $\text{MSE} = 195.3$. We propose to set the null hypothesis that $(\mu_4 - \mu_2) - (\mu_3 - \mu_1) = 0$. Here, $c_1 = 1$; $c_2 = -1$; $c_3 = -1$ and $c_4 = 1$. Also, $n - m = 34 - 4 = 30$. Accordingly, $c_1 x_1 + c_2 x_2 + c_3 x_3 + c_4 x_4 = -1$, and $(\sum c_i^2 / n_i)^{1/2} = 0.6921$. Since $f(0.05; 3, 30) = 2.92$, Eq. (A.9) yields $LB = -29.627$; $UB = 27.627$, and we fail to reject the null hypothesis (P -value ≈ 0.004). \square

A PROCESS DYNAMICS AND CONTROL EXPERIMENT

for the Undergraduate Laboratory

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While the variety of experiments contained in typical chemical engineering laboratory courses continues to broaden, it remains important to include experiments or projects involving process dynamics and control. And, in fact, modern hardware and software make such experiments more and more possible, realistic, and interesting. The experiment described here employs relatively simple and inexpensive equipment to demonstrate several important aspects of process dynamics and control, both model-free and model-based analyses of process dynamics data, and two related controller tuning methods.

This experiment permits the students to observe the response of a flow system to impulse injection of a tracer, to collect large amounts of data quickly, and to process the data rapidly using Excel and LabVIEW or QuickBASIC programs. It also permits students to observe, in action and with short time constants, the operation of a PID feedback control system. The students see the actuator (a stepper-motor driven valve) move, see dye enter and pass through a glass flow system, see the transducer (a spectrophotometer) respond to changes in the measured variable, and see the controller (a LabVIEW program) respond to changes in the measured variable and drive the actuator.

From a pedagogical standpoint, the experiment—described in enough detail to be accurately reproduced—provides a comprehensive treatment of a PID controlled flow system, including both standard and more advanced topics. It demonstrates also modern data acquisition and data processing techniques, including the use of LabVIEW. It is designed for use in either a junior- or senior-level laboratory, but should be preceded by or taught in parallel with a course in process dynamics and control.

APPARATUS

The apparatus is shown schematically in Figure 1. To remove dissolved air, house water is stored in a polyethylene carboy and supplied to the experiment by a magnetic-drive

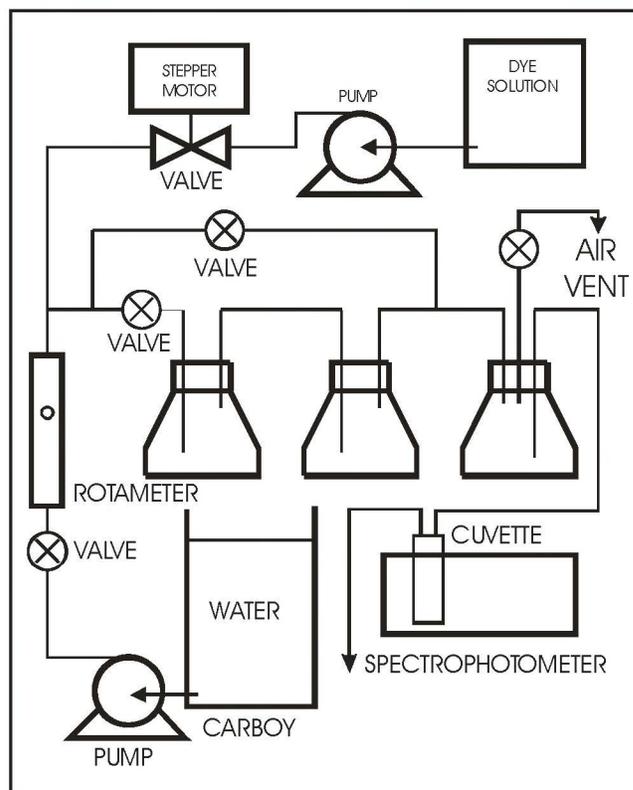


Figure 1. Schematic diagram of the apparatus, showing the three flasks and valving of the flow system, the water feed system, the dye feed system with stepper-motor controlled valve, and the spectrophotometer with a flow cuvette.



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centrifugal pump. A rotameter measures the flow rate, which is controlled by a manual metering valve. The flow system consists of three Erlenmeyer flasks, each of volume about 290 ml. The flasks are closed by Teflon stoppers sealed by o-rings, and are connected by 1/4 inch stainless tubing. A ball valve with a connection for a syringe allows impulse injection of dye solution at the entrance to the flow system. Two stainless ball valves allow three flow patterns, namely: (a) flow through one flask only, (b) flow through three flasks in series, and (c) partial flow through the first two flasks in series and full flow through the last tank. The tubing connecting the first two tanks is designed to prevent air accumulation in these tanks, while the last tank is designed to accumulate air, which can be vented via a valve before a run. This avoids the passage of air bubbles to the downstream spectrophotometer. A ball valve connected to a tee at the entrance to the flow system allows a dye solution (typically 10 ml of methylene blue dye at a level of 50 mg/L) to be injected using a syringe.

The transient dye concentration in the effluent water from the flow system is measured by a spectrophotometer (Milton Roy, Model Spec 20). A test tube with an o-ring-sealed Teflon stopper holding inlet and outlet tubes is inserted into the spectrophotometer and serves as a flow cuvette. The spectrophotometer is set at a wavelength of 640 nm, with the 0 to 1 volt analog output signal connected to a National Instruments A/D board (PCI-6043E).

Methylene blue solution (10 mg/L) held in a 20 L polyethylene carboy is pumped to stepper-motor (Arrick Robotics) driven needle valve. This valve controls the flow of the dye solution to a mixing tee upstream of the three-flask flow system. The stepper-motor is driven by signals from a LabVIEW VI that implements a standard PID (Stephanopoulos^[1]) control algorithm, corresponding to the following discrete-time algorithm

$$\text{Valve position} = \text{Base position} + K_C[\text{Present error} + (1/T_I) \text{Integral of past errors} + T_D \text{Derivative of error}]$$

Here K_C is the controller gain, T_I is the integral time, T_D is the derivative time, and error is the set point less the measured variable. The valve position is measured in stepper-motor steps (400 steps = 1 turn). The algorithm departs slightly from ideality in that the valve motion is limited to 100 positive or negative steps in a single iteration. When the system is close to the steady state and changes in valve position are small, this feature will have no effect.

The PID algorithm is iterated every four seconds, with a typical run involving 300 iterations, corresponding to 20 minutes. Users can change the set point and the three controller parameters at any time during the run, and a full record of the controller parameters and state variables is written to a spreadsheet file at the end of the run.

OPERATION

There are three modes of operation.

Impulse Response Mode

Prior to the run the spectrophotometer is zeroed and then set to 100 percent transmittance when the dye concentration is zero. The ball valves are set to give single-tank flow, three-tanks-in-series flow, or parallel flow. The rotameter is used to set the water flow rate to a value between 300 and 1200 ml/min. At time zero about 10 ml of methylene blue solution (100 mg/L) is injected rapidly through a ball valve at the entrance to the flow system, and at the same time a LabVIEW program (VI) is started. The program samples the spectrophotometer output signal at a selectable rate of roughly 2 samples per second, for a time long enough that the dye concentration has returned to zero. The program converts the transmittance signal to concentration, and also calculates the mean residence time from the concentration vs. time signal. The data are also written to a spreadsheet file for later plotting and processing.

Control Mode

With the flow rate and the flow system configuration set and the dye solution pump running, the LabVIEW PID control program is started. The students first set the controller parameters (K_C , T_I , T_D), and then the set point (typically about 50 percent Spec 20 transmittance, corresponding to 0.6 dimensionless concentration units). The program samples the transmittance signal every four seconds, converts it to dimensionless concentration, implements the PID algorithm, and plots the concentration, error, and valve position as functions of time. (Full valve travel is 3200 steps, equivalent to 8 turns, and the program limits the number of steps to 100 at each iteration.) At any time during the 20 minute run (300 points at 4 seconds per point) the students can change the set point or the controller gains or the flow system configuration. At the end of the run complete data on controller parameters, dye concentration, and valve position are written to a spreadsheet file for later plotting and analysis.

Step Response Mode

With the needle valve opened manually four turns, the system is allowed to reach steady state, and 400 baseline concentration points are acquired. Then the valve is manually opened two more turns, and 400 additional points are acquired. Subtracting the average baseline concentration from the step transient produces the desired step response, as shown in Figure 2.

MODELING AND PARAMETER ESTIMATION

The program used to acquire the impulse injection data also computes the mean residence time, based on the equation

$$\tau = \frac{\int_0^{\infty} tCdt}{\int_0^{\infty} Cdt} \quad (1)$$

where τ is the mean residence time, C is effluent stream dye concentration and t is time. If Q is the volumetric flow rate

and V is the volume of the flow system, then

$$V = Q\tau \quad (2)$$

Here the volume of the system is defined as the volume accessible to dye and enclosed within boundaries outside of which no dye can diffuse or move.

Since Q is known, the students can compare the calculated value of V with the known volume, 290 ml for flow through a single flask, and 870 ml for flow involving all three tanks. Note that this analysis is not based on the assumption that the flasks are well mixed, and in fact is not based on a model for the flow system. But linearity of the system with respect to dye concentration measurement, and that no dye can penetrate upstream of the injection point, are assumed.

In contrast, if we have some information about the structure of the flow system, we can attempt to estimate the value of one or more parameters of a model of the system. Such a model is shown in Figure 3. The model consists of three well-mixed tanks, corresponding to the three flasks in the flow system, and connected in the same way. The state variables of the model are the concentrations (x_1 , x_2 , and x_3) in the tanks, and the measured variable is the dye concentration (x_3) in the last tank. The undetermined parameters of the model, to be estimated by finding a least-squares fit to the data,^[4] are b_1 , the amount of dye injected, b_2 , the overall flow rate, and b_3 , the flow rate through the lower leg of the flow system.

The state equations of the model, used in the parameter estimation step, are as follows:

$$dx_1 / dt = -(b_2 / V_f)X_1, \quad x_1(0) = (b_1 / V_f)(b_2 / b_3) \quad (3)$$

$$dx_2 / dt = (b_2 / V_f)(x_1 - x_2), \quad x_2(0) = 0 \quad (4)$$

$$dx_3 / dt = (b_2 / V_f)x_2 - (b_3 / V_f)x_3, \quad x_3(0) = (b_1 / V_f)(b_3 - b_2) / b_3 \quad (5)$$

Here x_1 , x_2 , and x_3 are the dye concentrations in the three flasks, V_f is the volume of each flask, b_1 is the amount of dye injected, b_2 is the flow rate through the first two flasks and b_3 is the total flow rate through the whole system.

The best (least-squares) parameter values are determined by a QuickBASIC program implementing a standard Gauss-Newton non-linear regression algorithm.^[4] The program also computes the parameter correlation matrix and the variance-covariance matrix and the confidence limits for the estimated parameter values. Note that the amount of dye actually injected is not known, while the total flow rate is known and can be compared to the estimated value. Note also that parameter b_2 , the flow rate through the first two flasks, cannot be measured directly with the existing apparatus, which illustrates the power of using modeling and parameter estimation methods for indirect measurement of quantities that cannot be directly measured.

RESULTS

Impulse Response Runs

Figure 4 shows the concentration vs. time data, and also the best fit based on the model, for an impulse response run in which all the flow passes through a single flask only. Samples were taken every 0.40 seconds. The data correspond closely to the single exponential expected for impulse injection of tracer into a well-mixed tank. The first few points (not shown or fitted) were close to zero, due to the plug flow in the connecting tubing of the flow system. The concentration curve (solid line)

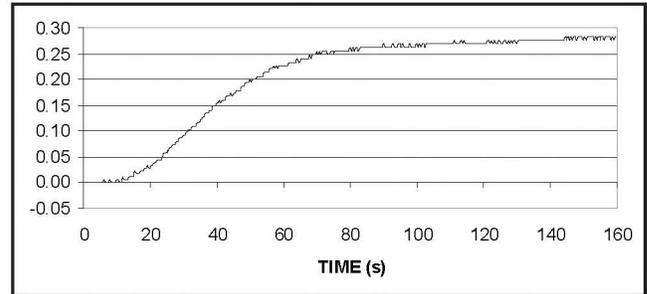


Figure 2. Shifted step response for three-tank flow configuration, valve opened 800 steps from base position.

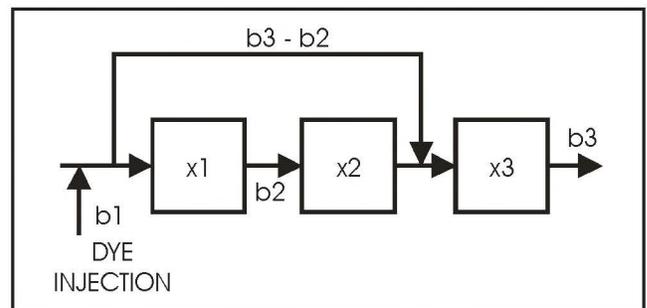


Figure 3. Schematic diagram of a model of the flow system. The parameters to be estimated are b_1 , the amount of dye injected, b_2 , the flow rate through the first two flasks and b_3 , the flow rate through the system. The state variables are dye concentrations x_1 , x_2 , and x_3 .

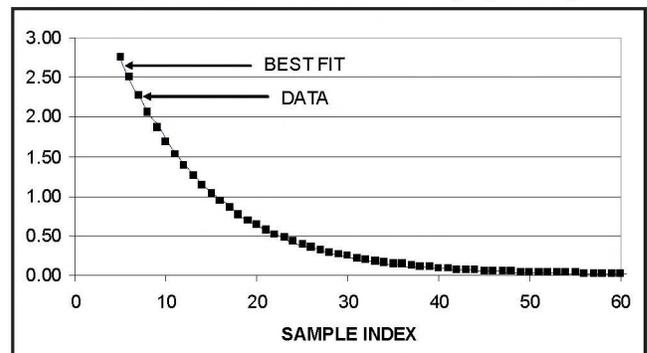


Figure 4. The experimental concentration vs. time data for an impulse injection run in which the lower ball valve was closed, thus allowing the total flow to pass through only one flask in series. Also shown, as a solid line, is the best fit based on the model.

based on the model fits the data almost perfectly, and is also an almost perfect exponential. Parameter b_2 , representing the flow rate through the first two flasks, was less than 10% of the total flow, but not the expected value of zero. Parameter b_3 , the total flow rate, was 956 ml/min, reasonably close to

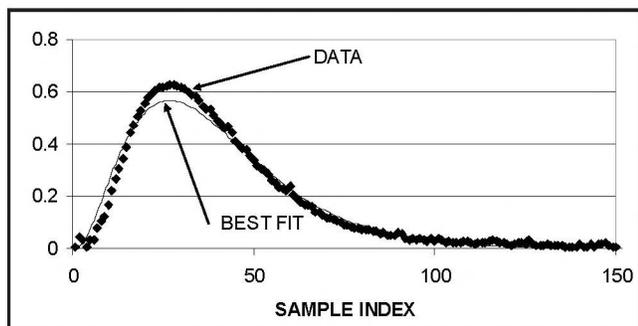


Figure 5. The experimental concentration vs. time data for an impulse injection run in which the upper ball valve was closed, thus allowing the total flow to pass through three flasks in series. Also shown is the best fit based on the model.

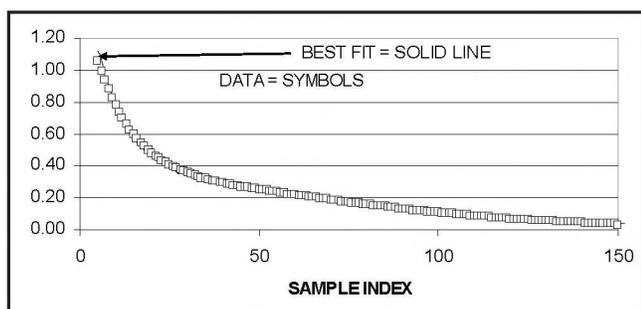


Figure 6. The experimental concentration vs. time data for an impulse injection run in which both ball valves were open, thus allowing some water to flow through three flasks in series, and the rest to pass through only the last flask. Also shown is the best fit based on the model.

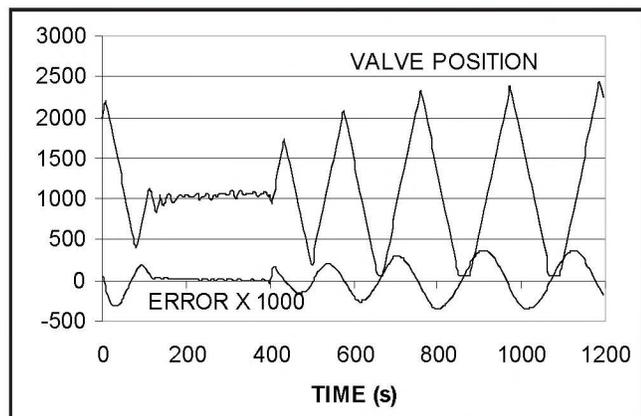


Figure 7. Error and valve position for PI control run, with $K_C = 5000$ and $T_I = 30$. Initially flow was through a single tank and the error approached zero relatively rapidly. At time = 400 seconds, the flow configuration was changed to three tanks in series, the system became unstable, and limit cycle oscillations resulted.

the measured value of 860 ml/min. These results reflect the normal uncertainty associated with parameter estimates.

Figure 5 shows the concentration vs. time data for an impulse injection run in which all the flow passes through three flasks in series, and shows also the best fit based on the model. Note that the fit is quite good, but not perfect. The estimated flow through the first two flasks is essentially equal to the total flow rate, in accord with the physical situation. The estimated system flow rate is reasonably close to the actual flow rate, as expected.

Figure 6 shows the concentration vs. time data for an impulse response run in which the flow passes partly through three flasks and partly through only one flask (parallel flow). The initial shape is very close to the single exponential corresponding to tracer injection into a single well-mixed vessel. Later dye that has passed through the first two flasks appears in, and increases, the spectrophotometer signal. The small delay near time zero corresponds to plug flow in the tubing that connects the flasks to each other and to the spectrophotometer. The run duration was 290 seconds, during which 200 data points were acquired and processed. There is no evidence of random behavior that might arise from turbulent poorly mixed flow in the flasks, although such behavior does appear at very low flow rates.

Figure 6 also shows the best fit based on the model. In general the fit is quite good. The best-fit value of b_1 , representing the amount of dye injected, could not be checked since the amount of dye injected was not known. The value of b_2 , the flow rate through the first two flasks, was 378 ml/min. The value of the overall flow rate, namely $b_3 = 780$ ml/min, was reasonably close to the measured value of 850 ml/min. The fair, but not perfect, agreement illustrates for the students realistic aspects of the power and limitations of modeling and parameter estimation methods. The students see also how quantities such as the lower leg flow rate, not directly measurable, can be estimated by using a model and parameter estimation.

PI Control Runs

A PI control run was made with gains $K_C = 5000$, $T_I = 30$, and $T_D = 0$ and (initially) flow through a single flask. As shown in Figure 7, the error exhibited a rapidly damped oscillation in the first part of the run, corresponding to an essentially stable system. (Note, however, a low-amplitude, high-frequency valve oscillation, probably reflecting the discrete-time nature of the PID algorithm.) Following a flow configuration change to three flasks in series, the system was no longer stable, began an increasing oscillation, and rapidly entered a large-amplitude, low-frequency limit cycle in which the valve position eventually reached its lower limit. This behavior shows clearly the potentially destabilizing effect of adding time lag to a feedback loop.

The fact that the system shows an oscillatory instability as the gains are increased is consistent with a root locus analy-

sis,^[1] based on a transfer function that corresponds to three well-stirred tanks (not of equal volume) under PI control. As an example of such a system we choose an open-loop transfer function

$$G(s) = K(s + 0.5) / s(s + 1)(s + 2)(s + 3) \quad (6)$$

This transfer function corresponds to the schematic root locus plot in Figure 8, which shows that the corresponding closed-loop system is stable for small positive gains K , exhibits an exponentially decaying oscillation as the gain is increased, and begins an exponentially increasing oscillation as the gain increases beyond a critical value. This is in qualitative agreement with the observed behavior, except that nonlinearities produce a limit cycle instead of an exponentially increasing oscillation.

Controller Tuning

While the gain parameters for a system equipped with a PID controller can be selected by trial and error, there are well-developed methods for calculating values that are in some sense optimal, or at least satisfactory. Perhaps the best known methods are those of Ziegler and Nichols.^[2,3]

In the open-loop Ziegler-Nichols version, the response of the system to a step change in the control variable is recorded and used to calculate values for the gain K_C , the integral time T_I , and the derivative time T_D . These parameters appear in the controller transfer function G_C as follows:

$$G_C(s) = K_C \left[1 + \left(1/T_I \right) \left(1/s \right) + T_D s \right] \quad (7)$$

A typical step response, corresponding to flow through three tanks in series, is shown in Figure 2. This response was generated by manually opening the control valve from 5 turns to 7 turns, and then shifting the concentration origin to zero. Based on the times corresponding to concentration increases of 28.3% and 63.2% of the steady state change, namely 28 and 45 seconds, the PID parameters were calculated as $K_C = 4771$, $T_I = 38.8$, and $T_D = 9.7$.

The PID controller parameters determined by the open-loop Ziegler-Nichols method were used in a control run, with the valve position and error as functions of time shown in Figure 9. The error, initially relatively large, rapidly returned to zero, corresponding to quite good control. After 300 seconds, dye solution was injected rapidly at the entry to the flow system. This produced a rapid decrease in the error. The error then became positive, followed by a rapid decrease to essentially zero. At about 750 seconds a larger amount of dye was injected, with qualitatively similar results. In general this shows that the Ziegler-Nichols open-loop tuning method is, at least in this case, quite effective. Very similar results were obtained using controller parameters determined by the Ziegler-Nichols closed-loop method.

In the closed-loop Ziegler-Nichols procedure, the controller involved proportional action only, with $T_I = 10,000$

(which effectively removes any integral action) and $T_D = 0$. As shown in Figure 10, the gain K_C was initially 12,000 and was later decreased to 9,000, at which point the error still oscillated. Then K_C was decreased to 6,000, at which value the oscillation disappeared. The ultimate gain was estimated at 7,500, and the ultimate period was 110 seconds. Based on these results the controller parameters were calculated as $K_C = 4500$, $T_I = 55$, and $T_D = 13.75$. We note that there is reasonable agreement between the open-loop and closed-loop

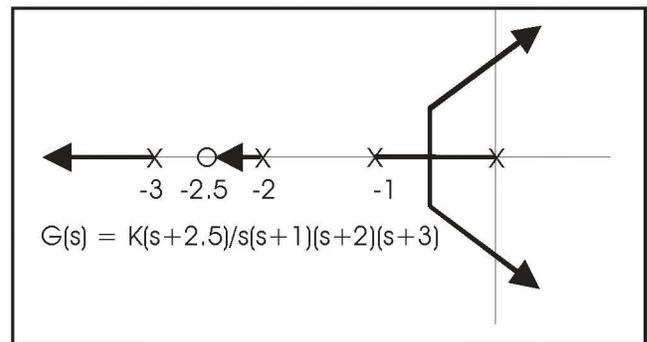


Figure 8. Schematic root locus plot for a PI control system with open loop transfer function $G(s) = K(s + 0.5) / (s(s + 1)(s + 2)(s + 3))$.

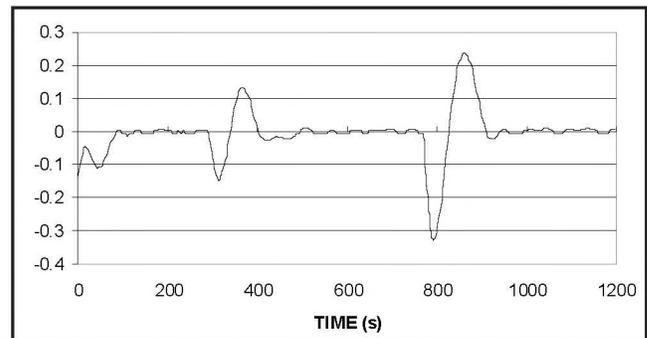


Figure 9. Error data for a PID control run with gains $K_C = 4771$, $T_I = 38.8$ and $T_D = 9.7$, corresponding to Ziegler-Nichols open-loop tuning. The flow configuration was three tanks in series.

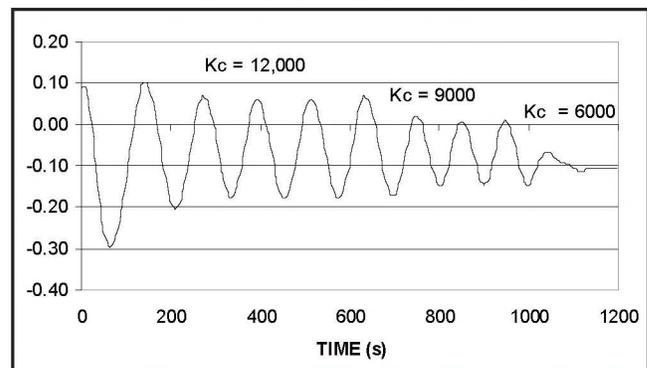


Figure 10. Oscillatory behavior for the closed-loop system with three tanks in series, for proportional control with $K_C = 12,000$, then 9,000, and finally 6,000.

Ziegler-Nichols procedure results. The open-loop procedure, however, requires only a single step-response run, while the closed-loop procedure requires a series of relatively long oscillatory steady-state runs.

DISCUSSION

The process dynamics and control teaching experiment described above is based on a relatively simple apparatus. It illustrates two basic and important aspects of the subject, namely the acquisition and processing of impulse response data, and the operation and tuning of a feedback controller. The impulse response data are analyzed using a nonlinear regression method to determine three parameters of a model of the flow system. In the control studies, the students use both the open-loop and closed-loop Ziegler-Nichols controller tuning procedures to estimate the parameters of the PID controller. Then they observe the behavior of the system under PID control using these parameter values.

The experiment allows the students to observe closely and in detail the interactions of the actuator, plant, transducer, and controller components of a single-variable feedback control system. In particular the opening and closing of the control valve, the resulting changes in dye concentration in each of the glass flasks, and the response of the concentration measuring spectrophotometer are clearly visible. And the key internal

variables of the PID controller program, implemented in the modern LabVIEW language, can also be followed as the system responds on a convenient time scale of tens of seconds. This provides an optimal environment for students to develop a practical—as opposed to purely theoretical—understanding of a realistic feedback control system.

The experiment also embodies several more general and relatively more sophisticated concepts, including the use of modern data acquisition software (LabVIEW), and nonlinear regression methods to estimate the parameters of a model of the flow system. The students see how a dynamic model of a flow system can be used in the estimation of several parameters of a model, and see also that the parameter estimates are subject to errors because the model rarely represents perfectly the modeled system.

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TAYLOR-ARIS DISPERSION

An Explicit Example for Understanding Multiscale Analysis via Volume Averaging

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The idea that the representation of a transport process is dependent upon the length-scale of observation is a perspective that has become widely adopted in chemical engineering education in recent decades; a graphical presentation of a system in which multiscale transport is important appears as Figure 1. Perhaps the clearest indication of this evolution in perspective can be found in the recent publication of the second edition of *Transport Phenomena* by Bird, Stewart and Lightfoot.^[2] A new focus in this second edition, as distinct from the first edition of 1960,^[3] is the multiscale structure of transport phenomena. This perspective appears throughout that text, and in particular is emphasized by the addition of a “Chapter 0” in which the connections among the molecular, microscopic, and macroscopic scales are discussed in the context of transport phenomena. It is becoming standard practice to refer to the smaller and more fundamental of the two scales involved as the “microscale” and the larger as the “macroscale” regardless of the actual dimensions that define the two scales, and this terminology will be used throughout the remainder of this discussion.

The concept of upscaling transport phenomena in complex, multiphase systems has been developed in the chemical engineering discipline extensively over the last 40 years. Although in principle this perspective is more fundamental in the sense that phenomena at different characteristic length scales are formally connected, the mathematical machinery required to understand and apply the theory has tended to keep it somewhat abstracted from applications.

New interest in the connection of transport phenomena among scales has developed in chemical engineering, however, (as evidenced, for example, by the second edition of Bird, Stewart, and Lightfoot,^[2] discussed above), driven partly by the need to understand multiscale systems and partly by evolving advances in experimental methods that allow measurements at small scales with unprecedented resolution. In particular, developments in nano- and micro-technology have made it clear that a thorough understanding of the micro-macro connection in transport phenomena is essential for understanding—and ultimately engineering—systems that involve nano- and micro-scale processes.

Upscaling is possible and appropriate for systems that have a significant amount of “redundant” information. Although the concept of redundant information has a concrete definition in the context of information theory (*e.g.*, Reference 4), from a pedagogical perspective we can think of redundant information as information that can be removed without affecting

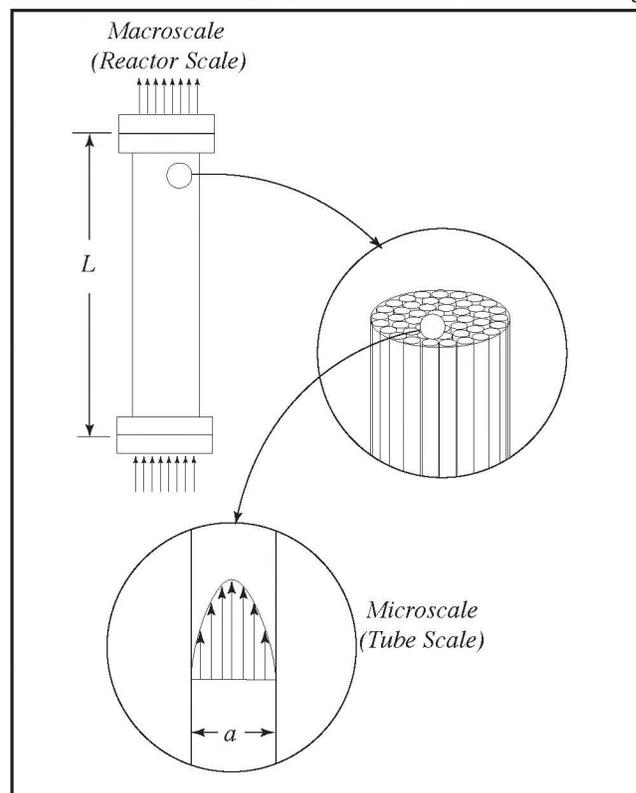


Figure 1. An example of a multiscale hierarchical system.



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the interpretability of the physical system. An example that I frequently use to communicate the ideas behind upscaling is that of the ideal gas. Viewed as a classical mechanical system, a mole of an ideal gas has an enormous number of degrees of freedom (6.02×10^{23} molecules times 3 position and 3 momentum coordinates gives something like 5×10^{24} degrees of freedom!).

If, however, our goal is to predict the pressure of an ideal gas in a fixed volume, then this constitutes a large amount of redundant information. Essentially, because of the extremely large numbers involved, the momentum and coordinates of any particular molecule of gas are not important for determining the pressure of the gas. Rather, the momentum coordinates can be grouped as a distribution, and we can take a statistical approach to computing the pressure of the gas. One can, in fact, show (*e.g.*, as explained by Feynman, et al.^[5]) that the system of roughly 5×10^{24} equations of motion (Newton's laws) for the ideal gas can be "upscaled" via averaging to the well-known result $PV = knT$, where k is the Boltzmann constant, n is the number of molecules involved, and T is the temperature. For this result to be obtained one also has to make a number of assumptions about the behavior of the system, and for the purposes of this paper I will refer to such assumptions as "scaling laws." In the case of the ideal gas, one must adopt the scaling laws of (1) a Maxwellian distribution of speeds applies to the population of molecules, and (2) the statistics do not depend on spatial location (*i.e.*, they are spatially homogenous). Under these conditions, averaging appropriately yields the ideal gas law, and the original 5×10^{24} degrees of freedom are replaced by a single degree of freedom—the temperature T (which is actually a proxy for the mean kinetic energy of the gas).

In Figure 2, a graphical summary of the upscaling process is presented. The essential features of upscaling are represented here as follows. Complete information for the system of interest (*e.g.*, the location and momentum of all molecules in the ideal gas example) is represented at the top of the figure, which we might think of as having, say, the number

N degrees of freedom. We are always at liberty to separate such a system into two components: a mean and a deviation from the mean. Note that here there are still N degrees of freedom; given one of these fields, the other can be obtained by subtracting from the microscale (complete information) representation. At this juncture, if redundant information can be identified, it can be eliminated by upscaling (this requires identifying a scaling law, which is nothing more than a statement about the assumed form of the redundant information). In the example of the ideal gas, we found that the redundant information was the list of velocity components and locations. All that was really needed from this information (at least for the purposes of deriving the ideal gas law) was the two assumptions of velocity statistics that follow a Maxwell distribution and spatial stationarity. The third row shows the results of the upscaled model; a reduction in the number of

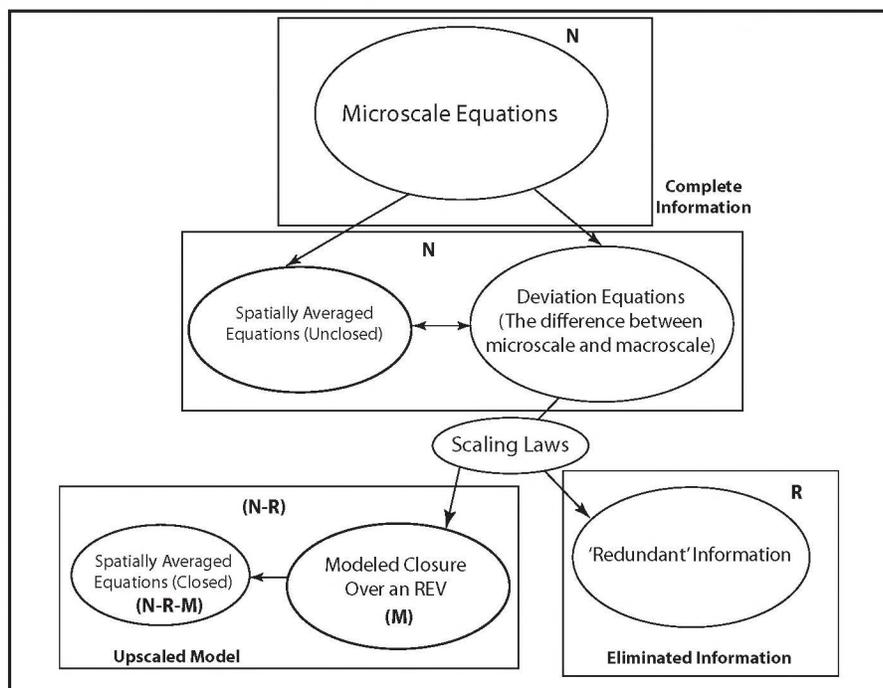


Figure 2. A graphical representation of information flow during the process of upscaling.

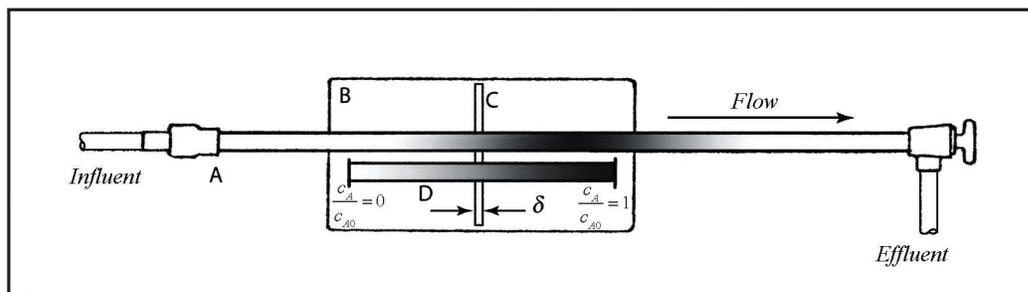


Figure 3. An experimental device used for examining dispersion of a visible dye in a tube, after Taylor.^[1] (A) The capillary tube. (B) A ground glass plate illuminated from behind. (C) The sampling window. (D) A tube containing dye at known concentrations for comparison to the experimentally observed values.

degrees of freedom has been accomplished by the elimination of the redundant information.

The purpose of this paper is to provide an example of up-scaling a multiscale system that has particular pedagogical value. Most students of chemical engineering become familiar with the concept of dispersion, and some will even study the specific example of Taylor-Aris dispersion in detail. The methods used to perform upscaling, in contrast, tend to be presented almost solely in advanced graduate-level courses, and even then there are generally few concrete examples in which students can test the upscaling methods themselves in a familiar context. The case of Taylor-Aris dispersion is an example that is both familiar and one in which a closed-form analytical solution for the effective dispersion coefficient can be developed without having to resort to the solution of a complex, multidimensional partial differential equation. The development also provides an opportunity to review the concept of moving coordinate systems, which are always problematic for students. The objective of this paper is to present a concrete example of upscaling in a manner that is suitable for undergraduate and graduate students alike, with a particular emphasis on generating an analysis where the assumptions and constraints are explicitly identified.

MICROSCALE FORMULATION OF THE PROBLEM

Background

Taylor-Aris dispersion has been studied for more than 50 years since the seminal works of Taylor^[1,6] and Aris,^[7] in the mid 1950s, and it continues to remain an archetypical example for development of new dispersion theory. Partly because it has been studied so extensively using a variety of mathematical approaches, it also represents an example that has been fraught with misunderstanding, even by established experts in the field (*e.g.*, see the exchange of Beard^[8,9] and Dorfman and Brenner^[10]). In principle, the concept of Taylor-Aris dispersion is straightforward. Because the fluid velocity profile in a capillary tube is parabolic (Figure 1), the fluid at the center of the tube moves faster than that near the tube walls. This causes an initially uniform pulse of solute to spread longitudinally due to fluid convection, which forms strong concentration gradients in the radial direction and allows radial diffusion to transport solute across convective streamlines; as time progresses, this tends to create a uniform concentration on planes perpendicular to flow. The question addressed by Sir Geoffrey Taylor (and amended later by Rutherford Aris^[7]) was essentially this: If one observes the average concentration in a capillary tube (using, for example, light transmission of a visible tracer) then is it possible, through knowledge of the microscale transport phenomena, to predict the effective longitudinal dispersion coefficient that would be observed for this averaged concentration? The answer to this question is ultimately yes, and the analyses by Taylor^[1,6] and Aris^[7] provide examples of those rare cases where a very satisfying,

Developments in nano- and micro-technology have made it clear that a thorough understanding of the micro-macro connection in transport phenomena is essential for understanding—and ultimately engineering—systems that involve nano- and micro-scale processes.

compact result is possible. Taylor investigated this problem both theoretically and experimentally; an illustration of Taylor's experimental device is given in Figure 3.

Microscale Description

To begin the multiscale analysis, one first poses the microscale mass balance equations describing solute transport in a capillary tube. It is useful to recognize at this point that the microscale equations can be, in principle, formally derived by upscaling the molecular scale transport phenomena. At the smallest length scale that we attempt to pursue, however, we must ultimately adopt the laws governing the balance of mass as axiomatic. That is, we must assume that the governing laws are true (*e.g.*, in the case of a classical molecular description, that Hamiltonian dynamics are valid^[11]) but are fundamentally unprovable. This feature is true of all upscaling efforts—they relate information among scales provided that one first has axiomatically defined the transport phenomena at a more fundamental scale (*i.e.*, the microscale).

For the case of transport in a capillary tube, we can pose the following microscale boundary-initial value problem for the solute [see Reference 7, Eqs. (3)-(6)]. A simplified version of Taylor's experimental system is presented in Figure 4, and the mathematical description of solute transport at the microscale is specified as follows.

$$\frac{\partial c_A}{\partial t} = -\nabla \cdot (\mathbf{v}c_A) + \nabla \cdot (\mathcal{D}_A \cdot \nabla c_A), \text{ in the fluid phase} \quad (1)$$

$$-\mathbf{n} \cdot (\mathcal{D}_A \cdot \nabla c_A) = 0 \text{ on the tube walls} \quad (2)$$

$$c_A(\mathbf{x}, t=0) = \mathcal{F}(\mathbf{x}), \text{ initial condition} \quad (3)$$

Here, c_A is the concentration of chemical species A, \mathcal{D}_A is the (isotropic) molecular diffusion coefficient, and \mathbf{v} is the fluid velocity vector. Fick's law has been adopted here for describing the diffusive flux, and this necessarily requires that the mole fraction of species A, x_A , be small enough such that $x_A \ll 1$. For the capillary tube, the velocity field is given by the well-known expression

$$\mathbf{v}(\mathbf{r}, \mathbf{x}) = 2U \left(1 - \frac{r^2}{a^2} \right) \quad (4)$$

where U is the average velocity (to be defined later), and r

and x are the radial and longitudinal coordinates illustrated in Figure 4.

Moving Coordinates

For the purposes of this analysis, it is convenient to put this problem in an inertial coordinate system that moves uniformly in the x -direction with the average velocity, U . In other words, the relationship between the nonmoving longitudinal coordinate z , and the moving longitudinal coordinate $x(t)$ is given by

$$\underbrace{x(t)}_{\text{current location}} = \underbrace{z|_{t=0}}_{\text{initial location}} + \underbrace{Ut}_{\text{amount of movement}} \quad (5)$$

Moving coordinate systems frequently confuse students, and this is not without good reason. The presentation of moving coordinate systems is frequently conducted by observation rather than by showing the detailed conversion from one frame of reference to another. For that reason, it is worth spending some time on this concept in class. To start, one can explain that Eq. (5) is the relationship between a point fixed in the fluid at the initial time ($t = 0$) and where that point would be located later if it were to flow with the fluid at the velocity U ; it is, essentially, the equation that describes a streamline for the mean velocity field. Sometimes it is easier to think about this in the reverse. In the moving coordinate system (Figure 4), any point $x(t)$ is related to the point that it originally came from (at the time $t = 0$), *i.e.*,

$$z|_{t=0} = x(t) - Ut \quad (6)$$

The velocity in the new frame of reference can be determined with reference to Figure 5. Here, $Z(t)$ represents the vector following a fluid parcel in the original (fixed) frame of reference. We can think of this vector as being broken up into two parts: the vector that traces the distance to the new coordinate system, and the vector that gives the displacement relative to the new coordinate system. In mathematical terms

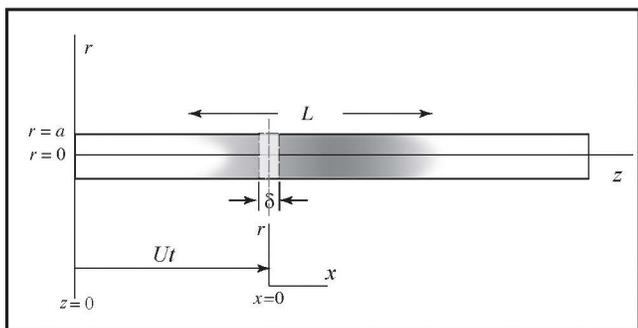
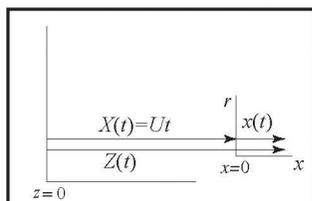


Figure 4. Geometry of the Taylor-Aris capillary tube.

Figure 5. Relationship among coordinate systems.



$$Z(t) = X(t) + x(t) \quad (7)$$

Taking the derivative of both sides of Eq. (7) and rearranging terms gives the following relationship

$$\frac{dx(t)}{dt} = \frac{dZ(t)}{dt} - \frac{dX(t)}{dt} \quad (8)$$

or, substituting in the definitions for velocities

$$v(x, r, t) = v(z, r, t) - U \quad (9)$$

For the particular case of interest, we are interested in steady flow. Referring to Eq. (4), we can put the function describing the velocity in the new frame of reference in the form

$$\begin{aligned} v(x, r) &= 2U \left(1 - \frac{r^2}{a^2} \right) - U \\ &= U \left(1 - \frac{2r^2}{a^2} \right) \end{aligned} \quad (10)$$

Simplifications

From these general balance equations, we can make some substantial simplifications by making the following reasonable assumptions: (1) the capillary tube is cylindrical, (2) the fluid is incompressible, (3) the fluid pressure on the cross-sectional area of the two ends of the tube is uniform (which leads to a cylindrically symmetric fluid velocity field), (4) the initial condition for the solute is cylindrically symmetric so that $\partial c_A / \partial \theta = 0$, and (5) there is no diffusive flux discontinuity at the center of the tube, so that $\partial c_A / \partial r = 0$ at $r = 0$. Under these conditions, we can rewrite Eqs. (1)-(3) in term of a cylindrical (but nonmoving) coordinate system (Figure 4) as follows

$$\frac{\partial c_A}{\partial t} = -2U \left(1 - \frac{r^2}{a^2} \right) \frac{\partial c_A}{\partial x} + \mathcal{D}_A \left[\frac{1}{r} \frac{\partial c_A}{\partial r} + \frac{\partial^2 c_A}{\partial r^2} + \frac{\partial^2 c_A}{\partial x^2} \right], \quad \text{in the fluid phase} \quad (11)$$

$$-\mathcal{D}_A \frac{\partial c_A}{\partial r} = 0, \quad \text{at } r = 0 \text{ and } r = a \quad (12)$$

$$c_A(r, x, t = 0) = \mathcal{F}(r, x), \quad \text{initial condition} \quad (13)$$

As a final step, we need to put these equations in the moving frame of reference. To do this, we start by noting from Eq. (10)

$$2U \left(1 - \frac{r^2}{a^2} \right) = U \left(1 - \frac{2r^2}{a^2} \right) + U \quad (14)$$

Substituting this into Eq. (11) and rearranging gives us

$$\frac{\partial c_A}{\partial t} + U \frac{\partial c_A}{\partial x} = -U \left(1 - \frac{2r^2}{a^2} \right) \frac{\partial c_A}{\partial x} + \mathcal{D}_A \left[\frac{1}{r} \frac{\partial c_A}{\partial r} + \frac{\partial^2 c_A}{\partial r^2} + \frac{\partial^2 c_A}{\partial x^2} \right], \quad \text{in the fluid phase} \quad (15)$$

As a final step, we note that by the definition of the total derivative we have

$$\frac{dc_A}{dt} = \frac{\partial c_A}{\partial t} + \frac{\partial c_A}{\partial x} \frac{dx}{dt} \quad (16)$$

which, by Eq (5), gives

$$\frac{dc_A}{dt} = \frac{\partial c_A}{\partial t} + U \frac{\partial c_A}{\partial x} \quad (17)$$

Substituting this result into Eq. (15) yields the form of the transport problem in the moving frame of reference

$$\underbrace{\frac{dc_A}{dt}}_{\text{Total Derivative (Moving Frame of reference)}} = -U \underbrace{\left(1 - \frac{2r^2}{a^2}\right) \frac{\partial c_A}{\partial x}}_{\text{Convection Term with Moving Frame of Reference Velocity}} + \mathcal{D}_A \underbrace{\left[\frac{1}{r} \frac{\partial c_A}{\partial r} + \frac{\partial^2 c_A}{\partial r^2} + \frac{\partial^2 c_A}{\partial x^2}\right]}_{\text{Diffusion Term in Moving Frame of Reference Remains Unchanged}} \quad (18)$$

in the fluid phase

$$-\mathcal{D}_A \frac{\partial c_A}{\partial r} = 0, \quad \text{at } r = 0 \text{ and } r = a \quad (19)$$

$$c_A(r, x, t = 0) = \mathcal{F}(r, x), \quad \text{initial condition} \quad (20)$$

Note that this should be a familiar operation—this is exactly what happens when one transforms a system into material coordinates in the study of fluid mechanics. The derivative in this case is a total derivative that is very similar to the material derivative that is used routinely in fluid mechanics; in our case, however, the velocity is the average velocity rather than the velocity of a material body, and therefore only the average velocity is incorporated into the total derivative.

AVERAGING

Averaging arises naturally in our experimental observations about systems, but we do not as often think about the relationship to our theoretical representation of the system. As an example, few would argue that Eqs. (18)-(20) represent a reasonable model for describing solute transport in a capillary tube. When we consider what is measurable for such a system, however, the answer is generally not “the microscale concentration, c_A .” Although with substantial effort it may, in fact, be possible to measure the microscale concentration directly, generally we would measure some macroscale property of the system, such as the flux-averaged concentration coming out of the capillary in the effluent, or possibly the spatially averaged concentration resident within the tube at a particular time and with a particular spatial resolution that depends on the instrument used. Although we frequently measure averaged or otherwise “filtered” properties in experimental systems, we rarely think about them as such. The problem of Taylor dispersion in a capillary tube is a cogent, specific example where this micro-macro duality is explicitly recognized, and a full analysis of the interrelationship among scales is possible.

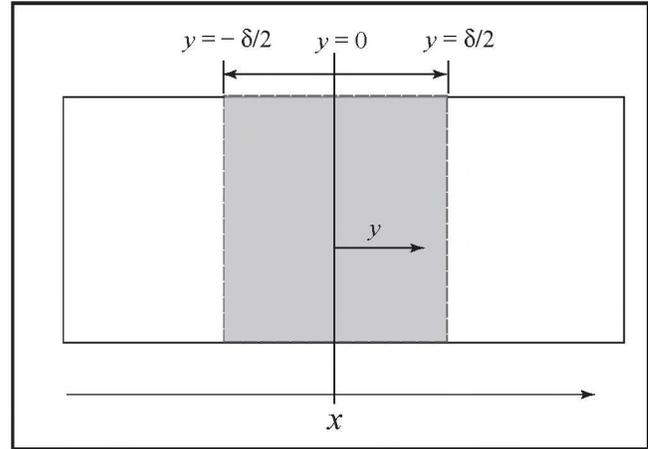


Figure 6. Integration domain for the averaging. Note that the average is still a function of the location, x . A volume average is well defined for each such location.

Ideally, then, we would like to develop a mass balance equation where the dependent variable is related to the quantity that we can actually measure. To this end, we can consider averaging the microscale mass balance equations using a weighting function that represents the influence of our instrument used for observation (*e.g.*, Reference 12). At first, this may seem like a curious perspective, but upon reflection one can recognize that this is actually more in line with our interpretation of laboratory results than is the set of microscale equations given by Eqs. (18)-(20).

Definition of the Average

To begin, we define an appropriate average. In the most general context, averages can be taken over any kind of weighting function that represents an instrument response. In applications of the volume averaging method in particular, however, the weighting function is usually taken to be a step function that is defined as being one inside an averaging volume, and zero outside. For our capillary system, the appropriate average is defined by

$$\langle c_A \rangle_x = \frac{1}{\pi a^2} \int_{r=0}^{r=a} \left(\frac{1}{\delta} \int_{y=-\delta/2}^{y=\delta/2} c_A|_y dy \right) 2\pi r dr \quad (21)$$

where y is a variable of integration. An illustration of the integration domain is given in Figure 6.

A little discussion is warranted here. Note that this is different from the area average that is conventionally used in the Taylor-Aris analysis. In part, this is due to the idea that we are attempting to generate an upscaled theory for a measurable property of the system, for example, the light transmitted through a small volume of the capillary tube (as a proxy for a dye tracer concentration) as Taylor did in his original experiments (Figure 3). The area average is not the measurable property, rather the average over some small observation window is (*e.g.*, as illustrated in Figure 3). We can, however,

imagine that when the concentration field does not have large gradients, and the thickness, δ , of the averaging volume is small we may be able to neglect the changes in the concentration, c_A , over the interval δ . This essentially converts our observation over a small volumetric window to one that is equivalent to the area average. More formally, we can do this by expanding the concentration in a Taylor series $c_A|_y$ around the point

$$c_A|_{x+y} + c_A|_x + y \frac{\partial c_A}{\partial x} \Big|_x + \frac{1}{2} y^2 \frac{\partial^2 c_A}{\partial x^2} \Big|_x + \dots \quad (22)$$

Substituting into the integral given by Eq (21)

$$\langle c_A \rangle_x = \frac{1}{\delta} \frac{1}{\pi a^2} \int_{r=0}^{r=a} \left(\int_{y=-\delta/2}^{y=\delta/2} dy c_A|_x + \int_{y=-\delta/2}^{y=\delta/2} y dy \frac{\partial c_A}{\partial x} \Big|_x + \int_{y=-\delta/2}^{y=\delta/2} \frac{1}{2} y^2 dy \frac{\partial^2 c_A}{\partial x^2} \Big|_x + \dots \right) 2\pi r dr$$

Note that the second integral in this expansion is identically zero. The third and higher terms can be neglected under the conditions that the concentration change over the distance δ is small compared to the distance L . To see this, we can pose the following restriction (see Reference 13)

$$\int_{y=-\delta/2}^{y=\delta/2} dy c_A|_x \gg \int_{y=-\delta/2}^{y=\delta/2} \frac{1}{2} y^2 dy \frac{\partial^2 c_A}{\partial x^2} \Big|_x \quad (24)$$

We can then make the following estimates

$$\int_{y=-\delta/2}^{y=\delta/2} dy = O(\delta) \quad (25)$$

$$\int_{y=-\delta/2}^{y=\delta/2} \frac{1}{2} y^2 dy = O(\delta^3) \quad (26)$$

$$\frac{\partial^2 c_A}{\partial x^2} \Big|_x = O\left(\frac{c_A}{L^2}\right) \quad (27)$$

Combining these yields with the restriction given in Eq (24) yields the constraint [See Reference (13)]

$$\frac{\delta}{L} \ll 1 \quad (28)$$

If the concentration field meets this condition, we expect the first term in Eq. (23) to provide a good estimate of the entire expansion. Under these conditions, the conventional area average concentration can be recovered.

$$\langle c_A \rangle = \frac{1}{\pi a^2} \int_{r=0}^{r=a} c_A (2\pi r) dr \quad (29)$$

The practical result of this is that, for the purposes of the upscaling effort, the conventionally adopted area average is an acceptable average to use, and should be equivalent to the concentrations found by observations of experimental systems provided that the constraint given by Eq. (28) is met.

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Upscaling

In the process of upscaling, simplifications are *necessarily* introduced if a useful theory is to be developed. This is because a useful macroscale representation is only possible if there is an underlying structure to the physics of the problem that allows one to reduce the number of degrees of freedom in the system without eliminating essential information. Approximations that allow a reduction in the number of degrees of freedom are called *scaling laws*. In the case of the Taylor dispersion problem, one scaling law that we are assuming is that the constraint given by Eq. (28) is valid. In other words, we require that the concentration field be *smooth enough* so that there are no large fluctuations on a length scale of δ ; if this condition is not met, the method may not work.

With the definition of the average identified, we can apply the averaging operator to both sides of Eq. (18) (essentially, this is done by multiplying both sides of the equation by $2\pi r$, and then integrating with respect to r from $r = 0$ to $r = a$). The result is

$$\begin{aligned} \left\langle \frac{dc_A}{dt} \right\rangle &= -U \left\langle \left(1 - \frac{2r^2}{a^2} \right) \frac{\partial c_A}{\partial x} \right\rangle \\ &+ \mathcal{D}_A \left[\left\langle \frac{1}{r} \frac{\partial c_A}{\partial r} \right\rangle + \left\langle \frac{\partial^2 c_A}{\partial r^2} \right\rangle + \left\langle \frac{\partial^2 c_A}{\partial x^2} \right\rangle \right] \end{aligned} \quad (30)$$

Noting that the averaging operator does not depend on x or t , we can exchange averaging and differentiation with respect to x and t .

For the second term on the right-hand side of Eq. (30), we can use integration by parts along with the two boundary conditions to show

$$\begin{aligned}
\left\langle \frac{\partial^2 c_A}{\partial r^2} \right\rangle &= \frac{1}{\pi a^2} \int_{r=0}^{r=a} \frac{\partial^2 c_A}{\partial r^2} (2\pi r) dr \\
&= \frac{1}{\pi a^2} \left[\frac{\partial c_A}{\partial r} (2\pi r) \Big|_{r=0}^{r=a} - \int_{r=0}^{r=a} \frac{\partial c_A}{\partial r} (2\pi) dr \right] \\
&= \frac{1}{\pi a^2} \left[- \int_{r=0}^{r=a} \frac{1}{r} \frac{\partial c_A}{\partial r} (2\pi r) dr \right] \\
&= - \left\langle \frac{1}{r} \frac{\partial c_A}{\partial r} \right\rangle \quad (31)
\end{aligned}$$

Combining these results gives a macroscale equation of the form

$$\frac{d\langle c_A \rangle}{dt} = -U \frac{\partial \langle c_A \rangle}{\partial x} + \mathcal{D}_A \frac{\partial^2 \langle c_A \rangle}{\partial x^2} + \frac{2U}{a^2} \left\langle r^2 \frac{\partial c_A}{\partial x} \right\rangle \quad (32)$$

Except for the last term on the right-hand side, this expression is a macroscale balance equation for the average concentration, $\langle c_A \rangle$. We can't simplify the last term as it stands because of the presence of the multiplier r^2 inside the averaging operator. To proceed further, we have to propose some method for expressing $\langle r^2 \partial c_A / \partial x \rangle$ in terms of the average concentration $\langle c_A \rangle$ rather than the microscale concentration, c_A . To do this, we define a *concentration decomposition* that relates the average and microscale concentrations as follows

$$c_A(\mathbf{r}, \mathbf{x}) = \langle c_A \rangle_{\mathbf{x}} + \tilde{c}_A(\mathbf{r}, \mathbf{x}) \quad (33)$$

where the quantity \tilde{c}_A is called the concentration deviation (from here on we will drop the explicit reference to the coordinates for all concentrations unless explicitly required). Using this in Eq. (32) gives

$$\frac{d\langle c_A \rangle}{dt} = -U \frac{\partial \langle c_A \rangle}{\partial x} + \mathcal{D}_A \frac{\partial^2 \langle c_A \rangle}{\partial x^2} + \frac{2U}{a^2} \langle r^2 \rangle \frac{\partial \langle c_A \rangle}{\partial x} + \frac{2U}{a^2} \left\langle r^2 \frac{\partial \tilde{c}_A}{\partial x} \right\rangle \quad (34)$$

Finally, note that the average of r^2 can be readily computed as follows

$$\begin{aligned}
\langle r^2 \rangle &= \frac{1}{\pi a^2} \int_{r=0}^{r=a} r^2 (2\pi r) dr \\
&= \frac{2r^4}{4a^2} \Big|_{r=0}^{r=a} = \frac{a^2}{2} \quad (35)
\end{aligned}$$

Combining this result with Eq (34) gives the simple-looking expression

$$\frac{d\langle c_A \rangle}{dt} = \mathcal{D}_A \frac{\partial^2 \langle c_A \rangle}{\partial x^2} + \frac{2U}{a^2} \left\langle r^2 \frac{\partial \tilde{c}_A}{\partial x} \right\rangle \quad (36)$$

Eq. (36) is starting to look like the spatially averaged equation that we are seeking. Recall that we put this analysis in a coordinate system that moves

with the average velocity; for this reason no convection term arises here. Our remaining goal, then, is to determine how we can obtain an expression of the form

$$\frac{d\langle c_A \rangle}{dt} = D_{A,\text{eff}} \frac{\partial^2 \langle c_A \rangle}{\partial x^2} \quad (37)$$

where $D_{A,\text{eff}}$ defines the effective dispersion coefficient. To accomplish this, we must find a way of *closing* the problem so that terms involving only the average concentration, $\langle c_A \rangle$, appear.

CLOSURE

To complete the analysis, we need to find some method of predicting the concentration deviation, \tilde{c}_A , in terms of the average concentration, $\langle c_A \rangle$. At first, this may seem like a tall order: it is not clear at this point that there is any reason to expect that we could express \tilde{c}_A as some function involving $\langle c_A \rangle$. We will see, however, that this is a tractable task. To start, we need to develop a balance equation for the concentration deviations.

The decomposition given by Eq. (33) suggests a relationship between the concentrations of the form

$$\tilde{c}_A = c_A - \langle c_A \rangle \quad (38)$$

and this suggests that a balance equation for \tilde{c}_A can be obtained by subtracting the balance equation for $\langle c_A \rangle$ from the balance equation for c_A . This is a straightforward operation,

To start, one can explain that Eq. (5) is the relationship between a point fixed in the fluid at the initial time ($t = 0$) and where that point would be located later if it were to flow with the fluid at the velocity U ; it is, essentially, the equation that describes a streamline for the mean velocity field. Sometimes it is easier to think about this in the reverse.

and the result is

$$\begin{aligned} \frac{dc_A}{dt} &= \mathcal{D}_A \frac{\partial^2 c_A}{\partial x^2} - U \left(1 - \frac{2r^2}{a^2} \right) \frac{\partial c_A}{\partial x} + \mathcal{D}_A \frac{1}{r} \frac{\partial c_A}{\partial r} + \mathcal{D}_A \frac{\partial^2 c_A}{\partial r^2} \\ &\quad - \left[\frac{d\langle c_A \rangle}{dt} = \mathcal{D}_A \frac{\partial^2 \langle c_A \rangle}{\partial x^2} + \frac{2U}{a^2} \left\langle r^2 \frac{\partial \langle c_A \rangle}{\partial x} \right\rangle \right] \\ \frac{d\tilde{c}_A}{dt} &= -\mathcal{D}_A \frac{\partial^2 \tilde{c}_A}{\partial x^2} - U \left(1 - \frac{2r^2}{a^2} \right) \frac{\partial \tilde{c}_A}{\partial x} + \mathcal{D}_A \frac{1}{r} \frac{\partial \tilde{c}_A}{\partial r} + \mathcal{D}_A \frac{\partial^2 \tilde{c}_A}{\partial r^2} - \frac{2U}{a^2} \left\langle r^2 \frac{\partial \tilde{c}_A}{\partial x} \right\rangle \end{aligned} \quad (39)$$

For the closure problem, we want a balance equation that involves only deviations and averages. Using the decomposition given by Eq. (33) to eliminate the microscale concentration in Eq. (39) and the boundary condition given by Eq. (2), we find a complete description of the closure problem that predicts the deviation concentration \tilde{c}_A is given by

$$\begin{aligned} \frac{d\tilde{c}_A}{dt} &= -U \left(1 - \frac{2r^2}{a^2} \right) \frac{\partial \tilde{c}_A}{\partial x} - \mathcal{D}_A \frac{\partial^2 \tilde{c}_A}{\partial x^2} + \frac{\mathcal{D}_A}{r} \frac{\partial}{\partial r} \left(r \frac{\partial \tilde{c}_A}{\partial r} \right) \\ &\quad - \underbrace{\frac{2U}{a^2} \left\langle r^2 \frac{\partial \tilde{c}_A}{\partial x} \right\rangle}_{\text{Nonlocal term}} - \underbrace{U \left(1 - \frac{2r^2}{a^2} \right) \frac{\partial \langle c_A \rangle}{\partial x}}_{\text{Source}} \end{aligned} \quad (40)$$

$$-\mathcal{D}_A \frac{\partial \tilde{c}_A}{\partial r} = 0, \quad \text{at } r=0 \text{ and } r=a \quad (41)$$

$$\tilde{c}_A(r, x, t=0) = \mathcal{F}(r, x), \quad \text{initial condition} \quad (42)$$

Note that in the development of this equation we have used the fact that $\partial \langle c_A \rangle / \partial r = 0$ (i.e., the average concentration depends only upon x). In principle, this equation can be solved (using, for example, Fourier transform methods) provided that the initial condition is known. This would then provide us with an expression that describes the time evolution of the deviation concentration.

From a practical perspective, it is useful to consider examining the “long time” solution to Eqs. (40)-(42), where the effective dispersion coefficient is essentially a constant. To begin the analysis of this approximation, suppose that the source term has a characteristic time scale of T^* . This implies that the dominant time scale for $\partial \tilde{c}_A / \partial t$ is also of order T^* . We can make the following estimates

$$\frac{d\tilde{c}_A}{dt} = O\left(\frac{\Delta \tilde{c}_A}{T^*} \right) \quad (43)$$

$$\frac{\mathcal{D}_A}{r} \frac{\partial}{\partial r} \left(r \frac{\partial \tilde{c}_A}{\partial r} \right) = O\left(\frac{\mathcal{D}_A \Delta \tilde{c}_A}{a^2} \right) \quad (44)$$

$$U \left(1 - \frac{2r^2}{a^2} \right) \frac{\partial \tilde{c}_A}{\partial x} = O\left(U \frac{\Delta \tilde{c}_A}{L} \right) \quad (45)$$

The key ideas of the Taylor-Aris analysis provide a structure for understanding upscaling in many other kinds of multiscale systems.

$$\frac{2U}{a^2} \left\langle r^2 \frac{\partial \tilde{c}_A}{\partial x} \right\rangle = O\left(U \frac{\Delta \tilde{c}_A}{L} \right) \quad (46)$$

$$\mathcal{D}_A \frac{\partial^2 \tilde{c}_A}{\partial x^2} = O\left(\frac{\mathcal{D}_A \Delta \tilde{c}_A}{L^2} \right) \quad (47)$$

Note that the estimates in Eqs. (45) and (46) are identical.

We begin simplification by imposing the restriction

$$\frac{d\tilde{c}_A}{dt} \ll \frac{\mathcal{D}_A}{r} \frac{\partial}{\partial r} \left(r \frac{\partial \tilde{c}_A}{\partial r} \right) \quad (48)$$

and using our estimates, this translates into a constraint of the form

$$\frac{a^2}{\mathcal{D}_A} \ll T^* \quad (49)$$

We can think of the term on the left-hand side of this expression as the relaxation time of \tilde{c}_A due to diffusion, whereas the right-hand side indicates the timescale for changes in the source term. This restriction indicates that diffusion must relax any radial gradients relatively “quickly” compared with changes in $\langle c_A \rangle$. Generally, this kind of relationship is known as a *quasi-steady* condition, and it is used frequently in engineering analysis.

We can make two additional restrictions to simplify the problem. Early on, we indicated that we expected radial diffusion to be “fast” relative to longitudinal convection. In the closure problem, we can formalize this by the restriction

$$U \left(1 - \frac{2r^2}{a^2} \right) \frac{\partial \tilde{c}_A}{\partial x} \ll \frac{\mathcal{D}_A}{r} \frac{\partial}{\partial r} \left(r \frac{\partial \tilde{c}_A}{\partial r} \right) \quad (50)$$

and making order-of-magnitude estimates as we did above, this yields a Péclet number constraint

$$\frac{Ua}{\mathcal{D}_A} \frac{a}{L} \ll 1 \quad (51)$$

Note that this same constraint also allows us to drop the nonlocal term on the right-hand side of Eq. (40) since it is of the same order of magnitude as the convection term that we just dropped.

Finally, we expect radial diffusion to dominate over longitudinal diffusion

$$\mathcal{D}_A \frac{\partial^2 \tilde{c}_A}{\partial x^2} \ll \frac{\mathcal{D}_A}{r} \frac{\partial}{\partial r} \left(r \frac{\partial \tilde{c}_A}{\partial r} \right) \quad (52)$$

Again using the estimates above, the associated constraint is

$$\frac{a}{L} \ll 1 \quad (53)$$

When these three constraints are met, we can describe the closure problem by

$$\frac{\mathcal{D}_A}{r} \frac{\partial}{\partial r} \left(r \frac{\partial \tilde{c}_A}{\partial r} \right) = \underbrace{U \left(1 - \frac{2r^2}{a^2} \right)}_{\text{source}} \frac{\partial \langle c_A \rangle}{\partial x} \quad (54)$$

$$-\mathcal{D}_A \frac{\partial \tilde{c}_A}{\partial r} = 0, \quad \text{at } r=0 \text{ and } r=a \quad (55)$$

$$\langle \tilde{c}_A \rangle = 0 \quad (56)$$

In Eq. (56), we have replaced the initial condition present in the original problem with the constraint that the average of the deviations must be identically zero. This is necessary because when we adopt the quasi-steady form the initial condition no longer enters the problem. Without some additional constraint, however, there is no longer enough information to solve the problem. The constraint that the average of the deviations is zero is consistent with the original initial condition, and allows the constants of integration in the solution to be explicitly identified.

We have made substantial simplifications here, but the benefits to these simplifications are (1) they were done in a manner in which explicit constraints were developed that indicate their domain of validity, and (2) the resulting balance still captures the essential physics of the problem, but is now significantly simpler to solve than the original problem. The solution to this problem is straightforward, and two integrations give the result

$$\tilde{c}_A = \frac{Ua^2}{4\mathcal{D}_A} \frac{\partial \langle c_A \rangle}{\partial x} \left(\frac{r^2}{a^2} - \frac{1}{2} \frac{r^4}{a^4} \right) + K \quad (57)$$

To determine the constant of integration, K , we use the constraint imposed on the problem [Eq (56)]. Taking the average of both sides of Eq (57) and using Eq (56) we find

$$K = -\frac{1}{3} \frac{Ua^2}{4\mathcal{D}_A} \frac{\partial \langle c_A \rangle}{\partial x} \quad (58)$$

so that the final solution is

$$\tilde{c}_A = \frac{Ua^2}{4\mathcal{D}_A} \frac{\partial \langle c_A \rangle}{\partial x} \left(\frac{r^2}{a^2} - \frac{1}{2} \frac{r^4}{a^4} - \frac{1}{3} \right) \quad (59)$$

The Macroscale Dispersion Coefficient

Recall that the unclosed macroscale transport equation that we developed took the form

$$\frac{d \langle c_A \rangle}{dt} = \mathcal{D}_A \frac{\partial^2 \langle c_A \rangle}{\partial x^2} + \frac{2U}{a^2} \left\langle r^2 \frac{\partial \tilde{c}_A}{\partial x} \right\rangle \quad (59A)$$

where the second term on the right-hand side represented the influence of mechanical dispersion due to the nonuniform flow field. Because we have determined the concentration deviation field by Eq. (59), we are in a position to close the macroscale equation. To do this, note that we will need the derivative of the concentration deviation field

$$\frac{\partial \tilde{c}_A}{\partial x} = \frac{Ua^2}{4\mathcal{D}_A} \left(\frac{r^2}{a^2} - \frac{1}{2} \frac{r^4}{a^4} - \frac{1}{3} \right) \frac{\partial^2 \langle c_A \rangle}{\partial x^2} \quad (60)$$

Substituting this into the macroscale transport equation above and regrouping terms yields

$$\frac{d \langle c_A \rangle}{dt} = \left(\mathcal{D}_A + \frac{U^2}{\mathcal{D}_A} \left\langle r^2 \left(\frac{r^2}{2a^2} - \frac{1}{4} \frac{r^4}{a^4} - \frac{1}{6} \right) \right\rangle \right) \frac{\partial^2 \langle c_A \rangle}{\partial x^2} \quad (61)$$

Note that this now takes the form of a dispersion equation, where the term multiplying the derivative on the right-hand side is the dispersion coefficient. It is straightforward to work out the term in the angled brackets explicitly using the definition of the average given by Eq (29). This result is

$$\left\langle r^2 \left(\frac{r^2}{2a^2} - \frac{1}{4} \frac{r^4}{a^4} - \frac{1}{6} \right) \right\rangle = \frac{a^2}{48} \quad (62)$$

Finally, substituting this result into Eq (61) yields the classical Taylor-Aris result

$$\frac{d \langle c_A \rangle}{dt} = D_{A,\text{eff}} \frac{\partial^2 \langle c_A \rangle}{\partial x^2} \quad (63)$$

where

$$D_{A,\text{eff}} = \left(\mathcal{D}_A + \frac{U^2 a^2}{48 \mathcal{D}_A} \right) \quad (64)$$

As a final step, we can put this equation back into a fixed frame of reference rather than one that moves with the mean flow. Doing this essentially adds back the (mean) convection term that we initially removed, and the final transport equation takes the form of the convection-dispersion equation. Using Eq. (17) we can easily convert our final expression back to the fixed frame of reference, yielding a macroscale convection-dispersion equation of the form

$$\frac{\partial \langle c_A \rangle}{\partial t} = -U \frac{\partial \langle c_A \rangle}{\partial x} + D_{A,\text{eff}} \frac{\partial^2 \langle c_A \rangle}{\partial x^2} \quad (65)$$

Note that the interpretation of this new equation, unlike the microscale equation that we started with, is that it describes the concentration averaged over the cross section of the tube. The microscale structure (geometry and flowfield) are represented in this equation, but only indirectly through the effective dispersion coefficient.

PERSPECTIVE

The essential ideas of the micro-macro duality of multiscale systems can be communicated to undergraduate and graduate students alike through the example of Taylor-Aris dispersion. Because of the simple geometry involved, this problem has a macroscale transport equation that is intuitively appealing, and the effective dispersion coefficient can be predicted in a simple, closed form from an analysis of the microscale flow and transport processes. The key ideas of the Taylor-Aris analysis provide a structure for understanding upscaling in many other kinds of multiscale systems. These key ideas can be summarized as follows.

1. Many systems have a complex, multiscale structure that would be infeasible or impossible to fully resolve at the smallest scale of interest (the microscale).
2. For such systems, a macroscale description of the phenomena of interest is sought that applies at a scale that is much larger than the microscale. Such a description seeks to represent the unresolved microscale processes in the system by a model. In this way, the net effect of the microscale processes are captured, even if they are not explicitly resolved.
3. Upscaling is a method of formally averaging the complete microscale description of a system in order to develop a valid macroscale representation. The goal in upscaling efforts is to make a connection between the microscale and the macroscale that allows one to predict the effective parameters that are developed for the macroscale transport equations. This is accomplished by breaking the problem into two separate systems of transport equations: (1) equations describing the transport of the average of the quantities of interest, and (2) equations describing the transport of the deviations from this average.
4. If we use the concept of numbers of degrees of freedom of a system, then upscaling is the process by which the number of degrees of freedom of the system is reduced by eliminating redundant information. For upscaling to be effective, there must be some identifiable structure or regularity of the deviation quantities in the system that leads to information that can be considered redundant.

A scaling law is a statement about the structure of the deviations in the system that allows one to accomplish this reduction in degrees of freedom. A few examples of scaling laws include (1) smoothness conditions (such as in the case of Taylor dispersion), (2) periodic geometric structure (such as is done in many analyses of porous media systems), and (3) statistically homogenous structure (as is done in turbulence).

Often, when upscaling concepts are presented to students who are unfamiliar with them, a “big picture” perspective is missing. If this can be first communicated, and then followed by a tractable example like the case of Taylor-Aris dispersion, the concepts underlying upscaling become significantly more tangible and much easier for students to understand.

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COMBINED STEADY-STATE AND DYNAMIC HEAT EXCHANGER EXPERIMENT

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Dow Chemical Co. provided a pilot-scale heat-transfer experiment to the Department of Chemical Engineering at Lehigh University about 20 years ago. This experiment has been an important fixture in our unit operations laboratory since that time. Only steady-state experiments and analysis were performed for most of this period. The equipment has been modified recently to permit experiments involving dynamic control studies.

The steady-state aspects of the experiment involve taking flowrate, temperature, and pressure data so that energy balances around each heat exchanger can be calculated. Flowrates are measured by orifice plates and differential pressure transmitters, but are also checked by the old reliable “bucket and stop watch” method. There are duplicate temperature measurements at some locations (thermocouple and dial thermometer) to give the students an understanding of the inherent discrepancy between different devices. Overall heat-transfer coefficients are calculated, and Wilson plots are made to determine inside film coefficients at different process-water flowrates. Experimental results are compared with the predictions of applicable correlations in the literature.

The dynamic aspects of the experiment involve dynamic tests (step and relay-feedback) and closedloop control of two process temperatures (process outlet temperature from the heater and process outlet temperature from the cooler) by manipulation of steam and cooling water flowrates, respec-

tively. Computer simulations of the system are developed, both steady state and dynamic, and results are compared with experimental data.

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Paul Bader is senior electronics technician in the Department of Chemical Engineering at Lehigh University. His special interest is the unit operations experiments. In the present work he designed and implemented the control loop for the heat exchanger experiment.



PROCESS DESCRIPTION

Figure 1 shows the flowsheet of the process. Figure 2 gives a picture of the apparatus. Water from a tank (0.71 m ID, 1.2 m height) is pumped by a 15 hp centrifugal pump to the heater, which is a two-pass tube-in-shell heat exchanger with 0.542 m² inside heat-transfer surface. Table 1 gives details of the heat exchanger equipment. Material of construction is stainless steel.

Saturated steam at 3.36 bar from a steam header passes through a pneumatically operated control valve (CV = 25, air-to-open, equal-percentage trim) into the shell side of the heater. Steam pressure in the shell side of the heater is about 1.8 bars under typical steady-state conditions, which corresponds to a saturation temperature of 117 °C. Condensate leaves the heater as saturated liquid through a steam trap. It goes to a three-way valve that permits bucketing the condensate flowrate or discharging into a drain.

The process water then flows into the cooler, which is a 4-pass tube-in-shell heat exchanger with 2.957 m² of heat-transfer area. Cooling water from a supply header at 3.7 bars flows into the shell side of the cooler. The temperature of the cooling water supply is generally around 7 °C. After flowing through the cooler, the cooling water passes through a pneumatically operated control valve (CV = 9, air-to-close, equal-percentage trim) and goes to a three-way valve that permits bucketing the cooling-water flowrate or discharging into a drain. The process water then flows through a control valve (CV = 12, air-to-close, equal-percentage trim) and back into the feed tank. Temperatures are measured at numerous locations and are shown on the flowsheet given in Figure 1. The three control valves are pneumatic, so the electronic signals (4 to 20 mA) from the computer control system are fed to three I/P transducers.

WILSON PLOT METHOD

In a tube-in-shell heat exchanger, the overall heat-transfer coefficient U is defined as follows.

$$\frac{1}{UA} = \frac{1}{U_o A_o} = \frac{1}{U_i A_i} = \frac{1}{h_i A_i} + R_{f0} + \frac{\ln\left(\frac{D_o}{D_i}\right)}{2\pi kL} + R_{fi} + \frac{1}{h_o A_o} \quad (1)$$

where A_i and A_o represent inside and outside heat-transfer surface areas of a single tube, h_i and h_o are inside and outside film coefficients, R_{fi} and R_{f0} are inside and outside fouling resistances, D_i and D_o are inside and outside diameters of the tubes, k is the thermal conductivity of the metal tube wall and L is the tube length. Using the inside surface area of the tubes as the basis,

$$\frac{1}{U_i} = \frac{1}{h_i} + A_i \left[R_{fi} + \frac{\ln\left(\frac{D_o}{D_i}\right)}{2\pi kL} + R_{fo} \right] + \frac{1}{h_o \frac{A_o}{A_i}} \quad (2)$$

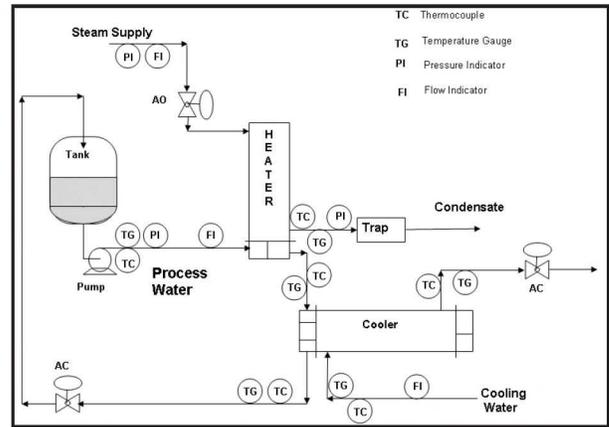


Figure 1.

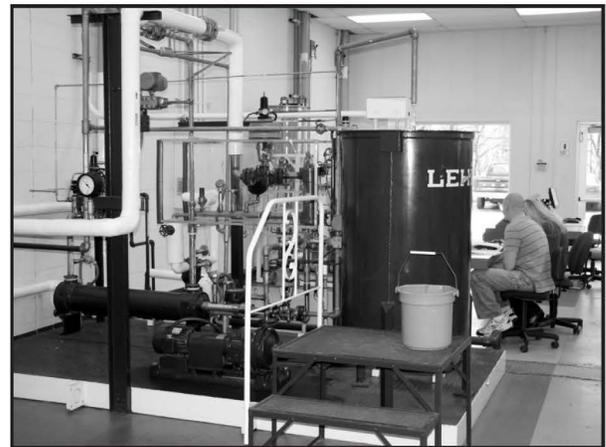


Figure 2.

Wilson^[1] suggested that experiments can be run to find a relationship between the overall heat-transfer coefficient (U) and the film coefficient inside the tube (h_i). In these experiments, the wall resistance, inside and outside fouling and outside film coefficient must be held constant, see also Hewitt, *et al.*^[2]

If we call the sum of the second and the third terms on the right hand side of Eq. (2) constant “A”

$$\frac{1}{U_i} = \frac{1}{h_i} + A \quad (3)$$

TABLE 1
Heat Exchanger Parameters

	Heater	Cooler
Number passes	2	4
Heat-transfer area (inside) (m ²)	0.542	2.957
Number of tubes	108	104
Tube ID (m)	0.00475	0.00775
Wall thickness (m)	0.0008	0.00089
Tube Length (m)	0.337	1.17
Shell ID (m)	0.105	0.206

$$\text{Where, } A = A_i \left[R_{fi} + \frac{\ln\left(\frac{D_o}{D_i}\right)}{2\pi kL} + R_{fo} \right] + \frac{1}{h_o \frac{A_o}{A_i}} \quad (3a)$$

For fluid flowing inside tubes, h_i can be expressed as

$$\text{Nu} = \frac{h_i D_i}{k} = C \text{Re}^m \text{Pr}^n \quad (4)$$

where C , m , and n are constants that depend on the fluid and flow conditions. Thus, h_i can be expressed as,

$$h_i = \frac{k}{D_i} \cdot C \left(\frac{\rho D}{\mu} \right)^m \cdot (v)^m \cdot \text{Pr}^n \quad (5)$$

Or, if we keep the properties of the fluid constant,

$$h_i = \frac{1}{B} \cdot v^m$$

$$\text{where } \frac{1}{B} = C \cdot \frac{k}{D_i} \left(\frac{\rho D}{\mu} \right)^m \cdot \text{Pr}^n \quad (6)$$

Introducing this into Eq. (3) gives

$$\frac{1}{U_i} = B \frac{1}{v^m} + A \quad (7)$$

Experiments can be carried out by keeping the operating parameters in “A” and “B” constant while varying velocity of the flow inside the tube. Measurements of overall heat-transfer coefficients then provide the values of the constants “A” and “B” if the parameter m is known. The data presented here were obtained from experiments that are carried out in the turbulent regime where $m = 0.8$. The constant “C” in Eq. (4) can also be calculated.

To keep the operating heat-transfer parameters constant on the shell sides of both heat exchangers, the following conditions are established:

- The temperature driving force ($T_s - T_{wall}$) on the shell side of the heater is kept constant in order to have similar film coefficients during condensation of the steam.
- Cooling water flowrate on the shell side of the

cooler is kept at its maximum value in order to have a fixed and a high film coefficient.

With the above conditions, the Wilson plot method can be applied to the data to extract tube-side film coefficients from the measured overall heat-transfer coefficients over a range of process water flowrates.

INSTRUMENTATION CALIBRATION AND DATA RECONCILIATION

There are two different temperature sensors at every location where temperature is measured (thermocouples and gauges). There are up to ± 2 °C differences between sensor outputs. Therefore all sensors are calibrated based on a reference temperature measurement device.

Flowrates are sensed using orifice plates and pressure differences and are recorded using a computer-based data acquisition system. Calibrations are carried out using the bucket and stopwatch method.

Even with these calibrations, the inaccuracies in the experimental data do not give perfect energy balances, so the students learn that some engineering judgment is required to reconcile the data. Temperature data is adjusted so that the calculated energy balances on both sides of both exchangers match perfectly.

EXPERIMENTAL DATA AND SAMPLE CALCULATIONS

Experimental measurements consist of recording of the following data:

- Process water inlet temperature to heater — $T_{PWH,in}$
- Process water outlet temperature from heater — $T_{PWH,out}$
- Process water outlet temperature from cooler — $T_{PWC,out}$
- Saturation temperature of the condensing steam on the

Description of Parameters	TP1	TP2	TP3	TP4	TP5	TP6
PW Inlet Temp. to Heater (°C)	23.25	36.16	34.00	34.00	34.59	35.67
PW Outlet Temp. From Heater (°C)	61.79	72.63	68.24	67.68	66.03	64.93
PW Outlet Temp. from Cooler (°C)	22.40	32.51	33.26	34.71	34.71	36.91
Condensate temperature (°C)	118.23	120.55	118.89	121.67	120.55	120.55
CW Inlet Temp. to Cooler (°C)	6.79	7.8	7.22	6.7	7.22	7.22
CW Outlet Temp. from Cooler (°C)	21.95	31.67	31.11	33.33	33.33	34.44
PW Flow Rate (kg/s)	0.241	0.667	0.8275	0.953	1.0435	1.099
Steam Flow Rate (kg/s)	0.0207	0.0473	0.0482	0.0491	0.0498	0.0514
CW Flow Rate (kg/s)	1.1	1.1	1.1	1.1	1.1	1.1

shell side of the heater— T_s

- Flow rate of the process water— F_{pw}
- Flow rate of the steam— F_s
- Flow rate of the cooling water— F_{cw}

Table 2 (previous page) gives raw experimental data for six runs with varying process-water flowrates.

To illustrate the calculations and data reconciliation, we take Run TP3 with a process water flowrate of 0.8275 kg/s.

A. Energy Balances

Under steady-state conditions, if there were no heat losses in the system, the heat gained by the process water in the heater would equal the heat lost by the process water in the cooler. Likewise, the heat lost by the steam would be equal to the heat gained by the process water, and the heat gained by the cooling water would be equal to the heat lost by the process water. Therefore, all four of the heat-transfer rates should be equal.

1. Heater:

The heat-transfer rate is calculated on the process-water side of the heater using Eq. (8) from the measurements of the process-water flowrate and its inlet and outlet temperatures.

$$Q_{PWH} = F_{pw} c_p (T_{PWH,out} - T_{PWH,in}) \quad (8)$$

$$Q_{PWH} = 0.8275 \text{ (kg/s)} \cdot 4.193 \text{ (kJ/kg-K)} \cdot (68.24 - 34.00) \text{ (}^\circ\text{C)}$$

$$= 118.8 \text{ kW}$$

The heat-transfer rate is calculated on the steam side of the heater using Eq. (9) from the measurements of the condensate flowrate, the supply pressure of the saturated steam and the temperature of the saturated liquid condensate. The enthalpy of the saturated vapor supply steam at 336 kPa is found in the steam tables (2730 kJ/kg), as is the enthalpy of the saturated liquid condensate at 192 kPa and 119 °C (499 kJ/kg). The heat transferred from the condensing steam is found using

$$Q_s = F_s (H_{supply} - H_{condensate}) \quad (9)$$

$$Q_s = 0.0482 \text{ (kg/s)} [2,730 \text{ (kJ/kg)} - 499 \text{ (kJ/kg)}]$$

$$= 107.5 \text{ kW}$$

Note that these two heat-transfer rates do not match perfectly.

2. Cooler:

The heat-transfer rate is calculated on the process-water side of the cooler using Eq. (10) from the measurements of the process-water flowrate and its inlet and outlet temperatures.

$$Q_{PWC} = F_{pw} c_p (T_{PWC,in} - T_{PWC,out}) \quad (10)$$

$$Q_{PWC} = 0.8275 \text{ (kg/s)} \cdot 4.194 \text{ (kJ/kg-K)} \cdot (68.24 - 33.26) \text{ (}^\circ\text{C)}$$

$$= 121.4 \text{ kW}$$

Of course, $T_{PWC,in}$ is equal to $T_{PWH,out}$.

The heat-transfer rate is also calculated on the cooling-water side of the cooler using Eq. (11) from the measurements of the cooling-water flowrate and its inlet and outlet temperatures.

$$Q_{CWC} = F_{cw} c_p (T_{CWC,out} - T_{CWC,in}) \quad (11)$$

$$Q_{CWC} = 1.1 \text{ (kg/s)} \cdot 4.193 \text{ (kJ/kg-K)} \cdot (31.11 - 7.22) \text{ (}^\circ\text{C)}$$

$$= 110.2 \text{ kW}$$

The four heat duties are not exactly equal, which is an important lesson for the students to learn and will always be the case using experimental data. The maximum difference of 11.2 kW corresponds to a maximum error of 10%.

It should be noted that some data are more accurate than others. The process water and cooling water flowrate measurements are more reliable than the measurement of steam flowrate because there is some flashing of the condensate even when an ice bucket is used to capture the condensate leaving the steam trap.

Temperature differences between the inlet and outlet conditions are used in the heat duty calculations. The larger the temperature difference, the more reliable the calculations. For example, during experiment TP3 the process water is cooled 35.0 °C in the cooler, while the cooling water is heated only 23.9 °C.

As a result, among the four heat duties calculated above, the two process water heat duties are the most reliable and should be used in any other calculations for the experiment.

B. Calculation of Overall Heat-Transfer Coefficients

1. Heater:

Since the steam condenses at a constant temperature, the temperature driving forces at the ends of the heater are

$$(\Delta T_H)_2 = T_s - T_{PWH,in} = 118.9 - 34.0 = 84.9 \text{ K}$$

$$(\Delta T_H)_1 = T_s - T_{PWH,out} = 118.9 - 68.2 = 50.7 \text{ K} \quad (12)$$

where T_s is the saturation temperature of the steam at the pressure in the shell of the heater. The log-mean temperature driving force is then (see Figure 3):

$$(\Delta T_H)_{LM} = \frac{(\Delta T_H)_1 - (\Delta T_H)_2}{\ln \left(\frac{(\Delta T_H)_1}{(\Delta T_H)_2} \right)} = 66.3 \text{ K} \quad (13)$$

The overall heat-transfer coefficient is

$$U_H = \frac{Q_{PWH}}{A_H (\Delta T_H)_{LM}} \quad (14)$$

$$U_H = \frac{118.83 \text{ (kW)}}{0.5421 \text{ (m}^2) \cdot 66.3 \text{ (K)}} = 3,306 \text{ W/K-m}^2$$

There is no multiple-pass correction factor because the steam-side temperature is constant.

2. Cooler:

Similar calculations are carried out for the cooler. See Figure 3.

$$\begin{aligned}(\Delta T_c)_1 &= T_{\text{PWH,out}} - T_{\text{CW,in}} = 68.2 - 31.1 = 37.1 \text{ K} \\ (\Delta T_c)_2 &= T_{\text{PWC,out}} - T_{\text{CW,out}} = 33.3 - 7.2 = 26.1 \text{ K} \quad (15)\end{aligned}$$

$$(\Delta T_c)_{\text{LM}} = \frac{(\Delta T_c)_1 - (\Delta T_c)_2}{\ln\left(\frac{(\Delta T_c)_1}{(\Delta T_c)_2}\right)} = 31.3 \text{ K} \quad (16)$$

$$\begin{aligned}U_c &= \frac{Q_c}{A_c (\Delta T_c)_{\text{LM}} F_{\text{corr}}} \\ &= \frac{121.4 \text{ (kW)}}{(2.957 \text{ m}^2)(31.3^\circ\text{K})(0.96)} = 1,368 \text{ kW/K} - \text{m}^2 \quad (17)\end{aligned}$$

The 1-shell pass/4-tube pass correction factor $F_{\text{corr}} = 0.96$ is obtained from Fig.13.18a of Cengel.^[3]

C. Velocities and Reynolds Numbers

The inside diameter of the tubes in the heater is 0.00475 m, and there are 54 tubes per pass. The velocity is

$$\begin{aligned}A_{\text{CS,H}} &= 54(\pi D^2 / 4) = 0.0009569 \text{ m}^2 \\ v_H &= \frac{0.8275 \text{ (kg/s)}}{0.0009569 \text{ (m}^2) 987 \text{ (kg/m}^3)} = 0.877 \text{ m/sec} \quad (18)\end{aligned}$$

The Reynolds number is

$$(\text{Re})_H = \frac{D_H v_H \rho}{\mu} = \frac{0.00475 \text{ (m)} 0.877 \text{ (m/s)} 987 \text{ (kg/m}^3)}{0.000552 \text{ (kg/m-s)}} = 7,444 \quad (19)$$

The inside diameter of the tubes in the cooler is 0.00775 m, and there are 26 tubes per pass. The velocity is

$$\begin{aligned}A_{\text{CS,C}} &= 26(\pi D^2 / 4) = 0.00123 \text{ m}^2 \\ v_c &= \frac{0.8275 \text{ (kg/s)}}{0.00123 \text{ (m}^2) 987 \text{ (kg/m}^3)} = 0.684 \text{ m/s} \quad (20)\end{aligned}$$

The Reynolds number is

$$(\text{Re})_c = \frac{D_c v_c \rho}{\mu} = \frac{0.00775 \text{ (m)} 0.684 \text{ (m/s)} 987 \text{ (kg/m}^3)}{0.000555 \text{ (kg/m-s)}} = 9,418 \quad (21)$$

TABLE 3. Operating Parameters for the Heater

m_{PW}	Avg. Temp.	Q_{PW}	Prandtl	Velocity	Re	U
(kg/s)	(°C)	(kW)	—	(m/s)	—	(W m ² K ⁻¹)
0.241	42.5	38.9	4.20	0.252	1860	969
0.667	54.4	102.0	3.36	0.70	6330	2920
0.8275	51.1	118.8	3.56	0.877	7440	3300
0.953	50.8	134.6	3.58	1.009	8530	3570
1.044	50.3	137.6	3.62	1.105	9260	3670
1.099	50.3	134.8	3.62	1.164	9750	3590

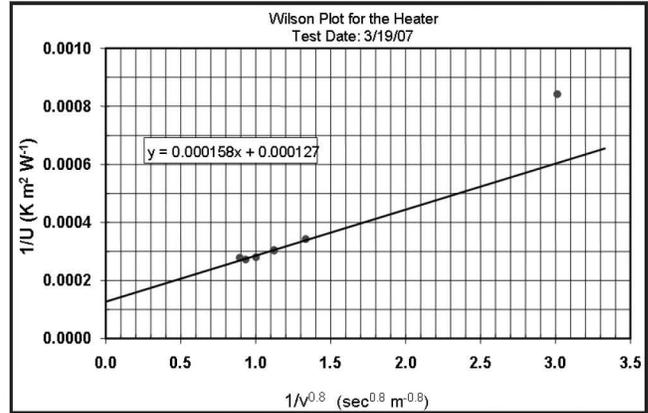


Figure 4.

WILSON PLOT FOR HEATER

A. Inside Film Coefficients:

Experimental data for a range of process-water flowrates are evaluated in a similar fashion as described above to calculate the overall heat-transfer coefficients and fluid velocities inside the tubes of the heater as well as the cooler. Results for critical parameters are presented in Table 3.

Since all but one data point have Reynolds numbers much greater than 2100, these data points are in the turbulent regime. Therefore, the constant “m” for the power of Re is assumed to be 0.8 according to the Dittus-Boelter correlation. For heating the fluid, again Dittus-Boelter suggests $n=0.4$ for the power coefficient of the Pr.

With these coefficients in mind, the Wilson plot for the heater data is shown in Figure 4. Several observations can be made from the Wilson plot.

- The five data points with high Re show a linear trend. This confirms that the power of Re is equal to 0.8, as was assumed when constructing the Wilson plot.
- The point with the low Re (1865) shows

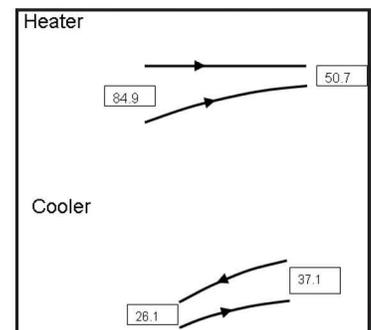


Figure 3.

a lower overall heat transfer coefficient as expected.

- The regression line for the data points in the turbulent regime intersects the ordinate at $1/U_i = 0.000127$. Since the ordinate is where the process water velocity is infinite (infinitely large heat transfer coefficient inside the tube), this value is equal to coefficient "A" of Eq. (3a). Assuming minimal level of fouling inside and outside of the tube ($R_f = R_{fo} = 0.00003 \text{ m}^2 \text{ K W}^{-1}$), the shell side film coefficient is calculated from Eq. (3a) to be $23,000 \text{ W m}^{-2} \text{ K}^{-1}$.
- The slope of the regression line is equal to the coefficient "B" in Eq. (7), which is used to calculate coefficient "C" in Eq. (4), as $C = 0.020$. The final correlation for the present experimental data is then:

$$\text{Nu} = \frac{h_i D_i}{k} = 0.020 \text{ Re}^{0.8} \text{ Pr}^{0.4} \quad (22)$$

Figures 5 and 6 compare experimentally found internal heat-transfer film coefficients to predictions by the Dittus-Boelter correlation. Figure 5 shows this comparison in a Nu/Pr^n vs. Re plot, and Figure 6 compares heat-transfer film coefficients. As indicated in Eq. (22), experimental results are 15% less than the predictions of the Dittus-Boelter correlation.

B. Repeatability:

The results of Wilson plot method are quite sensitive to

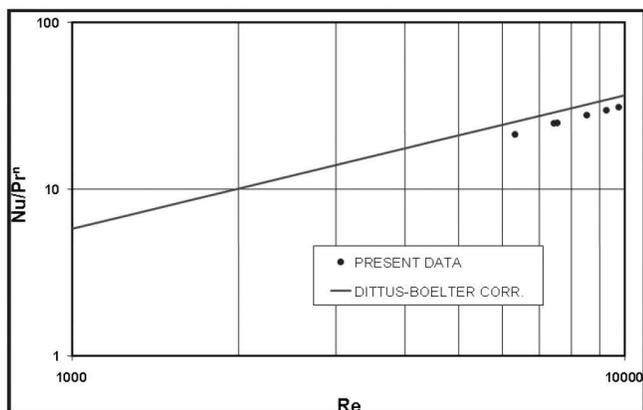


Figure 5.

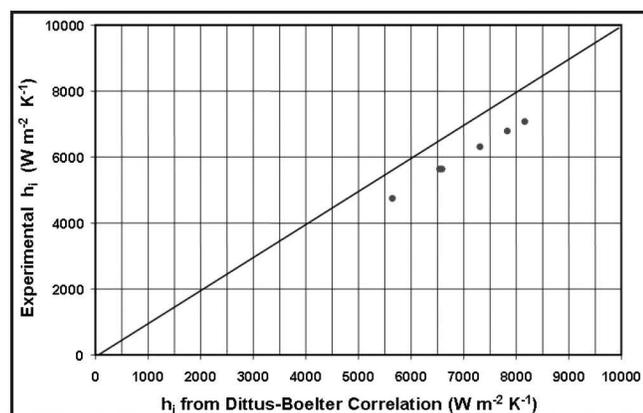


Figure 6.

the experimental uncertainty. This is illustrated in Figure 7, which shows two Wilson plots from the same facility but using data recorded on two different days. The circles are the data presented in Figure 4. The triangles represent results of the other experimental set of runs. It is seen that the two data sets provide two lines with different slopes. The slopes of the two data sets are 0.000158 and 0.0002, a difference of 25%. This difference will of course affect the film coefficients similarly. This illustrates one of the problems with the Wilson plot method. The long extrapolation of the data points to zero on the abscissa makes the value of the intercept on the ordinate quite sensitive to the accuracy of the data.

DYNAMICS AND CONTROL

The steady-state experiments described above are performed by manually positioning the three control valves. In the control part of the experiment, two experimental identification techniques are used to find important dynamic features of the process: step testing and relay-feedback testing. Transfer functions and frequency response plots are generated from the experimental dynamic data. PI controllers are designed, and their closed-loop performances are evaluated experimentally and compared with computer simulations of the dynamic process.

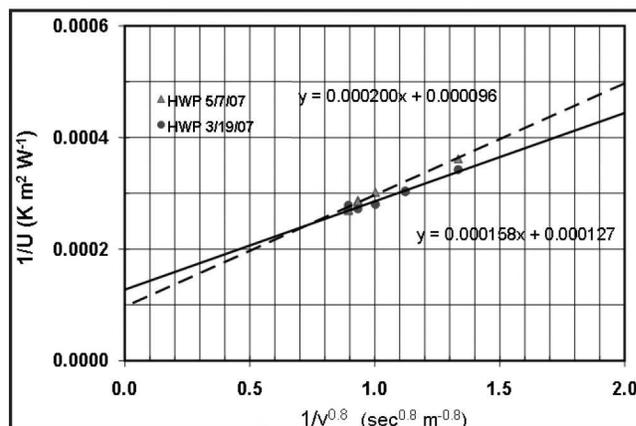


Figure 7.

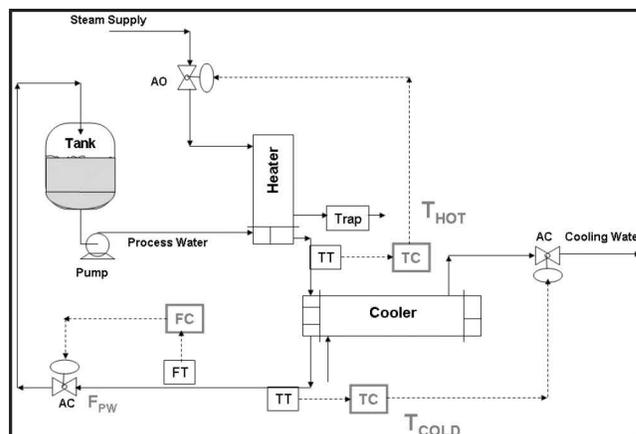


Figure 8.

One of the interesting control features of this experiment is dependence of the dynamics on the flowrate of the process water through the system. The higher the flow, the faster the dynamic responses of both heat exchangers. Controller tuning then depends on the process water flowrate.

A. Equipment and Control Structure:

Temperature and flowrate measurements are fed into a computer using A/D converters. LabView software has been developed that permits PI control with the three control valves positioned by three D/A converters from the computer. The steam valve is air-to-open, AO, so it will fail closed. The cooling water and process water valves are air-to-close, AC, so they will fail wide open.

The control structure is shown in Figure 8. There are three control loops.

1. Process-water flowrate is controlled by manipulating the process-water control valve.
2. The process temperature leaving the heater, T_{HOT} , is controlled by manipulating the steam valve.
3. The process temperature leaving the cooler, T_{COLD} , is controlled by manipulating the cooling water valve.

A screen shot is given in Figure 9 showing the three controller faceplates on the left. Each has a manual/automatic switch and displays for the setpoint (SP), the process variable (PV) and the controller output (OP).

B. Flow Control of Process Water:

The standard tuning of a flow controller is $K_C = 0.5$ and $\tau_i = 0.3$ minutes. The loop is quite fast since the flow transmitter and the valve respond quickly. Therefore a small integral time can be used. The gain is kept small so that the noise of the flow transmitter is not amplified.

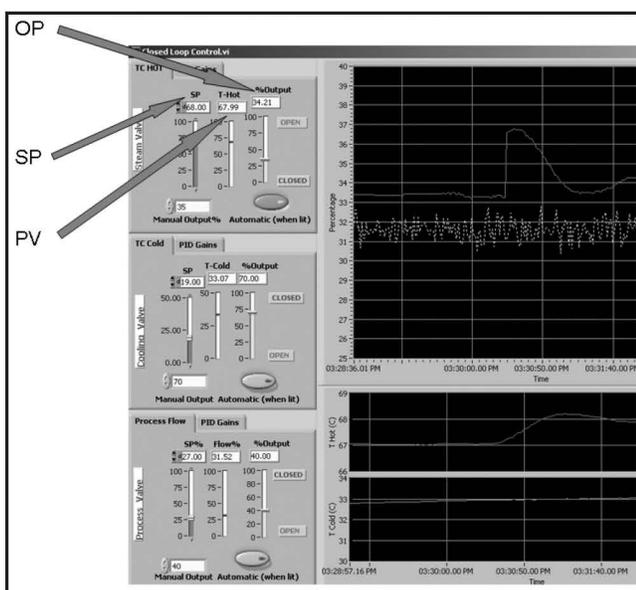


Figure 9.

The process water valve is AC, so the flow controller should have “direct” action (an increase in the flow transmitter signal PV produces an increase in the controller output signal OP to the valve, which reduces the opening of the valve). The equation of a PI controller is:

$$OP = Bias \pm K_c \left(E + \frac{1}{\tau_i} \int E dt \right)$$

$$E = SP - PV \quad (23)$$

A direct-acting controller should have a negative gain. Step changes in the setpoint of the flow controller are made to confirm that the tuning constants used give good flow control performance.

C. Step Tests:

With both temperature controllers on manual, positive and negative step changes in the heater exit temperature controller output signal to the steam valve are made to identify a transfer function relating the controller OP signal to process PV signal (T_{hot}). See Figure 10.

From the dynamic step response, an approximate transfer function of the form given in Eq. (24) is determined.

$$G_{M(s)} = \frac{PV_{(s)}}{OP_{(s)}} = \frac{K_p e^{-Ds}}{\tau_o s + 1} \quad (24)$$

where K_p is the process steady-state openloop gain, D is the deadtime and τ_o is the openloop time constant. The process gain K_p must be dimensionless, so the change in temperature must be divided by the temperature transmitter span (100 °C) to convert the PV signal to percent of scale. The OP signal is in percent of scale. The experimental data in Figure 10 show a deadtime of 0.2 minutes, a time constant of 1.1 minutes and a gain of 0.7.

The ultimate gain K_u and ultimate frequency ω_u are calculated from the transfer function using the relationships at the

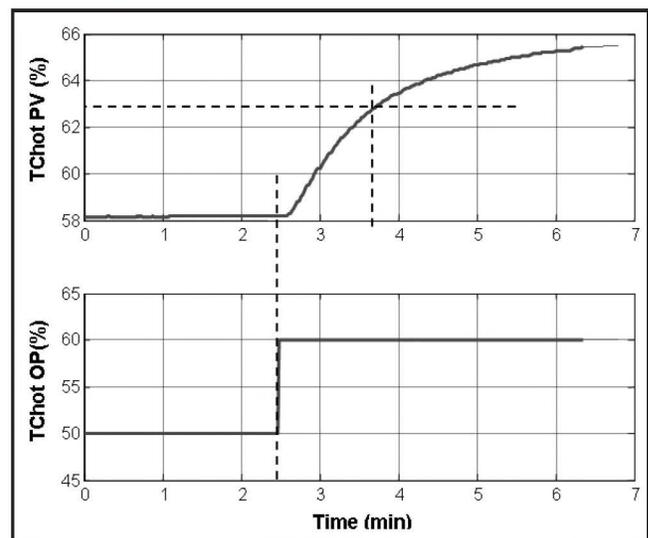


Figure 10.

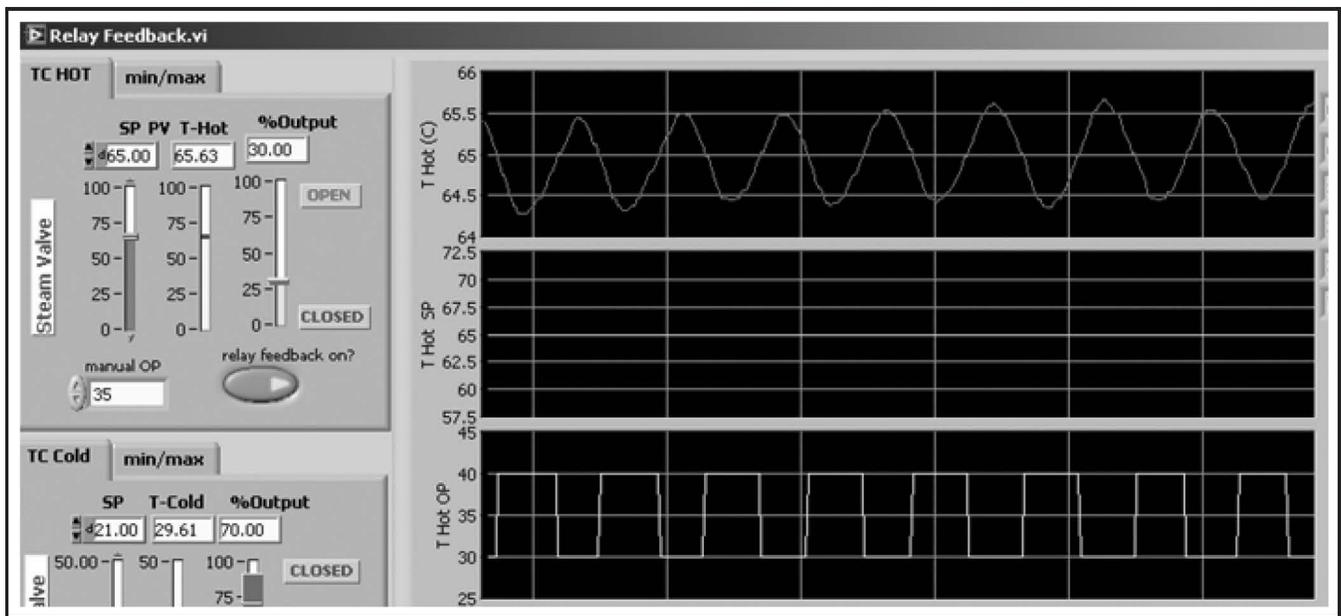


Figure 11.

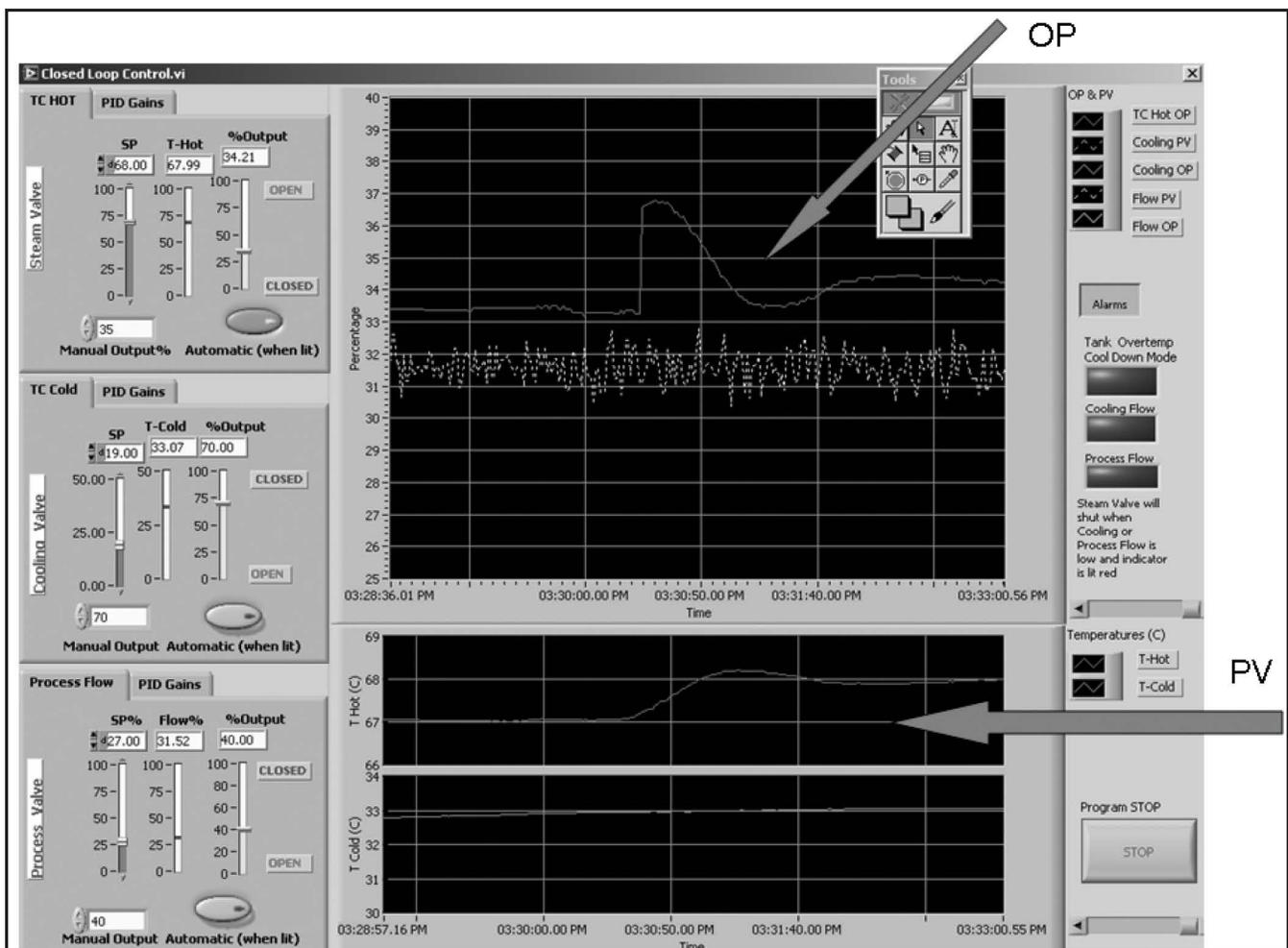


Figure 12.

ultimate frequency ω_u .

$$\arg G_M(i\omega_u) = D\omega_u - \arctan(\omega_u \tau_o) = -\pi \text{ radians.}$$

$$|G_M(i\omega_u)| = \frac{K_p}{\sqrt{1 + (\omega_u \tau_o)^2}} = \frac{1}{K_u} \quad (25)$$

The step test results predict an ultimate frequency of 8.4 radians/minute and an ultimate gain of 13.

D. Relay-Feedback Test

The relay-feedback test is a very simple, fast, and practical method for determining accurate information for tuning of feedback controllers. It is widely used in industry and is also included in commercial dynamic simulators to facilitate controller tuning. The test gives values for the ultimate gain and period.

A high-gain relay is inserted in the feedback loop that switches the controller output signal a specified “h” percent above or below the steady-state OP value as the PV signal crosses the SP setpoint signal. The SP signal is adjusted so that the signal to the control valve varies between the $\pm h$ limits in *symmetrical* pulses (approximately the same time at the low limit as at the high limit). Figure 11 gives a screen shot of the monitor when the relay-feedback test is running.

The amplitude “a” of PV temperature sinusoidal signal T_{hot} and the period P_u are read from a strip chart. The amplitude a must be in % of scale, using a temperature transmitter span of 100 °C. Note that h is also in percent of scale.

The ultimate gain and ultimate frequency from the experi-

mental curves are calculated and compared with the values obtained from the transfer function.

$$K_u = \frac{4h}{a\pi} \quad (26)$$

Figure 11 shows a plot of typical data. The value of a is 0.6 % with a 5% h, and the period is 0.7 minutes. The calculated ultimate gain is 10 and the ultimate period is 0.7 minutes, giving an ultimate frequency of 9 radians/minute. These results are fairly close to those determined from the step test data and are more reliable because of the closedloop nature of the relay-feedback test, which keeps the process in the linear region.

E. Closedloop Control

The Tyreus-Luyben tuning constants are calculated, and their performance for disturbances in setpoints and process water flowrate are observed.

Tyreus-Luyben:

$$K_c = \frac{K_u}{3.2} = \frac{10}{3.2} = 3.1$$

$$\tau_1 = 2.2 P_u = 2.2(0.7) = 1.5 \text{ minutes} \quad (27)$$

Figure 12 shows the closedloop step response of the T_{HOT} temperature controller for a change in setpoint using TL tuning. The setpoint is changed from 67 °C to 68 °C (a 1% of scale change). The OP signal jumps immediately from 33.3% to 36.4% from the proportional action ($K_c = 3.1$). There is a slight overshoot of the setpoint, and it takes about 3 minutes for the loop to settle out.

The closedloop response of the system for load disturbances is also explored by making changes in the flowrate of the process water. Process nonlinearity is studied by seeing how the dynamics of the process change at different process water circulation rates. Time constants decrease as process water flowrates increase.

COMPUTER SIMULATIONS

Our students use process simulation tools extensively in their design course to develop process flowsheets and study dynamic plantwide control. Applying these tools for the heat exchanger experiment provides an important exercise in comparing model predictions with real experimental data.

A. Steady-State Flowsheet Simulation:

A steady-state simulation of the two-heat exchanger and feed tank system is developed in Aspen Plus. Equipment sizes, operating conditions, and experimental heat-transfer parameters are used to match experimental steady-state conditions.

The *HeatX* unit is used in the *Short-cut* and *Design* modes. The inlet conditions of the steam and the process water are specified in the heater. In addition, the hot condensate stream leaving the heater is specified to have a vapor fraction of zero, as shown in Figure 13A. Figure 13B shows that the overall heat-transfer coefficient U is specified to be the experimen-

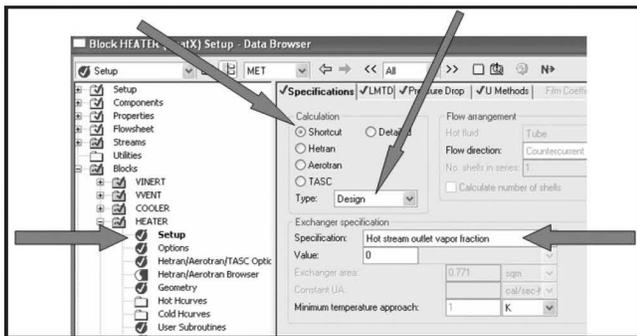


Figure 13A.

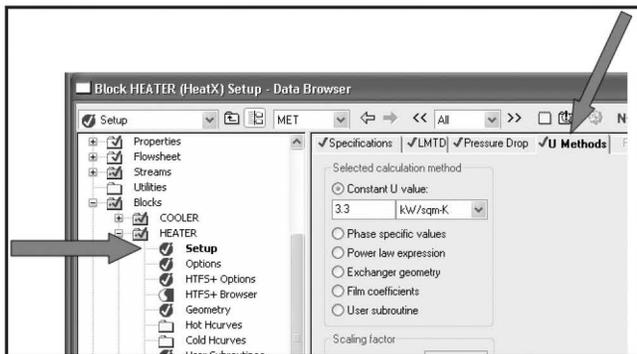


Figure 13B.

tal value ($3.3 \text{ kW m}^{-2} \text{ K}^{-1}$). The program then calculates the required area, which is almost exactly the real heat-transfer area of the heater.

The specification for the cooler, besides the inlet conditions of the cooling water and the process water, is the exit temperature of the process water, as shown in Figure 14.

The simulation is pressure driven, so pressures throughout the process must be specified. The pump discharge pressure is set at 5 atm in the simulation, and 1 atm pressure drops of the process water through each heat exchanger are assumed. The steam supply pressure is 3.3 atm with 1.5 atm in the shell side of the heater. The cooling water supply pressure is 5 atm, and the pressure drop through the cooler is assumed to be 1 atm. Since Aspen Plus does not permit the use of anything other than direct-acting control valve with linear trim, the steady-state positions of all control valves are set at 50% open in the simulation. Figure 15 gives the steady-state

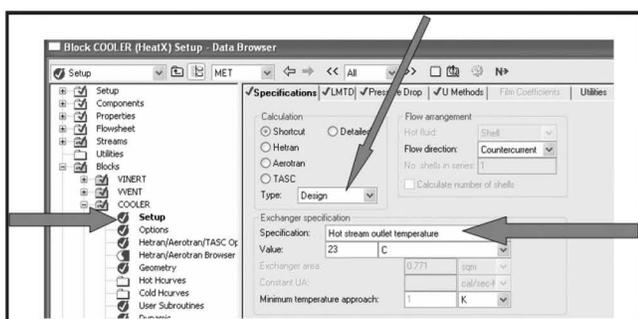


Figure 14.

	PWIN	PWOUTH	PWOUTC	STEAM	COND	CWIN	CWOUT
Temperature K	300.3	340.0	300.0	410.5	365.0	280.1	310.7
Pressure atm	5.00	4.00	3.00	3.30	1.50	5.00	4.00
Vapor Frac	0.000	0.000	0.000	1.000	0.000	0.000	0.000
Mole Flow kmol/hr	165.038	165.041	165.041	11.506	11.506	225.808	225.808
Mass Flow kg/hr	2974.355	2974.414	2974.414	207.288	207.288	4068.000	4068.000
Volume Flow l/min	50.023	52.087	50.008	1957.387	3.816	67.062	63.088
Enthalpy MMBtu/hr	-44.633	-44.186	-44.638	-2.596	-3.044	-61.407	-60.955
Mass Flow kg/hr							
WATER	2971.114	2971.173	2971.173	207.288	207.288	4068.000	4068.000
N2	3.242	3.242	3.242				
Mole Flow kmol/hr							
WATER	164.922	164.925	164.925	11.506	11.506	225.808	225.808
N2	0.116	0.116	0.116				

Figure 15.

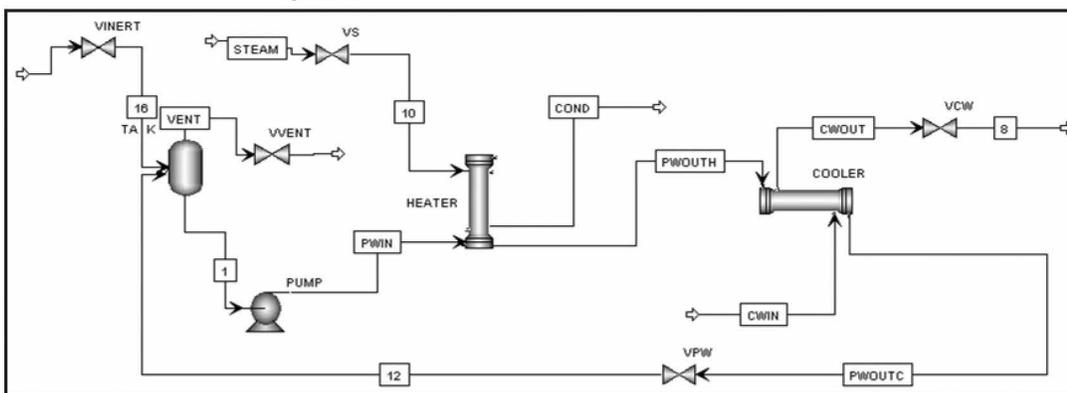


Figure 16.

stream information. The Aspen Plus process flow diagram is shown in Figure 16.

Note that a small nitrogen stream is fed into the feed tank and a vapor stream is removed. This is a simulation gimmick to account for the tank being open to the atmosphere.

B. Dynamics Simulation:

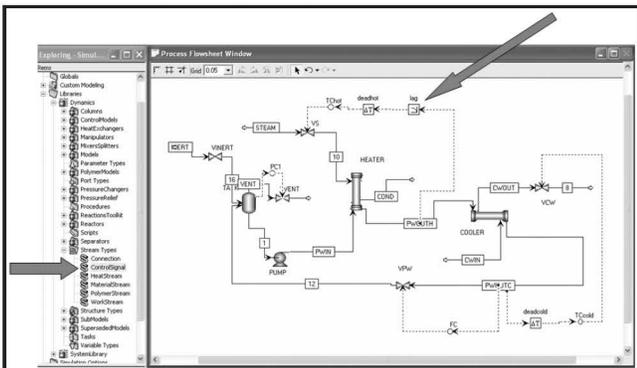
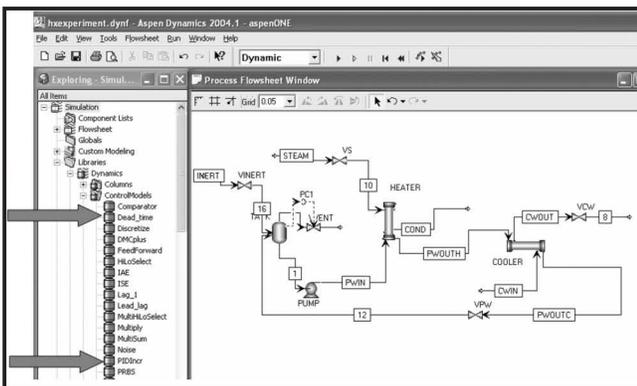
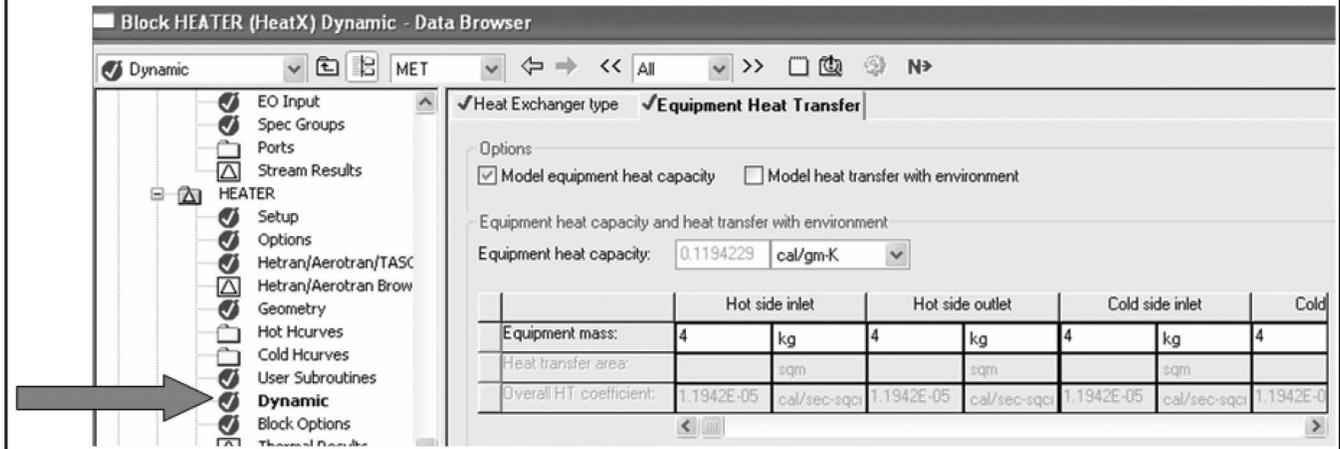
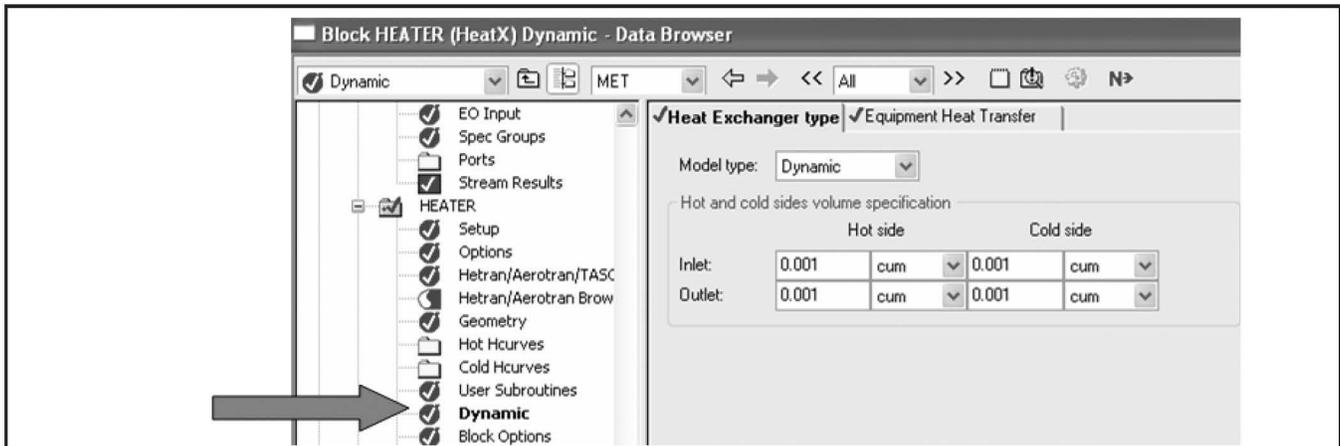
Before dynamics can be simulated, the volumes and weight of metal in the various units must be specified. These are calculated from the dimensions of the tubes and shell. Figure 17 shows how these are specified in the simulation by selecting the *Dynamic* item in the heater block. The file is pressure checked and exported into Aspen Dynamics as a pressure-driven simulation.

Figure 18 shows the initial process flow diagram generated in Aspen Dynamics. Controllers are installed by opening *Libraries, Dynamic, and ControlModels* in the *Exploring-Simulation* mode on the left side of the screen. A controller is inserted on the flowsheet by clicking on *PIDIncr* and dragging and dropping. Deadtimes are inserted in the same way.

The controllers are connected to the appropriate streams and valves by opening *Stream Types*, dragging a *ControlSignal* to the flowsheet and connecting its two ends to the appropriate spots. Figure 19 shows the TChot controller. It measures the temperature of the process water leaving the heater. The signal goes through a first-order lag and a deadtime before becoming the PV signal of the TChot temperature controller. The controller output positions the steam valve.

Figure 20 shows the controller faceplate. The third button from the right is clicked to open the window shown below the faceplate. The controller action is set to be *Reverse* since an increase in temperature should lower the OP signal. The dead-time in this loop is set at 0.1 minutes, and the lag time constant is set at 0.4 minutes. These values give an ultimate gain and frequency that match fairly closely the experimental values.

One of the unique features of the heater is the requirement that the condensate leaving must be saturated liquid (a vapor fraction of zero). In Aspen Dynamics, this condition is not the default. Instead the pressure is fixed. Of course, this is not what really happens. To increase flow of steam to the heater, the steam valve opens and the pressure on the steam side of the heater must increase to provide a higher temperature differential driving force. Therefore, some modifications must be made to simulate reality.

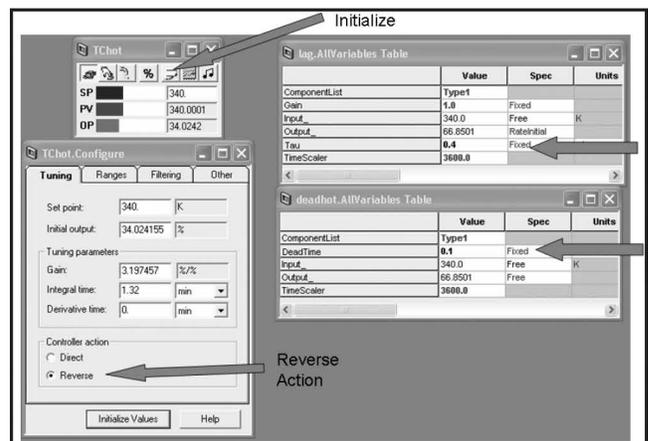


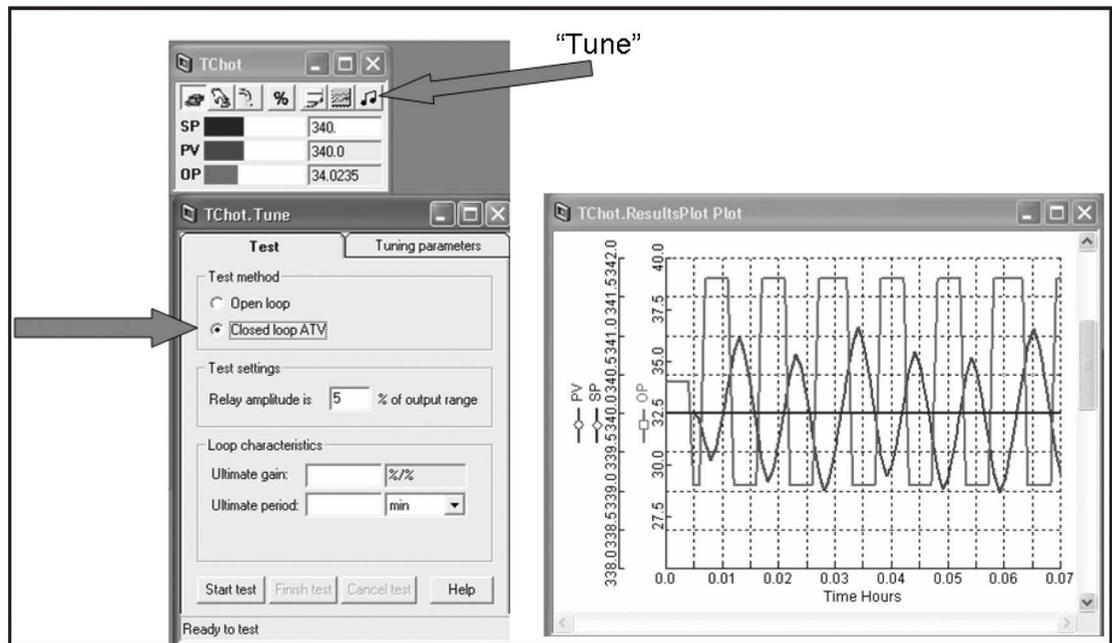
▲ Top: Figure 17.

◀ Left: Figure 18.

▶ Bottom left: Figure 19.

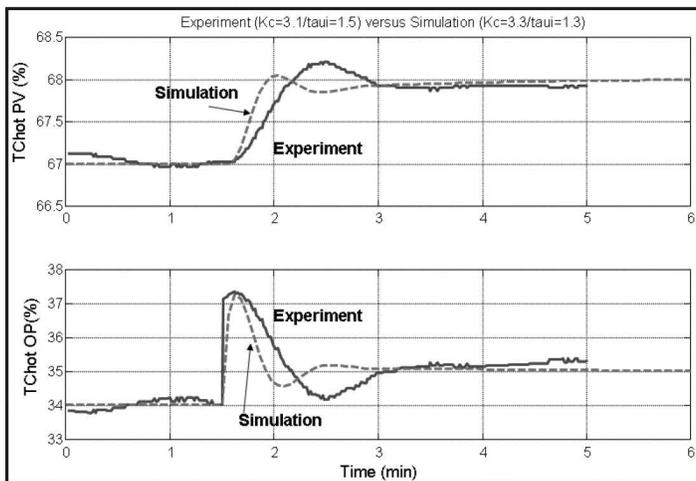
▼ Bottom right: Figure 20.





► Right: Figure 21.

▼ Below: Figure 22.



These are achieved by using *Flowsheet Equations*. The heater block is specified to have a hot stream leaving with a vapor fraction of zero.

$$\text{Blocks}(\text{"Heater"}).\text{Hotside.pflash2}(1).\text{vfr}=0;$$

In addition, the pressure of the condensate stream "COND" is changed from "fixed" to "free."

C. Dynamic Results:

Step changes are made by putting the controller on manual and changing the OP signal. Relay-feedback tests are run by clicking the *Tune* button on the controller faceplate (see Figure 21). The Closed loop ATV test is selected. The simulation is run until a steady state is obtained with the controller on automatic. Then the *Start test* button is clicked, and the process is allowed to run through several cycles, as shown in the strip chart in Figure 21. Clicking the *Finish test* button generated the ultimate gain and period: $K_u = 10.2$ and $P_u = 0.60$ minutes for the TChot controller.

Opening the *Tuning parameters* page tab, selecting the type of controller and the tuning rule and clicking the *Calculate* button produce the controller tuning constants. These settings are inserted into the controller by clicking the *Update controller* button.

Figure 22 gives a direct comparison between the experimental and simulation responses for a step change in setpoint of 1 K. The dynamics of the heater are fairly well predicted by the Aspen Dynamics simulation.

CONCLUSION

This paper has described an experiment that combines steady-state heat transfer analysis and dynamic controllability. The heat transfer analysis includes data reconciliation of redundant and conflicting temperature measurements by checking energy balances on both sides of the two heat exchangers. The Wilson plot method is used to calculate tube side film coefficients from the measured overall heat transfer coefficients.

Experimental dynamic data is obtained from step and relay-feedback tests. Both steady-state conditions and control performance are compared with the predictions of a commercial process simulator.

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USING SIMULATION MODULE PCLAB for Steady State Disturbance Sensitivity Analysis in Process Control

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Classical methods of teaching process control have been practiced in the classroom over the past several decades. These methods tend to focus on rigorous solution of differential and/or transfer function equations. The result is that students get caught up in mathematical algorithms rather than conceptualizing what happens in practice. It became evident to academics and practitioners that the way process control is taught to chemical engineers needs updating. It is believed that the strict classical teaching approach needs to be replaced by more practical and concrete approach.^[1] To give students insights into the process control courses they take, laboratory courses and simulation tutorials were introduced in most chemical engineering curricula as supplements. This, it was believed, would give students insight and experience into the actual practice of chemical engineering. This issue was raised and discussed by many academic researchers and instructors and by practicing engineers.^[1-8]

The introduction of simulation software has given students an outlet to follow their imagination. Simulation packages have caught up in all branches of engineering. This is because simulators have now acted as mergers between theory and practice that give students better understanding of processes before they venture into industry. The visualization of the process helps the student to form solid concepts on various aspects of chemical engineering.^[9, 10]

Process simulation technology has evolved dramatically over the past 10 years. Many packages are available that allow intuitive visualization with a user-friendly graphical interface that allows rapid control design using click-and-drag operations. Rivera, *et al.*,^[11] uses modules incorporated directly in process control computers. Young, *et al.*,^[1] presented workshops based on real-time simulation of industrial processes. Henson and Zhang^[2] have integrated simulation experiments

based on HYSYS into the undergraduate process control courses. Cooper, *et al.*,^[9,10] introduced a training simulator called Control Station. Other software packages for control education include PICLES,^[12] and ACS^[13]; however, these packages do not, in general, adequately handle large practical-scale problems.^[14] Doyle, *et al.*,^[15] have developed a process control module (PCM) simulator based on a MATLAB/SIMULINK environment that contains case studies illustrating various process control concepts. Despite the benefits of simulation-based experiments, one main criticism remains the lack of physical process that can be felt by students. It is argued, however, that training simulators can provide students with a broad range of experiences at low cost and in a safe environment. Moreover, students can achieve these experiences conveniently at their own desks.^[9]



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Process Control Laboratory (PCLAB) was developed in the chemical engineering department at King Saud University as an educational tool. General introduction of the tool is given elsewhere.^[16] The primary objective of this work is to unveil one of PCLAB's specific features—the steady state disturbance sensitivity analysis (SSDSA).^[17] We focus on SSDSA because it is a distinguishing contribution of PCLAB and because its approach is found to be effective in designing the control structure of multi-loops control problems.^[18, 19] Specifically, SSDSA will be carried out on a forced-circulation evaporator process, which is one of PCLAB's case studies. The purpose is to explore the disturbance effects on the output and controlled parameters and to conclude from the analysis which manipulated variable could be used to mitigate the effect of the disturbances.

PCLAB

PCLAB is interactive simulation software for process control analysis and training. It was developed using MATLAB tools and functions including SIMULINK (a graphical simulation toolbox). MATLAB was chosen as the programming platform because it became a standard among academic and industrial users alike for use both in research and education.^[14] Moreover, one can easily customize or add to existing modules of MATLAB. The flexibility of this platform allows for migration to many PC and workstation hardware platforms.^[14] The PCLAB software is designed in a user-friendly, menu-driven framework such that the process engineer can easily navigate through the various parts of the program, carry out simulation experiments, visualize the results, and draw conclusions on the effects of different parameters and control configurations. This is achieved by using the main-menu shown in Figure 1 which provides a Graphical User Interface (developed in the MATLAB graphics language). The software will run on any platform supported by MATLAB (WIN 95, WIN NT, UNIX). The software consists of several modules that comprise different case studies based on fundamental process models of industrial unit operations. The case studies of the current version of PCLAB shown in Figure 1 include process models adopted from the literature such as Forced Circulation Evaporator,^[20] Fluid catalytic Cracking Unit,^[21] Double Effect Evaporator,^[22] and Two CSTRs in Series.^[23] The case studies also include process models that are developed and validated by our research group such Polyethylene Reactor,^[18] Ethylene Dimerization Reactor,^[19] and Multistage Flash Desalination Plant.^[24] The selected modules in addition to the convenient visualization feature of the software provide the student with real-world hands-on experience. PCLAB is available for public use. Interested readers can download the program from the following Web site: <<http://faculty.ksu.edu.sa/Emad.Ali/Pages/PCLab.aspx>>

The main menu of the program, as shown in Figure 1, allows the user to choose from different case studies. When a case

study is chosen from the main menu, the software will trigger a submenu that contains the available exercises that can be carried out on the chosen case study. The submenu, shown in Figure 2, allows the user to select a specific tutorial from a variety of exercises, such as steady state analysis, process dynamic analysis, process identification, control structure selection and controller tuning for SISO systems, and multiple SISO loop tuning.

In this paper, we will discuss the SSDSA exercise applied on the forced-circulation evaporator case study to explore the versatility of the current version of PCLAB software. Application procedure of SSDSA on other case studies is similar.

FORCED-CIRCULATION EVAPORATOR

The forced-circulation evaporator is a common processing unit in sugar mills, alumina production, and paper manufacture. This process is used to concentrate dilute liquor by evaporating its solvent (usually water), as shown in Figure 3.^[20] A feed stream with solute of concentration C_1 (mass percentage) is mixed with high volumetric recycle flow rate and fed to a vertical evaporator (heat exchanger). The solution will pass through the tube. A saturated steam is used to heat the mixture by condensing on the outer surface of the tubes. The liquor, which passes up inside the tube, boils and then passes to a separator vessel. In the separator, the liquid and vapor are separated at constant temperature and pressure. The liquid is recycled with some being drawn off as product with solute concentration of C_2 . The vapor is usually condensed with water and used as the coolant.

A description of the process parameters and their values are given elsewhere.^[21] For this process we deal with three inputs: the coolant flow rate, F_{200} ; the steam pressure, P_{100} ; and the steam flow rate, F_{100} . Four disturbances are considered: the feed flow, F_1 ; feed temperature, T_1 ; feed concentration, C_1 ; and the coolant temperature, T_{200} . The process has four outputs: liquid level, L_2 ; output concentration, C_2 ; Column pressure, P_2 ; and outlet flow rate, F_2 .

PROCESS ANALYSIS

In this section, we discuss how steady state disturbance analysis can be implemented on PCLAB. This procedure is very useful for designing the appropriate control structure.^[18] When controlling a plant or a process with many inputs and outputs, it is usually difficult to optimally pair variables into a multi single loops structure. SSDSA is a tool that can help in this regard, although it cannot be implemented on real plant. Instead, simulation of the process can be used to perform the task. Figure 2 illustrates that one can simply click on the steady state disturbance analysis. As a result a new window will pop up. The new window is an SSDSA interface module for the evaporator case study as shown in Figure 4.

Figure 4 shows that the process has three inputs and four

possible disturbances, as discussed earlier. The procedure will focus on investigating the static effect of any disturbance or any combination of disturbances on the process outputs in open loop mode. This means that the inputs will remain fixed during the test. This is known as the open loop test. It reveals which process output is affected the most and which one is affected in nonlinear fashion. The test can also be run in closed loop mode. In this case, an output should be selected

as the controlled variable and a corresponding input should be selected to be the manipulated variable. The test will then examine the effectiveness of the chosen input to maintain the controlled variable at its nominal value in steady state when the process is under the influence of a range of disturbance values.

To start the procedure, simply click on the green button or the start button on Figure 4. By doing so, the SSDSA menu

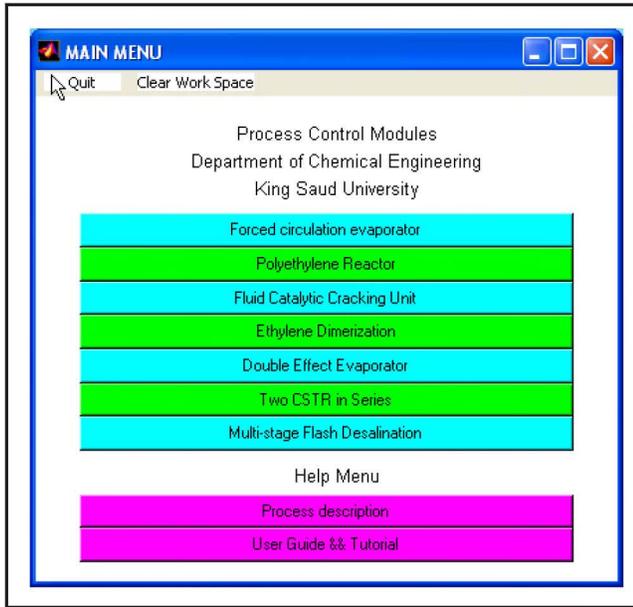


Figure 1. Main menu showing the main case studies.

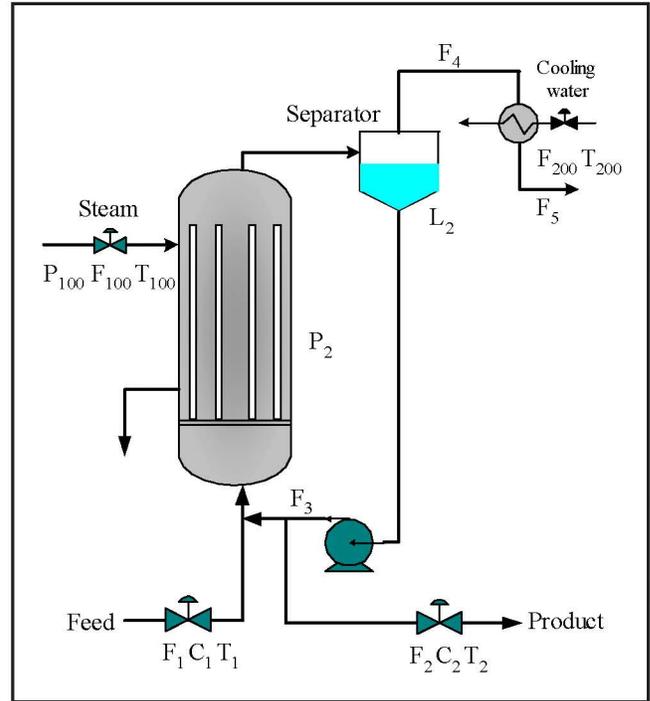


Figure 3. Flow sheet of Forced circulation Evaporator Process.

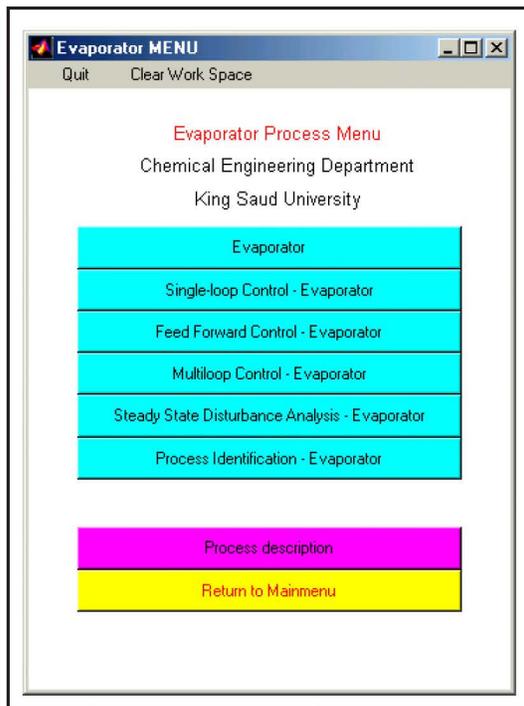


Figure 2. Sub Menu for Evaporator Case Study showing available control exercises.

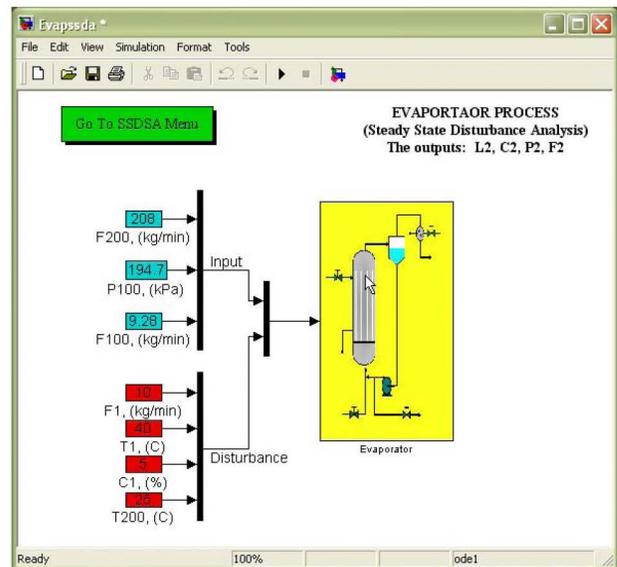


Figure 4. Steady State Disturbance Module for Evaporator Process.

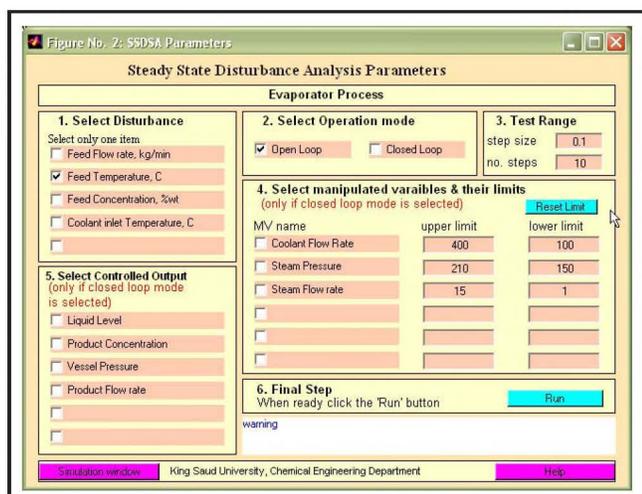


Figure 5. SSDSA menu for the evaporator process.

illustrated in Figure 5 pops up:

The menu in Figure 5 allows the user to enter the key parameters that controls the SSDSA analysis. Basically six steps are required to carry out the SSDSA analysis procedure, as discussed in the following two sections.

Open loop mode

First the user should select one of the four possible disturbances by marking the appropriate checkbox shown on Figure 5, for instance, the feed temperature. (Note that the other case studies of PCLAB will have a different list of disturbance variables according to the relevant process.) Next, mark the open loop checkbox. The third step controls the test range. For example, if the nominal value for the feed temperature is $T_0 = 40^\circ\text{C}$ and using step size of 0.1 and number of steps of 10, then the disturbance value will have the following range during the test:

$$T \in [T_0 + (10/2) * 0.1T_0, T_0 - (10/2) * 0.1T_0] \quad \text{Eq. (1)}$$

Increasing the number of steps at the same step size will increase the temperature range to be covered. The above values for the step size and number of steps cover a $\pm 50\%$ range, which is good enough from practice point of view. Decreasing the step size will help in producing smoother response curves but it will decrease the overall range. Therefore, if one decreases the step size for better resolution, one should also increase the number of steps to maintain the same operating range. It should be noted, however, that smaller step size requires a higher computational load.

In the open loop mode, steps 4 and 5 are bypassed. (If by mistake the user marks one of the boxes in step 4 or 5, an error message will be displayed in the warning box.) Next, press the run button and look at the results, shown in Figure 6.

Figure 6 illustrates how the four main process outputs respond at steady state to changes in the feed temperature

from 20 to 60°C . The graphs shows the response of the liquid level at the top followed by concentration response, then pressure response and finally the flow response to changes in feed temperature. It is obvious that the liquid level in the separator unit is not affected by this type of disturbance. Thus in the open loop mode, the user can gain information about the directional, magnitude, and nonlinearity effect of a disturbance. For example, as a directional effect, both C_2 and P_2 will increase when the feed temperature increases, while the outlet flow rate F_2 will decrease. One can also observe that the solute concentration (C_2) received the highest (magnitude) impact. Moreover, all outputs are altered linearly with the temperature variation. Thus, the user can learn how the process operation and product quality may be significantly influenced when the feed temperature is changing freely.

Closed loop mode

In this test mode, the student should unmark the open loop checkbox and mark the closed-loop checkbox instead. Furthermore, there is a need to specify a controlled variable. Let us choose, for example, the output concentration, C_2 . In addition, the user should select one of the manipulated variables listed in Step-Box 4 as the candidate. Let the candidate-manipulated variable be the coolant flow rate. See Figure 7 for example. The user then has the choice to either change the upper and lower permissible values for the candidate-manipulated variable or leave them at their default values. Note that the default values for the upper and lower limit can be restored at any time by simply clicking the “reset limit” button. It should be noted that in this simulation mode no typical control system is involved. The control objective, *i.e.*, the output deviation from its set point, is formulated as an algebraic constraint. These constraints along with the model algebraic equations are solved at steady state using the manipulated variables as the design parameters.

After the user finishes marking the required checkboxes in the SSDSA menu, he can simply click the run button in Step-Box 6. The result for the above specification is shown in Figure 8.

By inspecting the output response in Figure 8a, one observes that the controlled variable C_2 is well maintained at the nominal value. Not visible here, but on the computer screen, a red color is used for the controlled variable to distinguish it from the other uncontrolled outputs. Because the evaporator pressure is not controlled, it increases as expected with disturbance but this time with a larger magnitude. On the other hand, the feedback control caused the output flow rate to change slightly with disturbance.

More important is the response of the manipulated variable. In the right-hand plot, Figure 8b, red lines would be seen, showing the upper and lower limits for the coolant flow rate, which is set at 400 and 100, respectively. A white line represents the response of the coolant flow rate to disturbances,

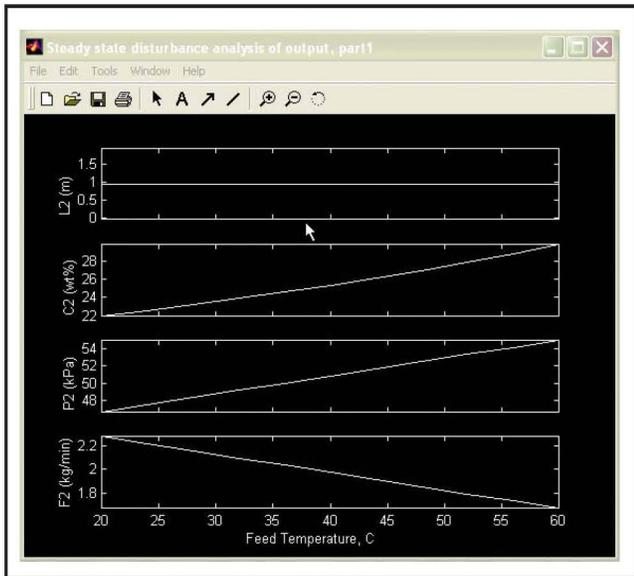


Figure 6. SSSDA results for open loop test showing the effect of feed temperature.

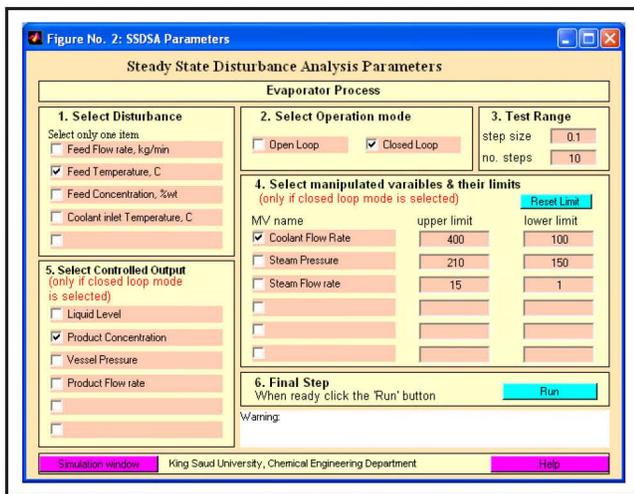


Figure 7. SSSDA menu for closed loop case option.

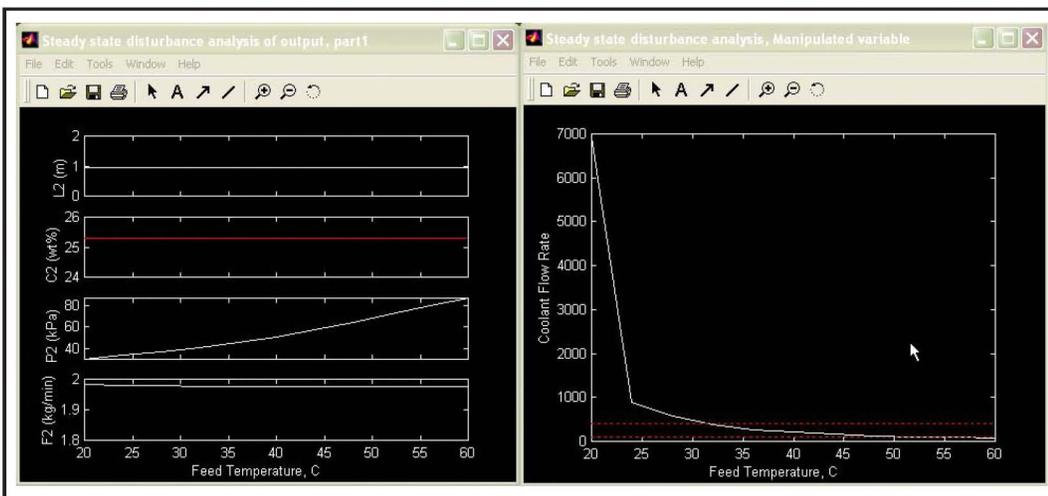


Figure 8. Output responses to disturbance in feed temperature when the coolant flow rate is used as manipulated variable.

allowing the user to maintain C_2 at nominal value. For large disturbances, *i.e.*, when the feed temperature exceeds 55 °C, the coolant flow should be reduced slightly below the lower limit in order to reject the effect of the disturbance. At feed temperature below 30 °C, however, the coolant flow rate must be increased multifold, especially below 25 °C, to maintain the required operation. Low feed temperature requires higher steam pressure to provide enough heat of vaporization, which in turn increases the process temperature. As a result a large amount of coolant flow is needed to absorb the extra heat and to cool down the vapor. The high demand on coolant flow may not be physically possible, however. Therefore, one can conclude that the coolant flow rate is not a good manipulated variable for negative disturbance in the feed temperature.

The user can also carry out a multivariable SSSDA. For example, one can add another controlled variable to the control structure, such as the column pressure. For this case, the user should consider a suitable manipulated variable, such as the steam flow rate. Rerunning the SSSDA as before, we obtain the results shown in Figures 9 and 10 (next page). Figure 9 shows clearly that the controlled variable and consequently the remaining outputs are well maintained at their targets. (Note that, on-screen, the controlled variables are distinguished by the red color.) On the other hand, Figure 10 shows how the selected manipulated variables change to counteract the effect of the disturbance and ultimately regulate the output at their set points. Notably, the first manipulated variable (*e.g.*, coolant flow rate) has not changed, while the second manipulated variable (*e.g.*, steam flow) decreased slightly as the feed temperature increased. One can accept this control structure because for a range of $\pm 50\%$ changes in the disturbance, the product concentration and column pressure are well regulated with minimum change in the manipulated variable. Moreover, this is achieved without violating the physical bound of the manipulated variables.

Although Yi and Luyben^[17] have used SSSDA for determining basic control structure, its outcome can help in building

an appropriate input-output pairing. In fact, the user can test various scenarios by examining other candidate-manipulated variable and by repeating the procedure for the other controlled variables. At the end, the user can build up a satisfactory control structure for the process, *i.e.*, can select the appropriate input-output pairing configuration.

Similar studies can be carried out on the remaining disturbances and find their effects on the controlled parameter. Furthermore the case study that was used here can be replaced by another case study and similar SSDSA analysis can be carried out.

CONCLUSION

In this paper, the process control laboratory PCLAB is introduced. PCLAB is based on MATLAB platform and designed in a user-friendly environment by using a convenient graphical interface. The current version of PCLAB thus far includes seven modules (case studies) that reproduce basic chemical processes. PCLAB has a number of control design problems (exercises) that can be applied to each of the seven case studies. One of the PCLAB exercises is the steady state disturbance analysis. The exercise is illustrated through a tutorial using the evaporator case study. The examples illustrate how the SSDSA can be carried out in either open loop or closed loop mode without tedious programming. The analysis helps in illustrating which disturbance has a detrimental impact on the process. Furthermore, different control structure configurations can be screened off line to determine the most appropriate input-output pairing. In addition to this exercise, there are other control projects that can be studied to enhance student learning. These exercises can help students to practice and visualize the theoretical concepts taught in the classrooms.

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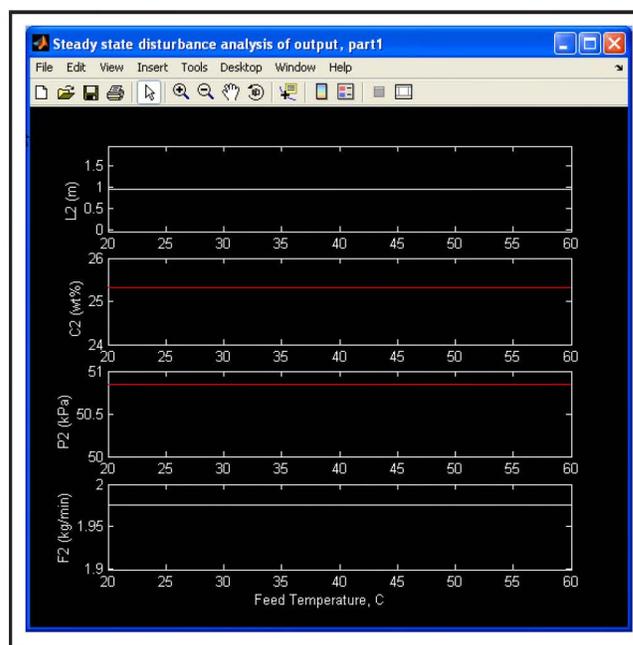


Figure 9. SSDSA result for multivariable case, output response.

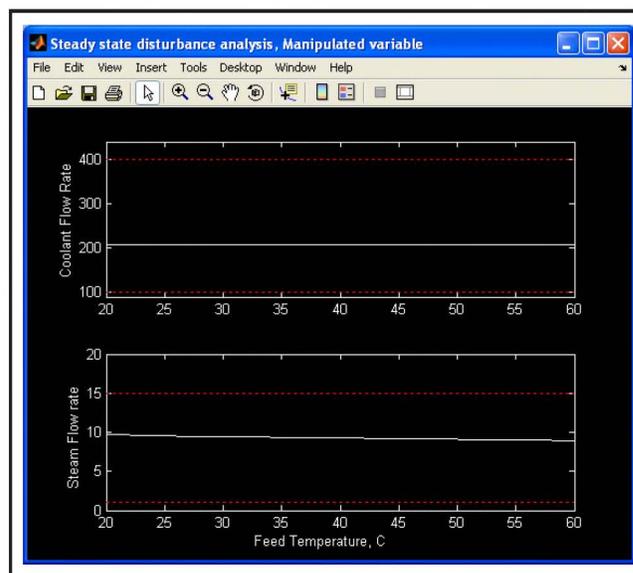


Figure 10. SSDSA result for multivariable case, the input response.

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PROCESS SYSTEMS ENGINEERING EDUCATION: LEARNING BY RESEARCH

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Chemical Engineering (ChE) education is a challenging task and is quite demanding for both teacher and student. The teacher has to effectively convey subject matter while the student must continuously develop knowledge and skill. In today's world, universities are becoming more and more competitive grounds for the elite educators serving students who are demanding concise higher education.^[1, 2] In this setting, the teacher must respond to this demand by providing a suitable and effective environment for learning. The broad question raised in this paper is "What constitutes such an environment?" In trying to answer this, we must recognize that the learning process is a complex interaction between the teacher, the student, the subject matter, and the learning environment. We further recognize that the teacher and the student carry with them inherent education attributes that also affect the learning process regardless of the subject matter and the environment.^[3, 4] In dealing with the question raised, we have come to realize the significance of the concepts of "facilitating" knowledge, project-based learning, and generic attributes, to which we will first direct some attention before we discuss the question at hand in the context of Process Systems Engineering (PSE) education.

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TO FACILITATE

Firstly, the notion of facilitator replacing teacher is welcomed as a key ideological change in the mind of the educator. Many academics recognize that learning is the responsibility of the students as much as it is the responsibility of the teacher, if not more.^[5] In many institutions we are starting to see the term teacher or lecturer being slowly phased out and replaced by the term facilitator. This is simply because these institutions see the teacher's role as that of a facilitator and a mentor rather than as someone who solely teaches. This is one aspect required for the creation of an effective environment for learning. Being among those who advocate this shift, we will use the word facilitator throughout the rest of this article to refer to the academic teacher.

In the past, teaching could be represented by Figure 1(a), which is a passive mode of instruction as practiced in the traditional lecture room. Bombarding students with knowledge during a lecture period does not achieve much learning nor does it contribute adequately to graduate attribute development. Enhancing the learning experience calls for active participation by the students in the subject matter. This is illustrated in Figure 1(b) by the active-learning model, where teacher-student interaction is promoted. A more advanced learning model is illustrated in Figure 1(c)—the interactive model, in which student-teacher contact is extended to allow for student-to-student interaction on the subject matter. Many educationalists advocate for this type of learning model, realizing that students tend to learn more from their peers and less from the teacher.

PROJECT-BASED LEARNING

Secondly, effective learning is inevitably related to the subject matter and to the degree the student enjoys the subject content. Making the learning of the content a matter of interest to the student becomes vital. One way of doing this is to provide students with real-life examples.^[6] The learning activity is always made more interesting and appealing when one can relate what is being taught to something from previous knowledge or experience, or to a problem relevant to real life. Problems and projects become important tools to the facilitator who is able to focus the student's mind on the ideas and concepts of the subject matter. Problem- and project-based learning are great environments that allow the embodiment of learned matter and thus promote deep learning as opposed to surface learning.^[7, 8] Thus, the con-

text the subject matter is delivered in is what has impact on student learning. For instance, if one of the course's learning outcomes is to understand model predictive control (MPC), we could have students read about the control technique and then instruct them on how to tune the controller parameters. As an alternative, we could challenge them to implement MPC algorithm on a real-life dynamic process. Or we could extend the learning to explore other dimensions influenced by the control problem such as how the control solution to be offered by the students impacts process operation, efficiency, economics, or even the environment. It is argued here that we should facilitate learning as exemplified in the third case, where the subject matter (MPC control strategy) is better and more completely comprehended by the students. This is because the students' level of interest is elevated because they relate to the problem and consequently delve into it beyond its theoretical boundaries. The learning environment benefits greatly from students' perceptions of the subject matter. The context in which the problem is posed to students plays a key part in achieving learning outcomes.^[9]

GENERIC ATTRIBUTES

Thirdly, the facilitator also has to consider students' non-technical development, viz. generic attributes. In this way, the facilitator is not only concerned with developing and extending students' engineering knowledge and technical know-how, but also with imparting a set of generic attributes necessary for post-graduation professional life. Three overarching attributes have been identified—a scholarly attitude to knowledge and understanding, global citizenship, and lifelong learning.^[10] These are in turn represented by more specific attributes contextualized differently in different disciplinary domains.

Students in the ChE undergraduate program are being trained to become engineers with a certain set of skills and knowledge, and so the course being delivered has certain aims and learning outcomes.^[11] Some of these outcomes directly relate to learning the subject matter, while others relate to student development. In this regard, the development of graduate generic attributes is now well recognized as an essential learning outcome and many progressive universities advocate developing them by imposing them in their academic policies. The generic attributes set by a higher education institution are a reflection of vision toward the development of graduates. Generic attributes are usually treated differently to subject matter and are typically found in university policy documents. They are less commonly found within the course outline document—which is usually stuffed with titles of content matter—and in the cases where they are found, they are referred to by simple statements that students rarely relate to. A key approach is to explicitly include the generic attributes within the course so as to recognize from both the facilitator's and students' ends that these attributes are part-and-parcel of the learning in the course. Students will appreciate that

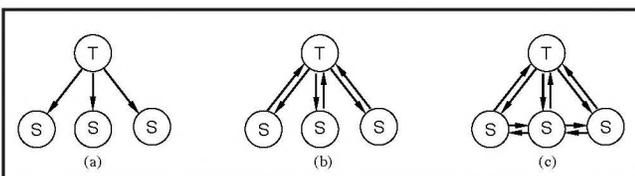


Figure 1. Learning models: (a) passive, (b) active, (c) interactive. (T) teacher, (S) student.

these attributes, when gained, will qualify them to progress forward in their profession. So, what generic attributes do you target and how do you manage their facilitation? We identify four attributes that students should develop through the PSE class:

1. *Research and inquiry: Students will be able to create new knowledge and understanding through the process of research and inquiry.*
2. *Critical thinking: Students should have certain thinking skills and exercise critical judgement. This involves rigorous and independent thinking that has logical and objective bases.*
3. *Communication: Students recognize and value communication as a tool for negotiating and creating new understanding, interacting with others, and furthering their own learning.*
4. *Professionalism: Students hold personal values and beliefs consistent with their role as responsible members of their engineering team.*

The facilitation of these attributes in the course can be achieved through use of key teaching tools. This is also very much related to, and should be aligned with, assessment.

Table 1 lists assessment items as well as what attributes these items target. Focusing on generic attributes stimulates student learning because students perceive this as personal development preparing them for the workforce. (This is our conjecture and is yet to be proven.) Beyond being a natural complement to learning, the development of generic attributes has direct positive influence on comprehending the subject matter. In the following sections, we discuss how we have integrated the three above-mentioned factors (*i.e.*, facilitation, project-based learning, and generic attributes) into the teaching and learning of the PSE course. We first describe the PSE course.

THE PSE COURSE

This course is offered to final-year students as an elective in the ChE degree program for the duration of one semester (13 weeks). The main objective is to make students familiar with strategies used by Process Systems Engineers in a team environment. The course involves students in many aspects of PSE and in a number of phases of process development,

including process conceptualization, fundamentals of process development, process integration, process modelling, simulation, synthesis and design, optimization, control, and operation.^[12]

This course, like the final-year design project, may be considered to be a capstone course in ChE, although the PSE course integrates in a more concentrated way the various concepts and principles from the earlier PSE stream of courses (ChE computation, process modelling, process control, advanced process control). The course is designed as a project-based course and is dominated by activities aimed at achieving a practical solution outcome.

The students encounter problems typical of those faced by a practicing chemical engineer. These problems are carefully selected from postgraduate research projects and are presented to the students at the beginning of the semester in the format of a manager assigning a project to a group of engineers. In this format the problem is ill-defined in the sense that insufficient data and information are provided. Having the problem very much open-ended makes the scenario like that of a real work environment. Problems given do not have a solution to begin with while any solution is the result of students' efforts and output. Groups of three or four students are formed by instructors to distribute intellectual strengths evenly. Groups work together to achieve project milestones, which form the assessment items to be graded.

The first milestone, a preliminary report based on a thorough literature review, is due at three weeks, after which the students present a detailed problem definition and project solution plan. A progress report due at the end of week 8 is the second assessment task. It requires students to report back on their advancement toward their solution, and whether changes are needed in their initial plan. A final report submission at the end of the course (week 13) is immediately followed by a final presentation and discussion. Throughout the course there is continuous review and feedback. Students are asked to provide confidential feedback on their contributions as well as their peers' within each group via the report submissions and across groups via the presentation. This peer review is used as guidance in the process of grading the students.

The coordination and facilitation of the course is illustrated in Figure 2. Regular meetings with the project advisors (postgraduate students) are scheduled on a weekly basis and it is the responsibility of the students to arrange these. The course tutors who are postgraduate students hold meetings with the course coordinator as needed. In Figure 2, the typical management hierarchy found in an engineering company is put beside the PSE course organization chart to illustrate the similarity to a real-life workforce environment.

The course emphasizes the concepts and tools used in process engineering. Moreover, students are introduced to a number of new topics in the field of PSE, including

TABLE 1
The Generic Attributes and Their Corresponding Teaching Tools

Attribute	Assessment Item
Research and inquiry	Literature search and review
Critical thinking	Problem analysis
Communication	Report writing, panel discussion and presentation
Professionalism	Peer evaluation and feedback

- Introduction to process systems engineering
- Cost-benefits analysis
- Process modelling (steady state and dynamics)
- Process optimization (theory and applications)
- Advanced process control concepts
- Data management and process data reconciliation
- Process integration techniques
- Computer aided process engineering (CAPE)—students are introduced to typical commercial packages used by process engineers

THE COURSE PROJECTS

In this section we report back on three projects previously given to students in the course and describe them in some detail.

Project 1. Model predictive control of a propylene glycol reactor

Model predictive control (MPC) was implemented on a dynamic HYSYS (Aspentech, USA) model of a propylene reactor. The controller was designed and built in Excel. The temperature of the reactor is controlled by manipulation of the heat input to the reactor. An MPC graphical interface shown in Figure 3 was developed in Excel and was connected to

HYSYS allowing real-time data transfer. The control of temperature by the MPC is compared to that of a conventional PID controller to determine its control performance. The students comprehended the advantages of MPC over PID control.

Project 2. Data Reconciliation in a VCM Plant

This project involved the application of data reconciliation to a Vinyl Chloride Monomer (VCM) plant. In this study, mass flow rate data from a fully measured and a partially measured plant were reconciled. The VCM plant studied was modelled in HYSYS. In developing a solution to the data reconciliation problem, a number of software packages were used and a data reconciliation interface developed (Figure 4, next page). The linking of these packages and development of the interface were also resolved. A solution for the detection of gross error in sensor measurements was undertaken and a sample result is shown in Figure 5 (p. 63). In the conclusion of the submitted final report, this group of students stated:

“...the model is capable of detecting faulty sensors by the use of a global error test. More importantly, the partially measured case study has shown that a reduction in the number of sensors from 35 to 24 is possible without any loss in accuracy. This, of course, results in a significant drop in the cost of the sensors if this model is used in an actual VCM plant.”

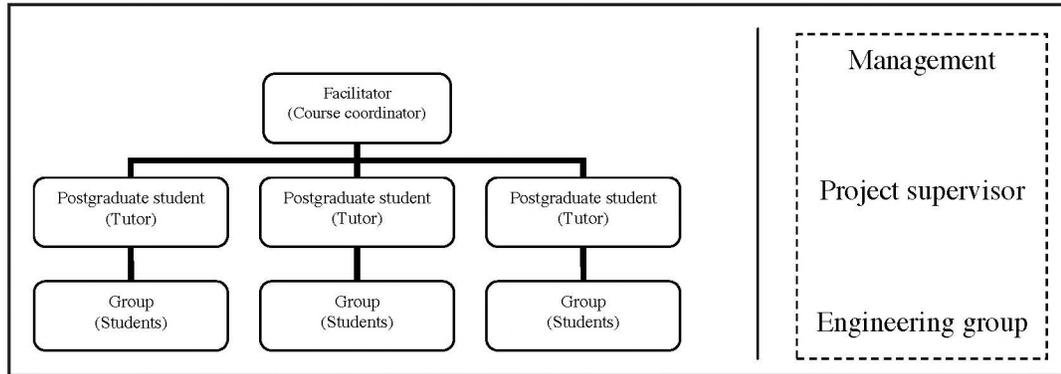
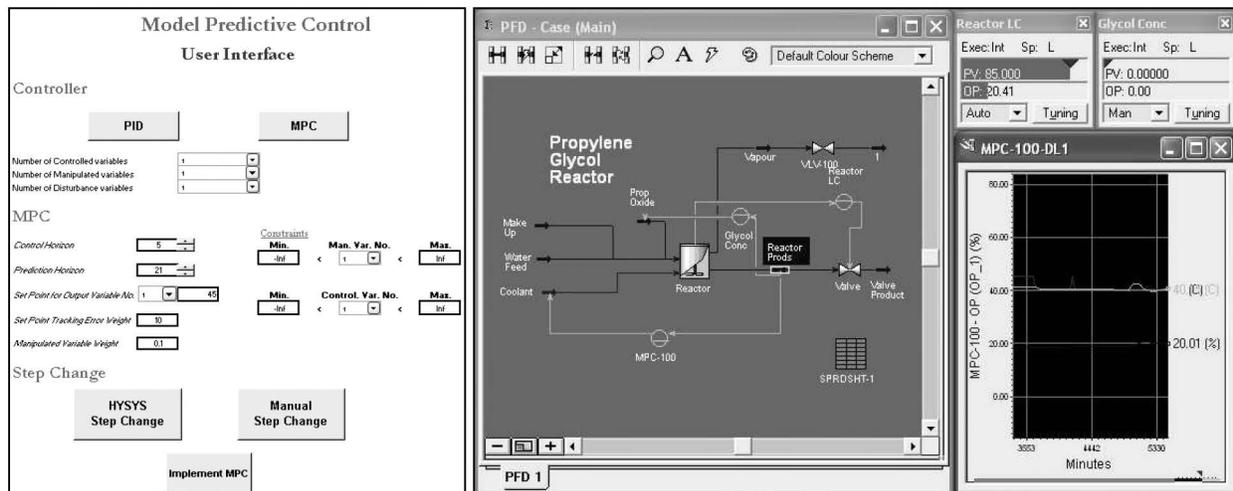


Figure 2 (left). PSE Course organization chart.

Figure 3 (below). Model predictive control of a propylene glycol reactor. Left side: Main graphical interface. Right side: propylene glycol reactor HYSYS flow-sheet with control and monitoring facilities.



Process Systems Engineering - Group 2
Data Reconciliation in a VCM Plant

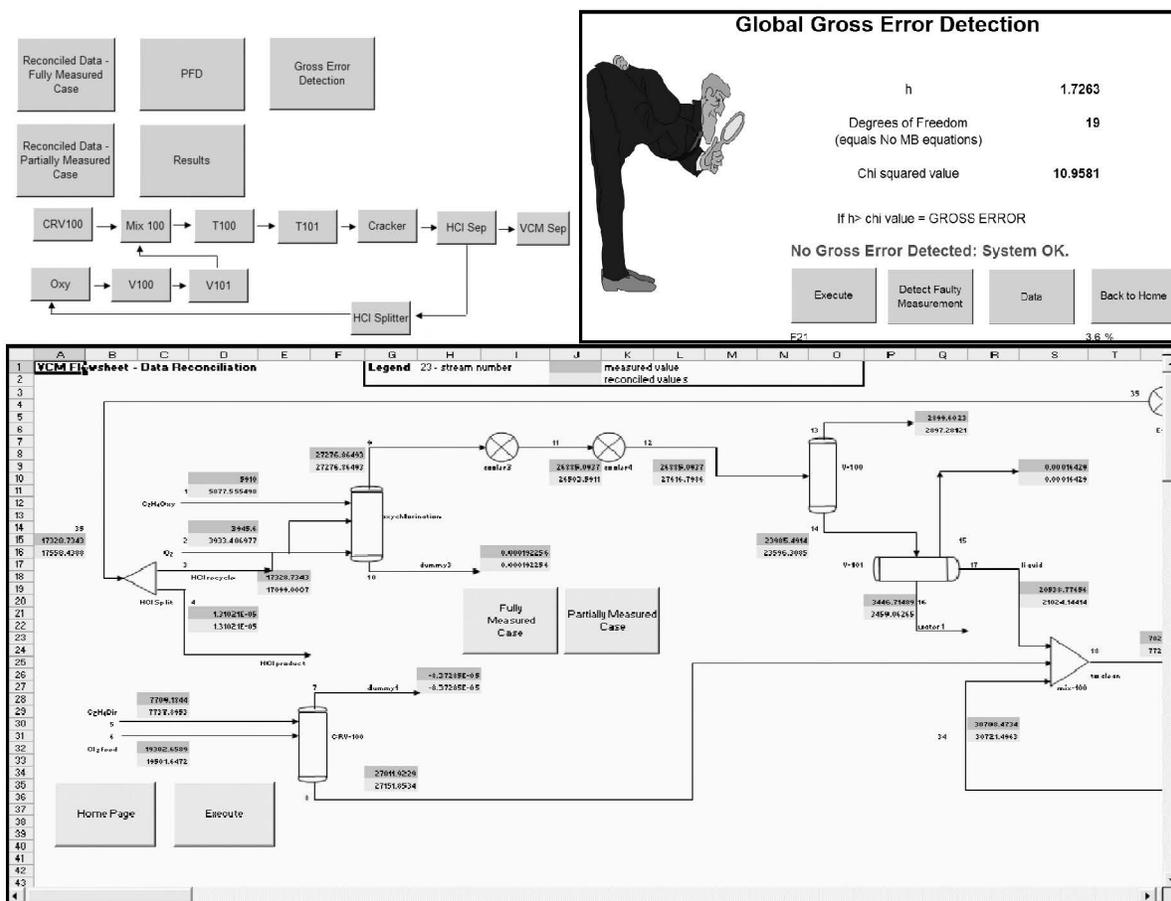


Figure 4. Data Reconciliation in a VCM Plant. Top left: Main graphical interface. Top right: Gross error detection interface. Bottom: VCM plant linked flowsheet.

Project 3. Pinch Target Analyzer

In this project, the students developed a good understanding of heat integration concepts and techniques and made use of this knowledge to develop an interactive Excel spreadsheet program that performs pinch analysis (Figure 6). The “Pinch Target Analyzer,” as this group of students named it, is a heat integration software tool that integrates data extracted from a process with the available utilities for optimum energy utilization and minimum utilities usage. It uses thermodynamic pinch analysis as the basis for designing a heat exchanger network where it employs three main concepts: the problem table, the grand composite curve, and the pinch point. This program takes the required data (streams and utilities information) either manually (by the user) or automatically (directly from HYSYS flowsheet) to decide on the minimum amount of utilities usage. It plots the grand composite curve and the problem table, which shows the enthalpy of the process streams as a function of temperature.

LEARNING AND OTHER OUTCOMES

The projects presented in the previous section are there for illustrative purposes to provide the reader with a feel for the kind of activities undertaken by students in this course. From the result one could judge that in reaching the deliverables presented here by the students, they would have had to become competent in the necessary knowledge, know-how, and soft skills. It didn’t take the students long to discover that what they had embarked on in this course is not what was previously experienced in the first years of their degree program. Their solution to their project problems was a unique one and was fashioned by their creativity. The main outcomes of this course can be summarized as follow:

1. Positive interdependence and teamwork: Students grasp the idea of team success when their individual success depends on group’s success. The groups are instructed to involve all members and determine the best way to use each member’s talents. Students

learned how to get along with others, how to manage their time, and how to integrate knowledge,^[13] areas in which they enhance their leadership and interpersonal skills. Students are highly encouraged to be active in the groups and continuous feedback is given to each student.

2. *Effective communication: Students worked together, talked and listened to each other, and respected each other. Good communication among group members was enforced and students used other communication tools such as e-mails and instant messaging. This improved their level of communicating ideas via report writing and oral presentation.^[14]*
3. *Ownership of learning and research: Students took charge of their own learning, leading each other toward a common goal. The realization that the learning was their responsibility had a great impact on the students, who found themselves in a new homework scenario where they had to research to learn about and solve a given problem, rather than relying on the instructor to provide the relevant knowledge.^[15] This also raised their level of interest as it drew upon their resourcefulness and creativity.*
4. *Individual accountability and personal responsibility: Group members shared the work of the project and individual accountability was evaluated based on the corresponding sections of the submitted reports and presentation. Students had enough flexibility to work alone as well as together in the team.*
5. *Engineers not students: Students are treated as professional engineers in an engineering consultancy environment where they are responsible for discovering solutions for open-ended problems. Students appreciated the complexities of real-life problems that lack necessary data for solution.*
6. *Research at undergraduate level: Teaching strategies such as peer teaching, collaborative learning, and individualized learning increase student involvement and comprehension—especially so in a research-based learning environment.^[16] Moreover, students gain research skills as they are asked to update their knowledge and techniques using journals and other sources rather than being dependent on the textbooks.*

STUDENT FEEDBACK, DISCUSSION, AND FUTURE DIRECTIONS

Students in this course worked much harder than they expected, learning how to do literature review and how to complete a substantial writing project. Later, many students expressed gratitude toward the course tutors since their experience in the course made it much easier for them to do and write their final-year theses and complete the final-year design project—and in one instance, find a job. Feedback was collected at the end of the course during interview sessions with all groups present. Other than administrative issues raised by the students, positive feedback was prevalent. Students indicated that this method of learning was new to them but they found it useful in developing their skills. Students appreciated the research environment and the contact with the postgraduate researchers. Many suggested that this type of course administration should be delivered earlier in the degree program. Some students suggested that more assistance be given in the beginning of the course with learning certain tools such as the simulation and modelling packages.

Some benefits of conducting the PSE course in this way include learning by research. Research being conducted by the academic and/or the postgraduate student would be used as learning material at the undergraduate level. The undergraduate student in turn learns by researching the topic presented to him/her. The efforts of the undergraduate students are harnessed and their research project output supports the efforts of the postgraduate student in the first instance and the facilitating academic in the second. This win-win situation represents, in our opinion, a necessity in the teaching and

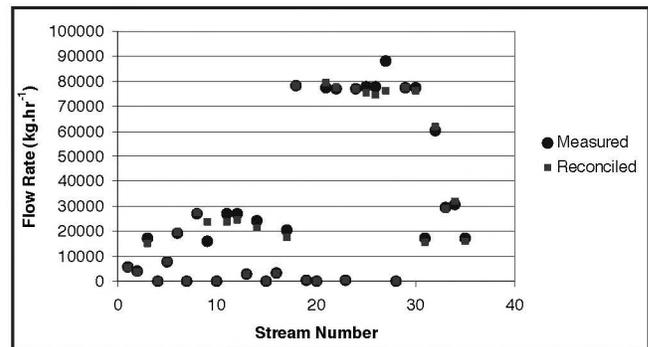


Figure 5. Case with two gross errors at streams 9 and 27.

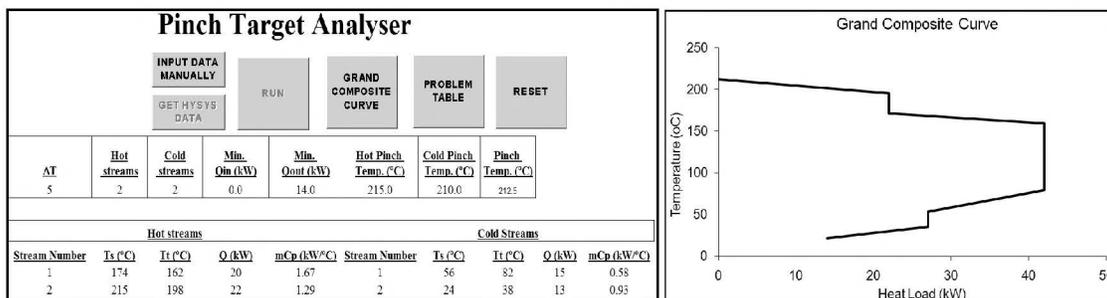


Figure 6. Pinch technology and energy conservation. Left: Main graphical interface. Right: Grand composite curve.

learning of higher education; all stakeholders in the teaching and learning process are rewarded for their efforts. The student benefits in gaining new knowledge and attributes, the postgraduate student's efforts in guiding the students provide him or her with help with the research, while the whole exercise is profitable for the facilitating academic and the research area. Effectively, in shifting toward this "learning by research" model of teaching, we are optimizing the time and resources available. Another benefit is the exposure of the students to the research environment, which may entice some to undertake postgraduate studies.

In this model of university teaching and learning, the ownership of learning is transferred directly to the student. To further enhance this, at the beginning of the course the students could be required to develop and sign a learning contract. The contract details the student's individual learning outcomes and methods for achieving them.^[17] This kind of "ownership of learning" requires students to plan their learning and develop a path toward their desired outcomes, ultimately leading to responsible deep learning that is individualised.

Inter-group interaction could be enhanced to provide more stimulus and convey the interdisciplinary nature of real-life engineering problems. For instance, the data reconciliation project could have been integrated with the MPC project. The purpose of data reconciliation is to eliminate random errors from plant data so that accurate decisions and control of a process can be made. By linking the two projects, the importance of data reconciliation in an industrial control can be further elucidated. The reconciled data would also help the control group in the development and operation of their control system. Integrating projects in this way poses several challenges and should be considered after several iterations of conducting the PSE course. A key challenge is to achieve the desired learning outcomes when integrating projects. To do this, the facilitator should refine the projects so they are set at the appropriate skill level for the students, while ensuring the link between projects does not negatively affect the progress of individual groups. For instance, the facilitator should provide sample data to work with while one group is waiting for data from another group.

CONCLUSIONS

A project-based group learning approach in the PSE elective course was presented, with emphasis on both technical knowledge development and generic attributes. Students

found this learning environment stimulating, especially because the assigned projects were derived from higher-level, real research problems and were challenging due to their open-ended nature. The course organization was presented, incorporating the academic supervisor and the postgraduate students, further enriching the learning environment for the PSE class. Three typical projects were described and corresponding student outputs were presented. These along with students' feedback demonstrate a deep level of learning and show the potential of this approach in PSE education.

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The object of this column is to enhance our readers' collections of interesting and novel problems in chemical engineering. Problems of the type that can be used to motivate the student by presenting a particular principle in class, or in a new light, or that can be assigned as a novel home problem, are requested, as well as those that are more traditional in nature and that elucidate difficult concepts. Manuscripts should not exceed 14 double-spaced pages and should be accompanied by the originals of any figures or photographs. Please submit them to Professor James O. Wilkes (e-mail: wilkes@umich.edu), Chemical Engineering Department, University of Michigan, Ann Arbor, MI 48109-2136.

First Principles Modeling of the Performance of A HYDROGEN-PEROXIDE-DRIVEN CHEM-E-CAR

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In this study, basic principles of thermodynamic, heat, and momentum transfer,^[1-3] are used along with the conservation laws of mass and energy to simulate the transient conditions of a reaction-driven car or so-called "Chem-E-Car." Chem-E-Car competitions are held in countries around the world to improve teamwork skills of university students in addition to providing them with a practical situation for applying their theoretical knowledge. Chem-E-Car is a shoe-box-size car that should be able to carry a specific load within a given range (*i.e.*, 0 to 500 g) up to a precise distance within a given range (*i.e.*, 15 to 30 m).^[4] Typically, these ranges are given to competitors a few months in advance, but the specific values of load and distance will be announced on the competition day. The closest car to the destination line will be the winner. Teams are free to use any chemical reaction to drive the car but they are not allowed to employ any mechanical brake to stop the car at the desirable point. Therefore, the car should be supplied with an accurate amount of fuel to stop as closely as possible to the final destination line. The most popular Chem-E-Car engines are based on the production of a pressurized gas by decomposition of a substance or by a reaction of an acid or base with a neutral salt. Also, combustion of

hydrocarbons and fuel cells are considered as other alternative methods. Several trial runs should be performed prior to the competition to identify the behavior of the constructed car. Simulation of the system has some great advantages both in the design stage and for decision making on the competition day. In the design phase, the model can be used to obtain the



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Figure 1. Schematic of the proposed car: fuel tank (A), reaction chamber (B), external load vessel (C), exit nozzle (D), connecting hose (E), and fuel valve (F).

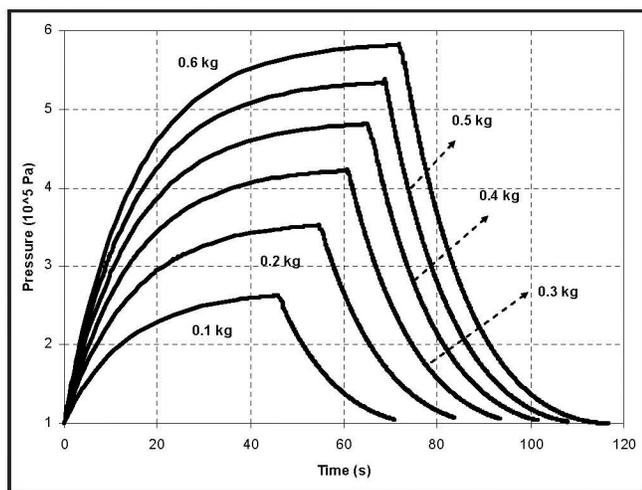
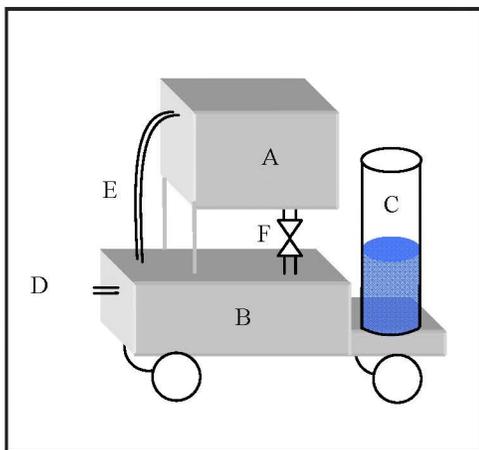


Figure 2. Absolute pressure vs. time for different initial fuel weights.

maximum expected pressure, thus, the machine's vessel can be constructed with a proper thickness. More importantly, sensitivity analyses of the different potential engines and vessel sizes would help determine a system that has the least sensitivity to the fuel's weight. After setting up the machine, the number of trial runs needed to identify the performance of the system could be reduced through simulation, which saves both experimental costs and time. Moreover, tuning the simulation parameters to the announced requirements right before the competition helps to find out the corresponding amount of the fuel. For example, the required traveling distance, load, surface friction, and ambient temperature would be used as the inputs of the simulation to obtain the weight of fuel that should be loaded into the fuel tank.

PROPOSED CAR DESCRIPTION

The performance of a car based on the production of pressurized oxygen from decomposition of hydrogen peroxide will be discussed.



The proposed car consists of a fuel tank, a reaction chamber, and an external load vessel (Figure 1). To maintain a uniform pressure within the system, vessels are connected together by means of a high-pressure hose. The bottom vessel is equipped with a nozzle at one end to let the oxygen exit the system at a high speed. At the beginning of each run, fuel (hydrogen peroxide 30%) is loaded into the fuel tank while the bottom tank contains a little amount of dissolved catalyst (KI). The reaction starts by opening the valve located between two vessels. Decomposition of hydrogen peroxide in the presence of KI solution is an instantaneous exothermic reaction.[5] Due to the short time of each run (~1 min), the heat dissipation to the surroundings is assumed negligible.

The physical and chemical properties of H_2O_2 are obtained from Reference 5, while *Perry's Handbook of Chemical Engineering*[6] was used for all other physical data.

MATHEMATICAL MODEL

To calculate the traveling distance of the car with given specifications, differential displacements of the car should be integrated over the range $t = [0, \infty]$.

$$x = \int_0^{\infty} v_1 dt \quad (2)$$

Also, by definition, the time derivative of the instantaneous velocity equals to the instantaneous acceleration.

$$a_c = \frac{dv_1}{dt} \quad (3)$$

There are three distinguishable steps in the movement of the car throughout each run.

- First, when the pressure is inadequate to create enough thrust force to overcome the static friction, the car remains stationary.
- Second, the pressure inside the chamber is high enough to cause a positive resultant force while the fuel is still being consumed.
- Third, from the maximum pressure time to the final traveling length. In this step, due to friction, the car's acceleration gradually becomes negative, which finally causes the car to stop.

$$F = F_t + F_\mu + F_d = m_2 v_2 - m_c \mu g + F_d = m_c a_c \quad (4)$$

$$m_2 = \rho_{\text{ox}} A_2 v_2 \quad (5)$$

The magnitude of the drag force, caused by the motion of the car, can be calculated using Eq. (6).

$$F_d = -\frac{\rho_A v_1^2 A_P C_d}{2} \quad (6)$$

Having a maximum velocity of about 1m/s and a projected area of about 20cm², the maximum amount of the drag force is calculated using Eq. (7):

$$F_d = -\frac{1.293 \times 1 \times 0.02 \times 0.3}{2} \approx 0.004N \quad (7)$$

Comparison of this value with typical values for the friction force (~0.1 N), makes it apparent that the drag force is two orders of magnitude smaller than the frictional forces, and thereby can be neglected.

By substituting Eq. (5) into Eq. (4), it can be seen that the car's acceleration is a function of oxygen velocity and density. The density of oxygen is simply calculated from the following equation.

$$\rho_{ox} = \frac{n_{ox} MW_{ox}}{V} \quad (8)$$

To obtain the number of oxygen moles in the system, a component mass balance is used.

$$\frac{dn_{ox}}{dt} = \frac{\dot{m}_1}{2MW_f} - \frac{A_2 v_2 \rho_{ox}}{MW_{ox}} \quad (9)$$

The velocity of oxygen at the exit nozzle is calculated from Bernoulli's equation.

$$v_2^2 = \frac{4RT(P - P_a)}{MW_{ox} P} \quad (10)$$

Eq. (10) is used to eliminate v_2 from Eqs. (4) and (9). Considering the very fast rate of decomposition of hydrogen peroxide in presence of KI catalyst, the reaction is assumed to be instantaneous. Therefore, the temperature of the system increases due to the heat of reaction.

$$\dot{Q} = \frac{\dot{m}_1 \Delta H}{MW_f} = f_h m_c C_{pc} \frac{dT}{dt} \quad (11)$$

Here, C_{pc} is the weight average specific heat of the car's components and f_h is the weight fraction of the car that is heated due to the heat of reaction. Taking derivatives of both sides of the ideal gas law equation with respect to time, it can be shown that the variation of the inside pressure is due to the simultaneous change in the total number of oxygen molecules and temperature.

$$PV = n_{ox} RT \quad (12)$$

$$\frac{dP}{dt} = \frac{RT}{V} \frac{dn_{ox}}{dt} + \frac{n_{ox} R}{V} \frac{dT}{dt} \quad (13)$$

Equal pressures in the reaction chamber and the fuel tank cause hydrogen peroxide to flow from the top tank to the reaction chamber under gravity. One can calculate the flow rate using Bernoulli's principle and a mass balance on the fuel tank.

$$\frac{\rho_f v_3^2}{2} = \rho_f gL \quad (14)$$

$$\dot{m}_1 = \rho_f v_3 A_1 = \rho_f A_1 \sqrt{2gL} \quad (15)$$

$$\rho_f A_3 \frac{dL}{dt} = -\rho_f A_1 \sqrt{2gL} \quad (16)$$

The variation of the depth of fuel in the fuel tank can be obtained by integrating Eq. (16).

$$\sqrt{L} = \sqrt{L_0} - \frac{A_1 \sqrt{2g} t}{2A_3} \quad (17)$$

$$L_0 = \frac{m_f}{\rho_f A_3} \quad (18)$$

By substituting the intermediate variables into Eq. (13), the following expression that describes the variation of pressure in the system is obtained.

$$\frac{dP}{dt} = \alpha_1 + \alpha_2 t - \alpha_3 t^2 + \frac{\alpha_4 P}{\alpha_5 + \alpha_6 t - \alpha_7 t^2} - \alpha_8 t - \alpha_9 t^2 + \alpha_{10} t^3 - \frac{\alpha_{11} Pt}{\alpha_5 + \alpha_6 t - \alpha_7 t^2} - P \sqrt{\alpha_{12} + \alpha_{13} t - \alpha_{14} t^2} - \frac{\alpha_{15}}{P} - \frac{\alpha_{16} t}{P} + \frac{\alpha_{17} t^2}{P} \quad (19)$$

Here, α_1 to α_{17} are positive constants that depend on A_1 , A_2 , A_3 , C_{pc} , ΔH , L_0 , MW_f , MW_{ox} , ρ_f , f_h , and T_0 . The Runge-Kutta method has been used to solve the differential equations.

RESULTS AND DISCUSSION

The pressure variation inside the system is independent of the car's weight, traveled distance, and friction factor between the wheels and the ground. Therefore, it is possible to analyze the transient pressure of the system regardless of its weight, position and friction factor (Figure 2).

Simulation results indicate that the maximum pressure occurs around the moment when the fuel is completely consumed, and after this moment the pressure inside the chamber starts to decline; this is because no more oxygen is generated while the existing oxygen gradually exits the reaction chamber from the exit nozzle.

After illustrating the variation of pressure with time, the movement of a car with a given weight and friction can be calculated using Eqs. (2) and (3). Expectedly, a great fraction of fuel is consumed just to overcome the initial static friction and to launch the car. After the initial movement, the traveling distance of the car is a strong function of the remaining fuel. Also, simulation demonstrates that the fuel is completely consumed before the car stops. In other words, after passing a specific time, the driving force (produced oxygen) is inad-

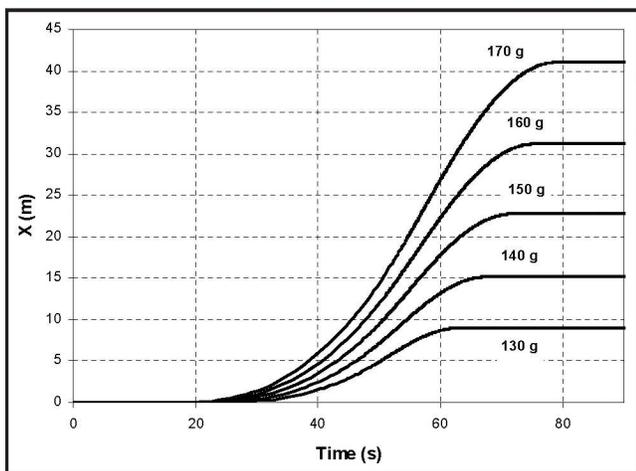


Figure 3. Distance vs. time for different initial fuel weights, weight of car = 750g, $\mu=0.01$, $T_0=300$ K.

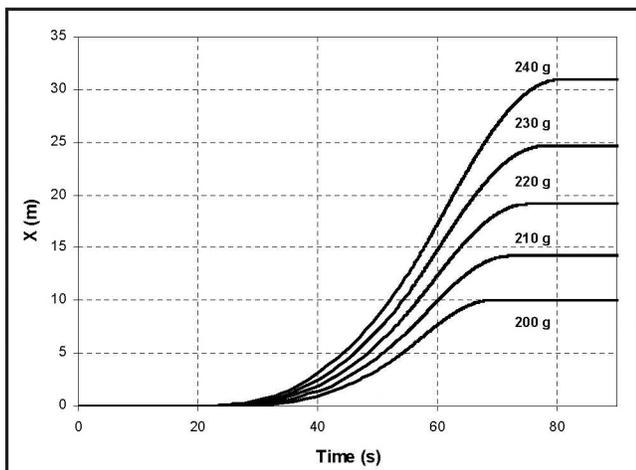


Figure 4. Distance vs. time for different initial fuel weights, weight of car = 1 kg car, $\mu=0.01$, $T_0=300$ K.

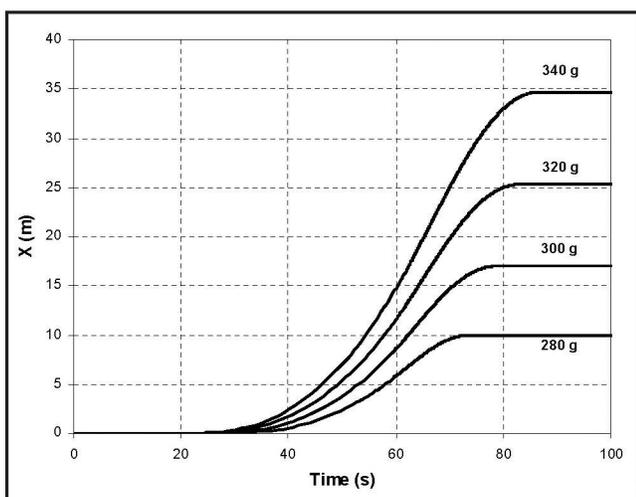


Figure 5. Distance vs. time for different initial fuel weights, weight of car = 1.25 kg, $\mu=0.01$, $T_0=300$ K.

equate to overcome the resistance force (dynamic friction force), which slows down the speed and finally causes the car to stop. (See Figures 3-5.)

To have a more clear picture of the car's performance over the possible ranges of weight, fuel and distance, the contours of iso-distance lines are created using the contour generator in MATLAB (Figures 6 and 7). These figures, or similar figures that are generated and calibrated before the competition, can help determine the appropriate amount of fuel to meet the competition requirements.

SUMMARY

The performance of a hydrogen-peroxide-driven Chem-E-Car was studied using basic engineering principles. The simulation showed that the car stops a few seconds after the occurrence of the maximum pressure inside the system. Also, a noticeable fraction of fuel is consumed to overcome the static friction and, after the very first movement, a little amount of fuel can keep the car moving. In other words, the ultimate traveled distance of the car is very sensitive to the weight of the remaining fuel right after the initial movement. Finally, contours of iso-distance lines are presented for a given friction coefficient and ambient temperature. One can use the same technique to obtain the corresponding contours for different initial conditions. Results are useful for both design purpose and decision making on the day of Chem-E-Car competition.

NOMENCLATURE

A1	Area of fuel supply pipe	m^2
A2	Area of the exit nozzle	m^2
A3	Area of the fuel tank	m^2
a_c	Acceleration of car	m/s^2
A_p	Cross section area of the car	m^2
C_{pc}	Average specific heat of car	$J/kg \cdot K$
F_n	Net force	N
C_d	Drag coefficient	-
F_d	Drag force	N
f_h	Mass fraction of car that is heated by the reaction	-
F_t	Thrust force	N
F_f	Friction force	N
g	Gravity	m/s^2
ΔH	Heat of reaction	J/mol
L	Depth of fuel	m
L_0	Initial depth of fuel	m
\dot{m}_1	Fuel mass flow rate	kg/s
\dot{m}_2	Oxygen mass flow rate	kg/s
m_c	Overall mass of car	kg
m_f	Initial mass of fuel	kg
MW_f	Molecular weight of fuel	kg/mol
MW_{ox}	Molecular weight of oxygen	kg/mol
n_{ox}	Number of oxygen moles	mol
P	Pressure inside the car	Pa
P_a	Atmospheric pressure	Pa

q	Rate of heat generation	J/s
t	Time	s
T	Temperature	K
T_0	Initial temperature	K
V	Total volume of the fuel tank and reaction chamber	m^3
v_1	Velocity of the car	m/s
v_2	Velocity of oxygen	m/s
v_3	Velocity of fuel	m/s
x	Traveled distance	m
μ	Friction coefficient	-
ρ_f	Density of fuel	kg/m^3
ρ_{ox}	Density of oxygen	kg/m^3
ρ_A	Density of air	kg/m^3

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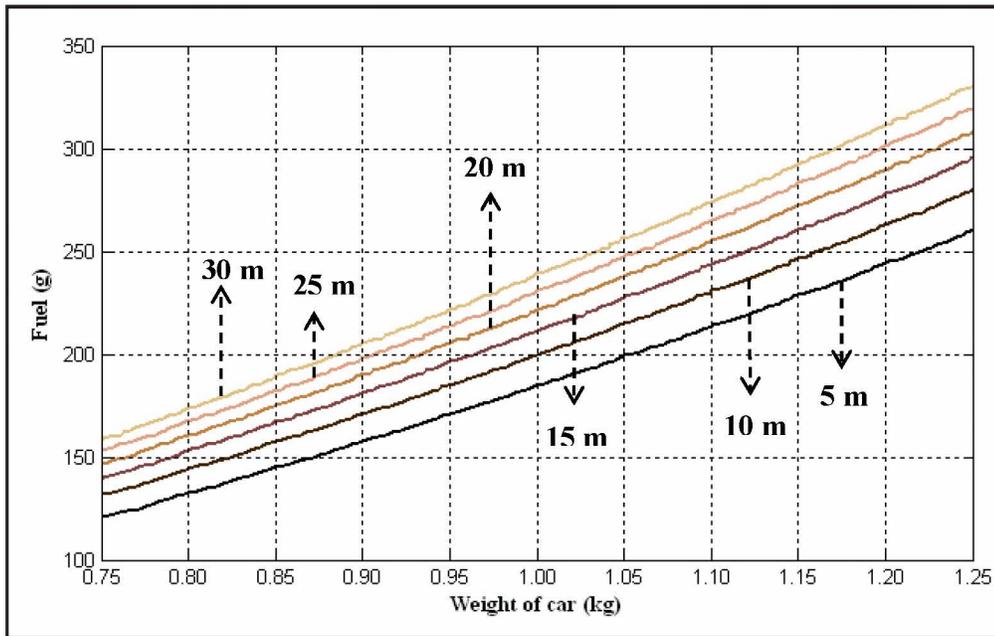


Figure 6. Contours of iso-distance lines, $\mu=0.01$, $T_0=300$ K.

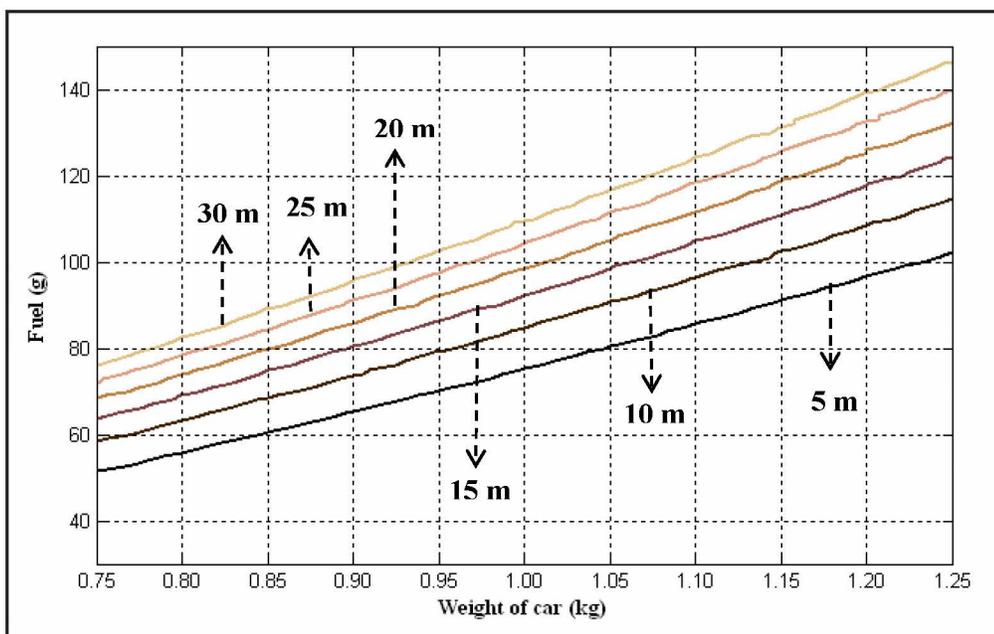


Figure 7. Contours of iso-distance lines, $\mu=0.005$, $T_0=300$ K.

TEACHING CHEMICAL ENGINEERING THERMODYNAMICS AT THREE LEVELS

Experience from the Technical University of Denmark

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According to the so-called “Bologna model,” many technical universities in Europe have divided their degree programs into separate 3-year Bachelor’s and 2-year Master’s programs (followed by an optional Ph.D. study). Following the Bologna model, the Technical University of Denmark (DTU) has recently transformed its 5-year engineering program into a 3-year Bachelor (B.Sc.) and a 2-year Master’s (M.Sc.) program. Master’s graduates that are interested and have achieved a good grade average are then in principle qualified for a 3-year Ph.D. In addition to the above, DTU has a 3.5-year industrial Bachelor’s program (“diplom” or B.Eng.), which directly qualifies its graduates for an industrial career. In all of these programs there are studies in applied chemistry and chemical engineering. Four different courses on chemical engineering thermodynamics are provided at the four levels mentioned above, thus satisfying the different needs of these programs. This manuscript discusses the different roles, context, teaching objectives, and educational methods used in the various courses. Examples are provided for all courses, with emphasis on the different types of exercises used. Finally, the suitability of thermodynamics textbooks for these courses is also discussed.

WHY 4 COURSES IN THERMODYNAMICS?

An evident question is why so many different courses are needed in “applied chemical engineering (technical) thermodynamics.” The necessity for the four courses in thermodynamics will hopefully become apparent from the brief description of their characteristics, illustrated in Tables 1-3, and the description of their similarities and differences

provided hereafter. In the discussion below, we follow the notation used in Table 1 for the courses, *i.e.*, A for the B.Eng., B for the B.Sc., C for the M.Sc., and D for the Ph.D course.

An important “common” characteristic of the four courses is that they all focus on aspects of thermodynamics that are of interest to chemical engineers. This characteristic differentiates them from more fundamental physical chemistry



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Approximation and Thermodynamic Models; Fundamentals and Computational Aspects.



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TABLE 1
Four Degree Programs and Four Courses in Thermodynamics at DTU

Degree Program	Course Name	Suggested Semester
A. B.Eng. (Industrial B.Sc.)	Chemical Engineering Thermodynamics	3
B. B.Sc.	Chemical Engineering Thermodynamics	4-6
C. M.Sc.	Phase Equilibrium for Separation Processes	> 7
D. Ph.D.	Thermodynamic Models: Fundamentals and Computational Aspects	—

TABLE 2
Comparison of Important Characteristics of the Four Thermodynamic Courses

Course/Program	Basic Objectives	Teaching Methods	Evaluation
A. B.Eng.	Estimation of physical-chemical properties for pure compounds and mixtures for use in chemical processes	Lectures Excel spreadsheets	Oral exam + projects
B. B.Sc.	Application of physical chemistry to solution of practical, industrial problems	Short lectures Excel spreadsheets using pre-developed modules that the students use and combine to simulate larger units and processes	Three projects on well-defined problems
C. M.Sc.	Presentation of thermodynamic models and theories for a wide range of fluid mixtures ranging from hydrocarbons and chemicals (and at both low and high pressures) to associating fluids, polymers, and electrolytes	Lectures Classroom exercises Available software with various models	One project at the end of the course based on research articles
D. Ph.D.	Fundamentals of thermodynamics, and how to program and debug fast and efficient computer codes for thermodynamic models and for a variety of advanced computational methods	Lectures Writing own programs	Final project requiring writing own Fortran code

TABLE 3
The Course Context of the Four Courses

Course	Course Context (in general lines)
B.Eng.	Equations of state for estimating properties (pure fluids and mixtures) including residual, partial molar, and excess properties. VLE, LLE and SLE calculations with activity coefficient models. Refrigeration and liquefaction processes. Phase diagrams for VLE/LLE/SVE as used for distillation and extraction processes. Colligative properties for binary mixtures.
B.Sc.	Same as for B. Eng., except for the colligative properties. Added are: compression processes, discussion of the assumption behind the choice of models, derivation of expressions for fugacity, enthalpy and entropy from a given EoS, and parameterization of cubic EoS
M.Sc.	Intermolecular forces. Cubic Equations of state with classical and advanced (EoS/G ^E) mixing rules. Random-mixing and local composition activity coefficient models. Corresponding States, group contributions and regular solutions. Association theories (CPA, SAFT). Phase diagrams and models for electrolytes and polymers—emphasis on free-volume concepts. Environmental thermodynamics.
Ph.D.	Fundamentals (state functions, equilibrium and stability, reference states, electrolytes, derivatives of thermodynamic functions, checking models for consistency). Models (equations of state, activity coefficient models, Debye-Huckel, ion exchange, adsorption equilibria). Computational methods (PT-flash: successive substitution, Rachford-Rice, higher order methods. Multiphase flash. General state function based specifications. Dew- and bubble-points, stability analysis, and the calculation of critical point. Chemical equilibrium calculation)

In terms of use of textbooks, only course D employs a specific textbook.^[1] Courses A-C are based on the authors' own teaching notes, but some recommended teaching is proposed.^[2-3] In Table 4, various recent thermodynamic textbooks are discussed, from the point of use of the programs of DTU. Despite the many positive features of all of these textbooks, we feel that none is suitable for all the purposes. For example, several of these textbooks do not contain chapters on polymer or electrolyte thermodynamics, environmental applications of thermodynamics, or the newest developments in equations of state—*e.g.*, association models (SAFT, etc) and the EoS/G^E mixing rules. These remarks by no means constitute criticisms of these excellent textbooks, rather an observation in relation to the needs of the courses taught at DTU. We do recommend several of these textbooks as supplementary reading material.

courses. Moreover, all of them put emphasis on “applied ways of learning,” but there are important differences both in the teaching methods employed and the level of difficulty, as will be explained later.

The audience of the three courses and also their interests and expectations from a course in thermodynamics are different. Only the B.Eng. (A) course is mandatory, while all the other courses (Bachelor, B; M.Sc., C; and, of course, the Ph.D. course, D) are elective. B.Eng. students, in particular, expect a brief “to-the-point” course that they can use almost immediately in relation to other courses in their (chemical engineering) degree, and naturally later in their future employment, *e.g.*, in the oil and gas and chemical industries. Since this course is mandatory and also at an early stage (third semester), it must remain relatively simple and appealing to broader audiences (including students with interest in biotechnology), while providing all the aspects of technical thermodynamics expected from a mandatory course. The students should also understand the role of thermodynamics in central disciplines of chemical engineering, especially separation processes and process design. B.Eng. students may not take more advanced courses in thermodynamics, so the A course should provide them with all the necessary background to build on when required.

The B.Sc. course is taken by students in the Chemistry/Chemical Engineering B.Sc. program (called “Chemistry and Technology” at DTU) and although elective, it is typically chosen by students in their fourth to sixth semester. It is also a basic course, but because the B.Sc. education—unlike the B.Eng.—is not an independent education but rather a prepara-

tion for the more advanced M.Sc. studies, several of the B.Sc. students may wish to take a somewhat more advanced course than the B.Eng. All the B.Sc. students will have taken, prior to attending course B, one or two courses in physical chemistry, and moreover they may, at a later point, choose to take course C (during their M.Sc. studies). Based on the rather loose structure of B.Sc. studies at DTU, the students who choose the B.Sc. course B may not have a “complete idea” of the role of thermodynamics in chemical engineering and will typically only take courses on process design and separations later in their M.Sc. studies. Most of the B.Sc. students taking course B will have interests in chemistry/chemical engineering but not so much in biotechnology, as the latter would take another bachelor-program line.

The M.Sc. course C has as a prerequisite one of the above courses (A or B), and builds from those. The audience of this course, however, is much broader, with not only students from chemistry and chemical engineering but also students from petroleum engineering, polymers, and environmental engineering (but, in general, not from Biotechnology). Thus, the thermodynamic models/methods and types of mixtures that should be covered and students’ expectations from course C are much broader.

Finally, the Ph.D. course builds also on courses A or B. A C-type course is not a prerequisite for the Ph.D. course but it may be useful. The Ph.D. course emphasizes computational aspects of thermodynamic models and phase equilibria calculations, and the students are then able to understand and write computer programs for phase equilibrium calculations including all sensitive aspects of stability and flash calcula-

TABLE 4
Discussion of Thermodynamic Textbooks

Textbook	Recommended for the course	Characteristics
Elliott and Lira ^[2]	B, C (partially)	Excellent new textbook. Includes exercises and also some advanced topics (association models). Nice discussion of local composition models and links between some models. Worked-out examples, software available.
Prausnitz, <i>et al.</i> ^[4]	C	Classical textbook—now in its 3rd edition. References to numerous models including the newest approaches. Includes chapters on polymers, electrolytes, EoS/G ^E mixing rules. Somewhat confusing presentation of far too many models and missing unified presentation of the different approaches.
Tassios ^[5]	A,B,C (partially)	Older textbook. Clear presentation of classical topics in thermodynamics including certain advanced topics (intermolecular forces, development of cubic EoS, statistical mechanics).
Vidal ^[6]	A,B,C (partially)	New textbook with emphasis on oil applications, <i>e.g.</i> , characterization, solids (wax, hydrates) are included. Chapters on EoS/G ^E mixing rules and polymers.
Israelaschvili ^[7]	Supplement to C	Excellent discussion of intermolecular (Part 1) and interparticle/interfacial forces in Colloids (Part 2)
Smith, <i>et al.</i> ^[3]	A,B,C (partially)	Classic in the field, now in its 8th edition. Includes chapters on intermolecular forces and certain advanced topics, <i>e.g.</i> , on solid-gas equilibria.
Sandler ^[8]	A,B,C (partially)	Interesting textbook with worked-out examples and certain advanced topics such as EoS/G ^E mixing rules. Somewhat confusing nomenclature.
Kontogeorgis and Gani ^[9]	C (supplement)	Chapters on several advanced topics (EoS/G ^E mixing rules, associating models, polymers, electrolytes, etc.). Not written in textbook form for students and expensive for use in universities.

No. of 4-hour modules	Topics	Type of Exercises
2	Pure components, Residual properties. Process applications	Excel exercises: Van der Waals EOS PR/SRK EOS (using pre-programmed macros)
2	Partial properties. Activity	Classroom pocket calculator
3	Phase diagrams, VLE/LLE/SLE	Classroom pocket calculator
2	VLE models: Ideal mixtures Activity models (Wilson, NRTL)	Excel exercises: Dew- and bubble-point calculations, flash calculations (using pre-pro- grammed Wilson/NRTL macros)
1	LLE calculations: NRTL	
1	Colligative properties	Excel exercises: Freezing curve
2	—	Project work (mainly Excel)

tions in complex situations.

As could be anticipated from the above presentation, the degree of difficulty (and also student initiative) rises from level A (B.Eng.) to D (Ph.D.), with courses A and B being rather close in both level and expectations (although under the assumptions discussed above). The students work on small projects in courses A and B and employ pre-programmed modules in Excel, typically with the thermodynamic models they should be using specified from the start. The students actively combine elements such as activity coefficients and vapor pressures to arrive to the final results.

In course C, software is used that contains numerous thermodynamic models and tasks (see more detailed description later), and student selection of appropriate models for specific applications and evaluation of results is expected, along with an in-depth understanding of the derivation and theoretical background of the models. Finally, at the final level (course D), students write their own codes, having been given basic thermodynamic codes (including derivatives) to start.

Following the general comparative description of the context and needs of the four courses presented in Tables 1 through 4, we will now present their most important characteristics with some special emphasis on the educational methods and the software and other tools employed.

ChE THERMODYNAMICS FOR INDUSTRIAL BACHELOR’S (COURSE “A”)

This is a new course that was taught for the first time in the Fall of 2006. The course is compulsory for the B.Eng. degree and is given jointly by the Department of Chemistry and the Department of Chemical Engineering. One-third of the course is devoted to physical chemistry (phase diagrams, activity,

partial and excess properties, colligative properties). The rest of the course is traditional chemical engineering thermodynamics with more emphasis on the application aspects and less on theory. The thermodynamic content of this course is therefore somewhat smaller than that of other “traditional” thermodynamics courses, *e.g.*, Course “B” for B.Sc. students.

The general objective of this course could be summarized as follows: Sizing and optimization of process units (distillation, extraction, compression, cooling, etc.) requires thorough knowledge of the thermodynamic properties of the chemical species (pure/mixture) present. Physical chemistry provides the theoretical framework, which makes the calculation of these properties possible with approximate models,

even with limited availability of experimental data. The goal of this course is to enable the participants to estimate thermodynamic properties of pure species and mixtures for application in sizing and optimization of process units.

A more detailed description of the content of the course is shown in Table 3, while the course layout and distribution of the various topics in the 13 4-hour modules devoted (at DTU) for a 5 ECTS point course is shown in Table 5.

The students are evaluated based on reports they write in small groups (three to four students) on three topics

- (i) *Ammonia cooling circuit*: Sizing of an ammonia compressor cooling circuit for cooling fermentor broth to 10 °C.
- (ii) *Binary mixtures Vapor-Liquid*: Calculation of partial and excess molar volumes based on experimental data. Calculation of phase diagrams (Pxy) given experimental data assuming either ideal behavior or an activity coefficient model (Wilson equation).
- (iii) *Freezing point depression, LLE extraction*: Calculation of freezing curves for a binary mixture (pure solid phase only). Calculation of the compositions of the two liquid phases for ternary mixtures.

Several of these problems are similar to those used in Course “B” and are described in the next section. Both during the course and in the above-mentioned project, Excel is used extensively (see also next section). Excel is a versatile tool that the students most likely will use in their professional careers, and more than 90% of engineers frequently use Excel for solving engineering problems, actually many more than those using commercial process simulators,^[10] according to a recent investigation of CACHE.

PROBLEM SOLVING IN CHE THERMODYNAMICS (COURSES “A” AND “B”)

The general concept—use of Excel in thermodynamics

Classical textbook problems in chemical engineering thermodynamics of the type:

“Carbon dioxide is compressed adiabatically from 300K, 1 Bar, to an outlet pressure of 4 Bar. Calculate the outlet temperature, assuming isentropic compression and ideal gas behaviour with a constant heat capacity”

solved with pen and paper and a pocket calculator, tend to bore students. One may, of course, make the problem more realistic by incorporating a temperature-dependent heat capacity. In itself, this does not really make the problem more fun to solve.

Much more interesting possibilities arise with the use of computers and easy-to-use tools such as spreadsheets. The above problem, for example, is easily solved with the spreadsheet PREOS.XLS from the textbook of Elliott and Lira,^[2] where an appropriate EoS (equation of state, in this case Peng-Robinson) allows us to solve the problem rigorously, without simplifying assumptions.

In our basic thermodynamic courses, the students solve three major problems, as also shown in the previous section for the B.Eng. course. In the case of the B.Sc. course, two of the projects are described below.

Problem related to “pure components”

The first project has carbon dioxide as its topic. Data are retrieved from NIST, and the students use Excel to derive Clausius-Clapeyron (by plotting $\ln P$ vs. $1/T$) parameters and next Antoine parameters (by nonlinear regression, using Excel’s solver) for the vapor pressure of CO_2 . Next they investigate, by comparing to the data for NIST, at what temperature and pressure ranges the gas phase can be calculated as ideal, and for a number of isotherms the data are also compared with those found using the van der Waals (vdW) equation.

Experimental vapor pressures are then compared with those calculated from the Peng-Robinson equation by means of

PREOS.XLS. The students are then required to modify the spreadsheet such that SRK is used instead and to compare the results with what this EoS gives (which is virtually identical to that of PR). Finally, they have to modify the spreadsheet to use vdW, which essentially is shown to be useless for the vapor pressure calculation.

For the final part of the first project, the students have to optimize a sequence of compressors with intercooling. Carbon dioxide has to be compressed from 1 Bar, 300 K, to 80 Bar in two, three, or four stages, with cooling to 300 K after each compressor. The objective is to determine the intermediate pressures such that the total work is minimized. PREOS.XLS can, of course, easily be used to calculate a single stage compression by

1. Calculating S and H at inlet conditions.
2. Solving for the outlet temperature where outlet entropy matches inlet entropy.
3. Calculating the enthalpy at outlet conditions.
4. Calculating the isentropic work as the enthalpy difference.
5. Calculating the real work as the isentropic work divided by the efficiency.

For a two-stage cascade it is possible to guess the intermediate pressure, calculate the work for each of the two steps, and by trial and error adjust the intermediate pressure to arrive at the minimum work. This process is tedious, however, and difficult to extend to additional stages.

We, therefore, supply students with an Excel module, written in Visual Basic, that has the same functionality as PREOS.XLS but can be called as an ordinary Excel function anywhere in the spreadsheet (all spreadsheets used in the course are available from the authors upon request). Actually, two routines are used:

1. An initialization routine,
=Cub_Ini(Mod,Tcr,Pcr,Omega,Cpcoef),

where Mod is a code for the model (PR or SRK), Tcr, Pcr, and Omega are critical temperature and pressure, and acentric factor for the compound, and Cpcoef are coefficients giving

TABLE 6
Course Layout of “Phase Equilibria for Separation Processes” (M.Sc. course, C)

No. of 4-hour modules	Topics	Specifics
2	Phase diagrams—Basic relationships—Intermolecular forces	—
4	Classical models	Cubic equations of state with vdWlf and EoS/ G^E mixing rules. Random-mixing and local composition activity coefficient models incl. group contributions.
1	Environmental thermodynamics	Octanol-water partitioning. Distribution of chemicals in environmental ecosystems.
3	Electrolyte thermodynamics	Standard states. Nernst equation, osmotic coefficients, and activity coefficient models.
1.5	Polymers	Phase diagrams. Basic approaches (solubility parameters, Flory-Huggins) and free-volume models. Equations of state.
1.5	Association models	SAFT and CPA—applications to petroleum, chemical, and polymer industries.

the ideal gas C_p as a temperature polynomial.

2. A calculation routine, =**Cub prop(T,P,X)**, where T and P are the actual temperature and pressure, and X is a text string specifying the property to calculate, e.g., "HL" for liquid enthalpy.

It is now possible to formulate the calculation of the compression cascade as a constrained optimization that can be solved in a single step by the solver in Excel. For a three-stage compression, we have

- 5 Decision variables: The 3 outlet temperatures and the 2 intermediate pressures.
- One objective function: The total work, i.e., the isentropic work, corrected by the compressor efficiencies.
- 3 Constraints: The condition of outlet entropy for the isentropic compression being equal to the inlet entropy.

There is no problem in determining the solution as long as suitable initial estimates are available. And here, the "classical" approach with the ideal gas, constant heat capacity assumption becomes useful, with its analytic solution to the problem.

What we gain by this approach is the following:

1. We are able to solve quite realistic problems without using tools where the students just have to "fill in the numbers."
2. The aid in form of the Excel module is transparent. The students can see the same thing done in PREOS.XLS and the module just represents a different and more useful, although less flashy, packaging.
3. The creative element of formulating the conditions and setting up the equations to be solved is still left to the students.

Problem related to mixtures

The final course problem has mixtures and equilibrium calculations as subject. For this problem, a new Excel module is provided, with the following capabilities for multicomponent mixtures:

1. Activity coefficient models. We provide the following:
 - Wilson
 - UNIQUAC
 - NRTL
2. Equations of State for mixtures. We provide the following:
 - Soave-Redlich-Kwong
 - Peng-Robinson
3. A Rachford-Rice equation solver.

The property routines include an initialization part in which the model parameters (i.e., interaction energies and size parameters for the activity coefficient models, critical properties, and interaction coefficients for the equations of state) are specified, and a calculation routine that given composition and temperature returns a vector of activity coefficients (for the

activity models), or given composition, temperature, pressure and liquid state returns a vector of fugacity coefficients for the equations of state. Finally the Rachford-Rice function returns, given a composition vector and a K-factor vector, the vapor composition.

These tools are used for solving the following problems:

- Calculating nonideal Pxy and Txy-diagrams.
- Calculating an ideal solution PT-flash.
- Calculating PT-flash using an EOS for the model description.
- Regressing energy parameters from experimental Pxy or Txy-data for a binary mixture.
- Constructing a ternary type I diagram using an activity coefficient model with specified parameters.

The nonideal flash is solved by successive substitution, as follows:

- Initial estimates for the K-factors are calculated.
- The Rachford-Rice equation is solved.
- New compositions are calculated.
- New properties (activity or fugacity coefficients) are calculated that yield new K-factors.
- If calculated K-factors agree with assumed, terminate; Otherwise repeat from second step.

This requires that we set Excel to permit iteration. Initially students are instructed to set the maximum iteration count to 1 to see how rapidly convergence occurs. The back-substitution of the calculated K-factors to the assumed is accomplished by means of a flag that selects the assumed K-factors either from the calculated or from the initial estimates. This enables an easy restart when things go wrong. For calculating the ternary diagram, the students start by specifying a feed containing equimolar amounts of the two immiscible components. The nonideal flash is used to calculate the corresponding equilibrium compositions, which yields one tie-line. Then, a small amount of the miscible component is added to the feed, and a new flash is converged. This process is continued until the entire diagram is calculated. In the process it becomes necessary to adjust the proportions of the immiscible components to not exit prematurely, too far from the plait point.

The setup gives the students a very good feel for the difficulties in doing calculations in the vicinity of the plait point. Even when the iteration count is increased to 1,000, the calculation often has to be repeated several times to converge, and the feed specification frequently is in the single-phase region, resulting in convergence to the trivial solution of phases of equal composition.

THE COURSE "PHASE EQUILIBRIA FOR SEPARATION PROCESSES" (M.Sc. COURSE, C)

Table 6 presents the course outline of the MSc course.

We have found it particularly useful to employ varying forms of teaching methods in almost every one of the course's 13 4-hour blocks including short lectures (via PowerPoint presentations with notes available in advance to the students), classroom exercises, and computer exercises. The course material is currently being enhanced and prepared in the form of a textbook.^[13] Different types of exercises have been employed in this course as well. These include simple derivations or pocket-calculator calculations, *e.g.*, illustrations with activity coefficient models, polymer solutions, or derivations of EoS/ G^E mixing rules and association schemes for novel association models, up to the somewhat more advanced applications—*e.g.*, those where equation of state calculations are involved that are performed using an in-house software package (SPECS). This software resembles the thermodynamic part of a process simulator in the sense that students can choose among a large variety of thermodynamic models, databases (“ordinary” systems, polymers, oil, electrolytes), and tasks (VLE, LLE) including, if necessary, different models for different phases and different mixing rules for the equations of state. Several up-to-date thermodynamic models are included (CPA, PC-SAFT, Entropic-FV for polymers, etc.).

The course is currently being taught in the present format for its sixth consecutive year, and based on student evaluations and other considerations, some enhancements have been made, including:

1. The “introductory” part, *i.e.*, the classical models including local-composition models and cubic EoS, includes several exercises aimed at illustrating similarities and differences among the various models but also strengths and weaknesses of the models, both from the theoretical and the application points of view. Although course C has courses A or B (or similar ones) as prerequisites, we have found that this structure also facilitates the understanding of complex concepts for students having different backgrounds, *e.g.*, those from petroleum, polymer, or environmental engineering.
2. A topic addressed in the introductory lecture is the “needs of thermodynamic data and models,” mostly from an industrial point of view. This is accomplished via references to selected articles written by colleagues from industry and in particular we have found the articles of Zeck^[11] and Dohrn and Pfohl^[12] to be particularly useful in this context, as example of one older and one more recent account of thermodynamic needs in the chemical industry.
3. Early in the course, a lecture is devoted to intermolecular forces and their application in understanding phase diagrams, as well as developing and understanding thermodynamic models. We constantly refer to the use of intermolecular forces in all subsequent lectures, including during the software and other exercises, *e.g.*, when selecting models, interpreting phase diagrams. A multiple choice is used in this lecture to illustrate

several aspects and “play around” with the various implications of intermolecular forces.

4. A lecture on “environmental thermodynamics” is included after the activity coefficient models, so that students encounter relatively early in the course a somewhat “different” but exciting application of thermodynamics.
5. The evaluation used in this course is a short project (individual or in small groups) provided during the last lecture, but based on the students’ own choice of area of interest, *e.g.*, oil & gas, polymers, electrolytes, environment, association theories (students are asked a week before to complete a relevant questionnaire). To ensure a satisfactory evaluation of the whole course, the evaluation will also include, besides the final project, exercises on selected sessions from the whole course.
6. The course project is based on one or more (recent) articles in the field of interest to the students (but chosen by the teachers) and the final report will include several components, *e.g.*, summary of the articles, derivations, and calculations including using the software of the course. Critical discussion of models and results is typically included. The list of articles is continuously updated and students, in some cases, may provide suggestions for articles themselves, but even in this case, the choice and formulation of questions will be made by the instructors.
7. We have found it necessary to provide “overview” tables and summaries of the lectures outlining the most important messages (available upon request from the authors). Tables of “recommended models for specific types of applications (phase equilibrium calculations and separation processes)” have been also provided. One example is given in Table 7, while additional tables have also been provided outlining strengths and weaknesses of the models mentioned in Table 7. Of course such tables are not complete (they do not contain all available models) and they are necessarily somewhat biased or limited to the models covered in this course, but they provide a general picture of the different models or approaches needed/typically used for different applications.

THE PH.D. COURSE

The objective of this course is that students become able to write robust and efficient computer programs for solving phase-equilibrium problems. An essential part of the course therefore is to implement the theory in algorithms of increasing complexity. Programming is done in Fortran.

We provide the students with precompiled modules for routine tasks such as solving sets of linear equations, and, in addition, with routines for calculating thermodynamic properties from a cubic equation of state. These routines contain a small component database of predominantly hydrocarbons. The students, given temperature, pressure, and molar amounts of the mixture species, are able to calculate volume and fugacity coefficients,

and, in addition, the derivatives of these properties, with respect to temperature, pressure, and the molar composition.

The major part of the first week is used to build up a solver for the PT-flash. The students start by writing and testing a simple routine for solving the Rachford-Rice equation (calculation of vapor fraction, given K-factors and mixture overall composition). This routine is then used to implement a solution routine that uses successive substitution. In the next step, acceleration by the dominant eigenvalue method is implemented and tested, and finally, stability analysis is incorporated. The students who can find time for this conclude by implementing second-order methods.

The second week is used on more complex tasks. The first is to write a bubble- and dew-point routine, based on a partial Newton's method (where composition derivatives are neglected). This is followed by a phase envelope calculation where a full Newton method has to be implemented, and where the routines developed by the students are required to be able to

pass the critical point of the mixture. The next problem is the multiphase flash, where the first step is the implementation of a general multiphase Rachford-Rice solver, and the following steps are successive substitution, accelerated successive substitution, and stability analysis.

The final problem during the formal part of the course (first two weeks) is to write an efficient solver for a mixture of dimerizing and cross-dimerizing components described by the ideal gas law. Essentially, this is the type of solver that is required in SAFT-type association models.

The participants are graded based on a report they write afterwards relating to an individual problem they solve (in teams of two). One example is given below:

“Correlation of VLE frequently requires the calculation of the equilibrium curve for binary mixtures at fixed temperature (Pxy-curves) or at fixed pressure (Txy-curves). Write a program for automatic calculation of such equilibrium curves. The program should be capable of

TABLE 7
Types of Phase Equilibria and Choice of Thermodynamic Models for Specific Applications

Application (e.g. separation process)	Systems	Phase Equilibria Types	Models (tools)
Distillation/Absorption	hydrocarbons gases, non-polars	VLE, GLE	cubic EoS (vdW1f)
—	polars incl. gas/polars	VLE, GLE high pressures	cubic EoS (EoS/G ^E rules e.g. MHV2, PSRK LCVM)
—	—	low pressure VLE & LLE	act. coef. models (van Laar, Wilson, NRTL, UNIQUAC, UNIFAC, RST)
—	polars, associating	multicomponent (V)LLE	UNIQUAC, CPA, PC-SAFT
Azotropic and Extractive Distillation	Polar, associating,...	VLE and LLE	UNIQUAC, CPA, PC-SAFT
Extraction	polars, associating water	LLE	UNIQUAC, CPA, PC-SAFT
Polymers	solutions, blends gas/polymers, etc.	VLE (act.coefs.), GLE, LLE, SLE, etc.	solubility parameters, FH, UNIFAC-FV, Entropic-FV, cubic EoS (vdW1f & EoS/GE), PC-SAFT, various complex EoS e.g. Sanchez-Lacombe
Environmental thermodynamics	water, air, complex pollutants/chemicals, biota	Kow, infinite dilution act. coefs., VLE/LLE, SLE	UNIFAC-water, Kow-correlations, advanced models
Many others	solids, electrolytes, pharmaceuticals,	SLE, LLE, SSLE, SGE	all the above and more...
(adsorption, SCFE, crystallization, complex products,...)	biomolecules, surfactants, colloids,...	—	—

Abbreviations

act.coef. = activity coefficient
 EoS = equation of state
 CPA = Cubic Plus Association
 FH = Flory-Huggins
 FV = Free-Volume
 GLE = gas-liquid equilibria
 Kow = octanol-water (partition coefficient)
 LCVM = lineac combination Vidal and Michelsen mixing rules
 LLE = liquid-liquid equilibria
 MHV2 = modified Huron-Vidal mixing rule
 NRTL = Non-random two-liquid activity coefficient model

PC-SAFT = Perturbed Chain Statistical Associating Fluid Theory
 PSRK = predictive Soave-Redlich-Kwong EoS
 RST = regular solution theory
 SCFE = Supercritical Fluid Extraction
 SGE = solid-gas equilibria
 SLE = solid-liquid equilibria
 vdW1f = van der Waals one fluid mixing rules
 VLE = vapor-liquid equilibria
 UNIFAC = Uniquac Functional activity coefficient
 UNIQUAC = Universal quasichemical activity coefficient

calculating the equilibrium curve for mixtures in which one of the pure components is supercritical.”

CONCLUDING REMARKS

Four different courses in Chemical Engineering Thermodynamics have been presented, fulfilling different needs and offered at different degree levels: Engineering Bachelor, B.Sc., M.Sc., and Ph.D. The context and learning objectives of the courses have been comparatively presented with special emphasis on the different teaching methods employed, *e.g.*, use of software at various levels and degrees of complexity. We consider it a problem that there is a lack of suitable textbooks that present chemical engineering thermodynamics in an applied, thermodynamic framework. Despite this difficulty, however, the very-positive evaluations of all the courses and other indicators (*e.g.*, increasing number of students) point out that the changes implemented in teaching chemical engineering thermodynamics at DTU have led to improved courses and enhanced both understanding and interest of students in chemical engineering thermodynamics.

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