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Experiments for a Computing Class

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Abstract

The course description for Numerical Computing for Chemical Engineers course at Missouri University of Science and Technology states that students will "add to their programming skills by exploring numerical computational techniques for … chemical engineering processes." The challenge is that the course is taught early in the curriculum before the students know what those chemical engineering processes are. The course has been structured as a flipped class with class time devoted to solving problems with the numerical tools. To provide relevance for the material, an experimental component has been added to the course. In the laboratory sessions, the students conduct a brief experiment or activity and then analyze that process using the computational technique for the week. The activities and experiments take no more than 10 minutes to conduct and use inexpensive materials. In this paper, the author will present how the course was flipped to accommodate the lab sessions, describe the experiments used in the course, and relay the student response to this course.

Introduction

ChE 3111 Numerical Computing for Chemical Engineers was part of a major revisioning of the chemical engineering curriculum at Missouri University of Science and Technology and was first taught in 2018. I had prior experience with teaching computing tools (e.g., Aspen) as lessons in other courses and found them frustrating. Typically, half of the students would work at the rate that you were presenting material. Some students would work ahead and then move on to other activities. Unfortunately, this was often watching videos or playing games which caused a distraction to others who would see their screen. Then there were the students who would stop you halfway through the class saying that they need help opening the software. It seemed that only a small remnant of the class was still with me by the end of class and abilities to use the tool or skill later were only modestly retained. I had, therefore, begun recording these lectures for students to review on their own when they needed a refresher. As video technology improved, I had moved to assigning the videos as homework. When I was given the task of designing this new course in numerical computing, I chose to embrace the flipped model I had been using for these lessons.

So, what was I to do with the class time? Another idea that I had gleaned from conversations with students was that they didn't remember much from their computer science Introduction to Computing courses because it seemed impractical. "Hello, world" and other programs they had been asked to write were not related to what they saw as their future career. My goal, therefore, was to demonstrate relevance to my students. Thus, each problem they were asked to solve needed to relate to chemical engineering. This was made more challenging by the fact that the students had very limited knowledge of what chemical engineering was at the time they were taking this course. My plan was to demonstrate a variety of chemical engineering concepts to the students and have them perform the calculations to answer questions relating to the other courses in the curriculum. In class we would talk about a practical chemical engineering problem, do a simple experiment to gather data or provide a physical context, I would present a very abbreviated, non-mathematical explanation of the theory and the final equation to be solved. Their task would be to solve the problem in class. For homework they would have a different application (without an experiment) and problem to solve. The exam would then give them yet another opportunity to solve a similar problem, but these problems would be purely mathematical and stripped of the physical application.

The course was intended to cover numerical solutions to basic topics from algebra, calculus, and ordinary differential equations. The students were first-semester Juniors and they had an option to take an additional more advanced numerical computing elective course during their senior year. The mathematical and chemical engineering topics covered in the course are shown in Table 1.

Table 1. Topics covered in Che 3111

Lesson	Math Skill	Lab Topic	Homework Topic
1	Infinite Series	Heat Transfer: Conduction in a plane (no experiment)	Mass Transfer: Diffusion and Fick's Law
2	Nonlinear Equations (part 1)	Safety: Upper and lower flammability limits	Separations: Underwood equation for distillation
3	Nonlinear Equations (part 2)	Fluid Flow: Friction factor	Thermodynamics: Multicomponent flash
4	Matrix Math	Worksheet only – overlaps with career fair	None
5	Linear Systems	Mass Balances: Find a recipe	Mass & Energy Balances
6	Differentiation and Integration	Absorption: H_{oy} calculations	Reactors: Reaction rate and sizing a reactor
7	Optimization	Thermodynamics & Economics: Recipe for lip balm at minimum cost	Economics: Minimize cost or maximize profit
8	Curve Fits and Interpolation	Kinetics: Reaction rate for Alka Seltzer in water	Heat Transfer: Exchanger U and exit temperature
9	Nonlinear Systems	Fluid Flow: Pipe network	Reactors: CSTR with multiple reactions
10	1^{st} Order ODEs	Safety: Evacuating an air tank	Reactors: Semi-batch reactor operation
11	Runge-Kutta for higher order ODEs or systems of ODEs	Predator-Prey model	No homework

Discussion with alums and industry partners indicated that VBA for Excel would be a good choice of programming language to use with Python as a close second. Students would be coming in without a common background as our university teaches a variety of introductory programming courses and student choose which language based on schedule availability. VBA in Excel was selected for initial offerings of the course.

The Lab Setup

The primary purpose of the course is to teach the students the numerical techniques and tools for solving chemical engineering problems. The hands-on activities are only included to convince the students that these skills can be useful for the practical problems they may one day see on the job or the homework problems for future courses. Years of hearing students say "why do we have to learn this" was the primary incentive for adding this element to the course. The activities, therefore, needed to be quick and inexpensive. With the flipped format, the goal was to spend the first 5 minutes reviewing key items from the video lessons and another 5 minutes discussing how to select the appropriate technique of the variety that had been presented. The next few minutes would be devoted to describing an application, defining variables, and giving the students the key equations to be solved. They would then spend 5 minutes doing an activity or quick experiment. The remainder of the class session was used for students to work on the calculations alone or with their classmates. The undergraduate teaching assistant and I would then help as they encountered roadblocks while doing their work.

The classroom where this course is taught is attached to the undergraduate unit operations laboratories. The room can hold more than 40 students, but with these activities it is best to keep the enrollment in a single section to 24 or so. Thus, two sections are usually necessary each semester. The room has long tables with electrical outlets every few feet. Two sinks are available in the lab space a few steps outside of the classroom, so water access and cleanup are easy. Another advantage of using this classroom is that the students can see the laboratory equipment that they will be using in the next year.

A set of inexpensive equipment was purchased for use in this course. The core set includes sets of scales, graduated cylinders, pumps, buckets, tubing and fittings for use with 6-8 teams for most of the activities. These were purchased at a local hardware store or through Amazon. See Table 2 for a summary of the key items with information for purchasing through Amazon in 2023. Some additional items are borrowed from the department break room or the instructor's kitchen as needed.

Table 2. Equipment for Hands-On Lab Activities

Item	Picture	Amazon Product Name	Price (02/2023)
Scale (3000 g reads to 0.1 g)		Digital Kitchen Scale 3000 g 0.01 oz/0.1 g Pocket Cooking Scale	$10.99
500 mL graduated cylinder		500mL Graduated Cylinder, Premium Polypropylene, Hexagonal Base, 5 mL Graduation	$14.99
Submersible Pumps		A variety of submersible pumps ranging from 80 GPH to 200 GPH	$6.99 - $25.99
Thermometers		Meat Food Candy Instant Read Thermometer	$7.49
Buckets		Dollar Tree Plastic Storage Tubs (not Amazon)	$1.25
Plastic Tubing		A variety of sizes (1/4”, 5/16”, 3/8” ID are the most frequently used) clear vinyl tubing	$6.88 for 10 ft of 3/8”
Tubing Tees		Barb 3 Way Hose Fitting	$6.99 for set of 5 @ 3/8”

The Lab Activities

The first weeks of the semester focus on helping the students learn the patterns of the course since the course is highly non-traditional. Thus Weeks 1 and 2 do not really have an experimental component. An experimental addition for Week 1 using candle warmers and metal blocks with infrared thermometers was introduced one semester but seemed to add chaos and not provide the added relevance. For Week 2, the students are taken into the lab and taught to read the manometer so that they can determine the upper and lower flammability limit of a chemical stored in a cannister. (The container is actually empty, but it helps to bring a container into the room for added relevance.)

Week 3 is the first actual experiment. The students are provided graduated cylinders, buckets, tubing, and submersible pumps. They measure the flowrate and calculate the friction factor using the Nikuradse equation (which was selected because it is highly nonlinear so they will not be tempted to solve it analytically). At this point the students have become accustomed to the pacing of the course. The hands-on activity requires them to talk to others in their group which also increases the interaction between students as they try to solve their problem and de-bug their programs.

Week 4 typically coincides with the career fair, so a review of matrix mathematics is scheduled for that week. Students have a worksheet to do on their own time and Khan Academy videos to watch if they need additional help.

Week 5 is a "cooking" experiment. The students are given 4 ingredients to make a food product. Typically, the four ingredients are melted chocolate, cereal, small crackers, and peanuts. This requires a crockpot and scales as well as many disposable bowls and spoons. The students weigh out and mix together their choice of ingredients and develop a nutrition fact label. They then must create a system of linear equations to determine the recipe to make a product with a particular nutrition fact label. The basic equations are the same for both problems, but one is a direct calculation and the other requires them to use the matrix techniques covered in lecture.

Week 6 has the students numerically integrate to find the height of packing for an adsorption column. I do not have the students operate the equipment, but I do have them don hardhats to tour that portion of the unit operations lab and I show them the control system to run the equipment.

Week 7 is an optimization problem. Typically, I have them optimize a product to minimize cost or maximize profit. The product is selected each semester to use up remaining supplies from recent K-12 outreach activities in the department. The experiment may take a little longer than the usual 5-minutes, but it is usually fun. This past semester the challenge was to minimize the cost of producing lip balm that had a melting point 1°C higher than skin temperature.

Week 8 the students need to gather data for curve fits and interpolation. Alka seltzer in water of different temperatures works well for this. When measured on the scales in Table 2, the data is relatively smooth. Noisier data can be obtained using the scales from the unit operations laboratory.

Week 9 has the students solving a system of nonlinear equations that represent a pipe network. The students build a small version of the pipe network on the screen using tubing and tees with the submersible pumps and buckets. They verify that they have flow in all legs of the network and measure the flow through the total system. I have them solve the system of equations to estimate the flow through each leg.

Week 10 is the final week of regular classes and the topic is first-order ordinary differential equations. For this experiment, I borrow an experiment from Ed Clausen (Christie 2017). The students model the rate that air leaves a tank through a small hole. The experiment is done by the class as a whole with student volunteers operating the equipment.

Week 11 is "reading week" at the university, so an in-class discussion of the predator-prey model followed by an opportunity for students to solve the problem is the final activity of the course.

My Observations and Summary

The students generally find this course to be both fun and useful. Students have opportunities to use these skills during the same term for their other courses and they use them during internships. It is not uncommon to overhear students discussing ways to solve problems in later courses and hear them refer to the numerical skills in terms of the classroom activity that week. "Use the code from the air tank experiment" is a phrase heard in the student lounge recently.

The format of the class also encourages students to attend class. Colleagues are often afraid to try the flipped class because students will stop attending. I rarely have more than 5% of my class out on any given day and the students are all engaged. Because the activities are not essential to understanding the numerical technique, it is also easy to accommodate students who need to be absent due to illness or travel. Classes are recorded for them to watch their classmates perform the activity if they so desire.

A common question is whether or not the students actually watch the videos. Most students have a week where they are unable to watch the videos before coming to class. It is obvious that they have not because they are not prepared to do the computations with everyone else. Sometimes they watch them in class as they are trying to do the computations for the week's assignment or they ask their friends to catch them up. Most often, these students excuse themselves for the day to watch the lesson and do the week's work as homework. It is extremely rare for students to make this mistake more than once. Since my videos are publicly hosted on YouTube, the record of views is anonymous and is confounded by viewers beyond my students. However, the traffic picks up the week before lab with the highest peaks in the last day or two before class. There will also be a small peak right before an exam as students review. I can also observe bumps in the number of views at times when my colleagues in other courses make an assignment using one of these skills.

As the instructor, this course has become the highlight of my week. Class sessions are fun. Gathering the materials takes a little extra time before class, but cleanup is usually done during class as the students do their calculations. Most of my time during class is spent walking around the room and talking to students and answering their questions. I feel confident that the students are learning the material and I enjoy the time to build relationships with the students.

References

Christie, M.A., J.A. Dominick III, R.E. Babcock, W.R. Penney and E.C. Clausen. 2017. "Comparison of Experimental Data and Model Results for the Depressurization of an Air Tank." *Proceedings of the ASEE Midwest Regional Conference.* Stillwater, OK.