

A Web-based Learning Tool that Introduces Engineering Concepts by Simulating a Chemical Reactor

Jay B. Brockman, Jucaïn Butler, and Mark J. McCready
University of Notre Dame

Abstract

The arrival of the World Wide Web signaled the beginning of fundamental changes in how teaching, training, and self-directed learning will occur at all ages and stages of life. Because of its versatility as a learning tool in the realm of higher education, the Web has woven its way into engineering classes and laboratories. As a supplement to a Chemical Engineering project in an Introduction to Engineering Systems course at the University of Notre Dame, we are developing a self-paced, web-based learning tool that primarily demonstrates feedback control, and the use of mass balance equations with reaction to describe a chemical reactor, and secondarily demonstrates basic aspects of fluid flow. Included in the learning tool is a set of reference materials that explain technical concepts, a web-based simulator of a continuously flowing reactor in which the neutralization of acetic acid with sodium hydroxide is carried out, and an assessment engine built around the simulator to measure if students acquire simple skills, and follow students through their work to see if the path to a solution seems logical. This learning tool will be used by over 300 first-year engineering students who go on to major in various engineering disciplines. Because the learning tool is web-based, it will also be available to any institution that wishes to use it. The project is being developed with support of the NSF through the Course, Curriculum, and Laboratory Improvement (CCLI) program.

In this paper we discuss our motivation for creating this tool, its design, and the current status of the implementation.

Goals and Objectives

The goal of this project is to provide an example of and a template for education modules in engineering that integrate experimental work, web-based text and resources and numerical simulation of the laboratory experiments with a web-based assessment tool, based on primary trait analysis [1] to evaluate student progress. With a properly designed web-based evaluation tool, it should be possible not only to measure if students have acquired simple skills, but also to follow students through their work on complex problems to see if the path to a solution makes sense. In doing this, the instructor can evaluate and even quantitatively measure, the degree to which students have mastered the *process* of solving, e.g., design problems that require integration of understanding and knowledge by the student.

The "deliverables" of this project will be complete plans, materials and purchased equipment list for a ~0.5 l sized acid neutralization reactor, extensive web-based textual materials on the main

topic including pages appropriate for reading with various web-links and PowerPoint lectures on the key topics, a complete Java-based simulation of the laboratory experiment that would allow extensive exploration of the behavior of the reactor and the controller, and integrated assessment tools to track and analyze student progress. A hierarchical approach to the text materials will allow more advanced students to find new, deeper, facets of the problems to investigate. Further, the experimental setup will be robust enough to allow both basic and advanced studies. To evaluate student progress to understanding the information, the simulator will have an assessment engine wrapped around it so that instructors will be able to quantitatively evaluate student progress.

Of the main topics of the proposal, *feedback control* is central to mechanical, electrical and chemical engineering, *use of balance equations* is central to chemical and environmental and has applications in other fields, *fluid flow* (to feed the reactor) and *mixing* are of interest to chemical and mechanical engineers. Further it is emphasized that we are not just trying to produce this one comprehensive module, but to determine the key elements for such modules and how they are put together to most effectively enhance student learning and assessment of this learning.

While the preliminary work for this proposal has been done for first year students at Notre Dame, our interest is general and is intended to address: (a) **Engineering student retention**—which is a continuing problem at Notre Dame as well in the US in general—primarily by exciting students, at an early stage of their educational careers, about the creative as well as the analytical nature of engineering and (b) **enhance student learning** by providing a well **integrated package** in which the web-based textual materials define the topic, carefully organize the presentation, and give feedback to students and faculty through "quizzing", a powerful simulation package that allows students to efficiently *explore* (letting them determine a path to their learning) all aspects of reactor and controller and a physical experiment that gives "hand-on" experience and lets them see how engineering models and engineering experiments are used together to solve engineering problems.

The evaluation of this project will be done at the within the context of "EG111/112: Introduction to Engineering Systems" course [2] by tracking student progress to the learning goals. As this is a new course that is receiving a lot of attention from the University administration, considerable effort will be put on assessment of all aspects of instruction and student learning.

Project Scope and Topics

The motivation for this project arose out of the need to create a comprehensive learning experience based on a laboratory experiment for first year engineering students that demonstrated feedback control and use of the mass balance equations with reaction to describe a chemical reactor. Secondary learning goals for the module are basic aspects of fluid flow and (for the students) continued enhancement in their ability to use computers. It was decided that the main learning goals could be met using a small, continuously flowing reactor in which the neutralization of acetic acid with sodium hydroxide was carried out and for which a Proportional-Integral controller was used to adjust the sodium hydroxide flow rate to control the pH in a range from 4-6. As a result of this course, working versions exist of the experimental apparatus, the simulator (but only in Matlab), lectures and some pdf files of "how to" for the topics of module and the experiment. Interactions with the students as they ran the experiment and simulator have given significant insight into the flaws and good parts of this project. Below, we describe the fundamental topics of the module prototype and the manner in which they are addressed.

Feedback control

Feedback control is a concept that is of interest in most engineering disciplines. First students must understand the concept of feedback in that a measured output is being compared to a desired *setpoint* and then an action (e.g., change the base flowrate) is being taken. The plan for the module is to use both *proportional* (where the neutralizing base flowrate is proportional to the error in the pH) and *integral* (where the neutralizing base flowrate is proportional integral of the error in the pH) control. Students will be shown that both are necessary to control the chemical reactor. A key to getting first year engineering students to understand feedback and control schemes is showing them how to explore the control of the reactor with the simulator. They will be enticed into doing this by lecture and text materials such as shown in Figure 1. It is seen that a purely proportional controller does not get the set point. The purely integral controller is prone to severe overshoot and oscillation. However, when the two schemes are used together, the performance could show only mild overshoot, right on the setpoint.

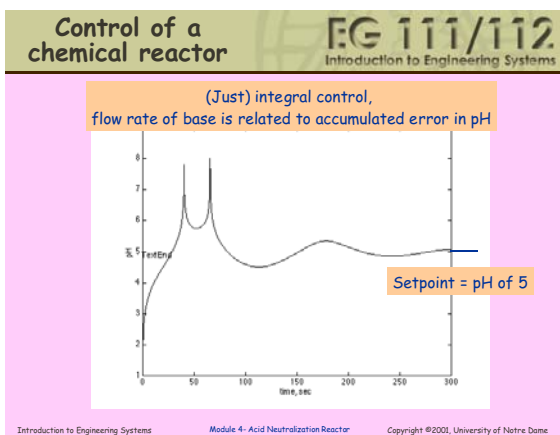
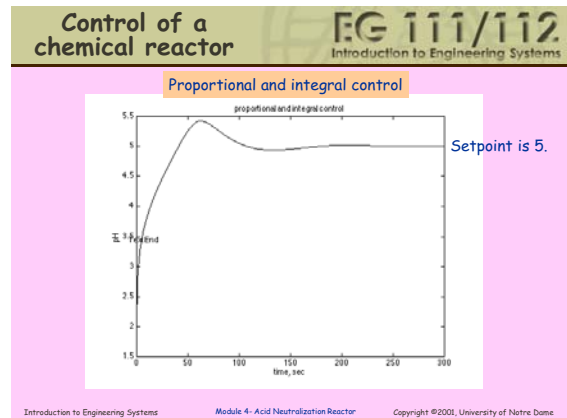
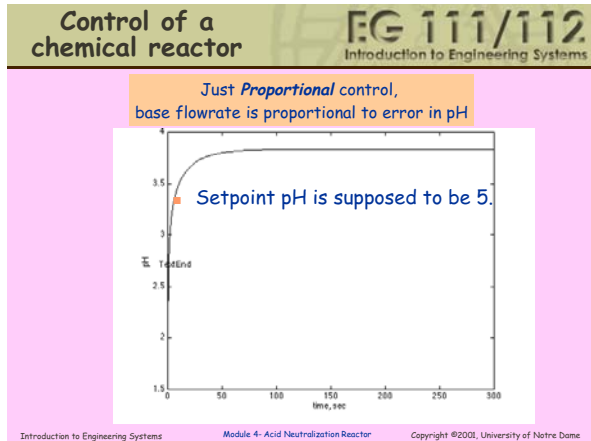


Figure 1. Transient simulations (pH versus time) of the reactor showing proportional control, integral control and combined proportional and integral (PI) control showing the benefit of using a PI controller.

Once motivated, they will be first led through the use of a simulator by asking them to run specific cases. Then, they will be given more open-ended questions that require them to think through how the different control schemes behave. They will need to model the reactor before running the experiment, to find some reasonable *controller constants*¹. After running the physical experiment, they may need to run the simulator again to understand the differences between the experiment and the model. Through this procedure, they should get a good introduction to the use of a simulator as an engineering model.

¹ Once a control strategy, e.g., proportional-integral, the controller needs to be "tuned". This involves adjusting one or two constants until the controller gives the desired response. Formal schemes exist for tuning and will be shown in the advanced material. First year students will be given some simple heuristics and bounds.

Mass Balance for a transient flowing system

The important concept is the "thought processes" necessary and the mathematical terms involved in writing a general conservation equation for a fixed volume in space. In this module only *mass* will be conserved but such equations for *energy* and *momentum* conservation are used at later stages in the curricula.

In contrast to many introductory texts on mass balances, e.g. [3] we follow Russell and Denn [4] by including the derivative term that describes the transient behavior of the process. Intuitively, students understand that the system can be transient. We show them how to get solutions for first order (one, or more than one) differential equations by using an Euler numerical integration scheme, which first had been introduced in the Fall semester (EG111) course. Having this skill, students can be shown how steady states² often arise as an expected outcome -- rather than a steady state being an *assumption* made necessary by the omission of the derivative term. Further with this integration procedure they can calculate a "titration" for which they are adding quantities of base to a fixed volume of acid while always calculating the pH. This problem is crucial to understanding the weak-acid -- strong base system (in which the weak-acid buffering capacity defines at which pH range the reactor can be controlled).

Basic fluid mechanics for a draining tank

For convenience and cost, the acid feed to the system is gravity driven. To help students understand how the flow rate of a draining tank will vary with the depth, we will give a brief introduction into fluid flow that is governed by Bernoulli's equation. For just gravity draining, this equation can be derived with a simple example of the conversion of potential to kinetic energy. This material ties in well to fluid mechanics courses that are taught in the Junior year of chemical, mechanical and civil engineering.

Elementary acid-base chemistry and behavior of buffer solutions

The chemistry necessary for this project includes concepts of pH, pH of a weak acid solution, pH of a buffer solution and pH during a titration of a weak acid by a strong base, are all contained in the first year chemistry course. This module will serve as a review of these concepts and show students how information from a basic science forms an important foundation for what is very much an engineering problem. Another crucial issue that relates to chemistry is that the reactor would be very difficult to control in certain ranges of the titration curve where small changes in concentration lead to big changes in pH [5]. The flat region of a weak-acid/strong base titration curve (where the buffering action of the acid and its conjugate base is most effective) presents the opportunity for effective control. A strong acid/strong base where no buffering is present has a very sharp change between the low pH and high pH region and thus control would be very difficult. Students would not understand the subtlety if they did not understand how the buffering action works.

² Steady states in this context are input and output conditions that are not changing in time.

Methodology

Putting Assessment at the Heart of Module Development

A well-known flaw of the traditional grading system is that it provides little or no opportunity for directed feedback or corrective action. Under this “open loop” approach, teachers present information, students try to assimilate it, the teachers assign a grade to the students’ work, and then the class moves on to the next topic. By contrast, our proposed approach is based on a technique called *Primary Trait Analysis* (PTA) that places assessment of student learning outcomes at the heart of module development, providing students and teachers alike with the information that they need to improve their performance. A major contribution of our research will be to develop a framework for integrating Primary Trait Analysis with web-based instruction, using the module on chemical reaction control as a model.

Primary Trait Analysis is a scoring rubric that captures the learning objectives of a particular course or project and the standards and criteria deemed most relevant by the teachers of the course or project. It was created for the National Assessment of Educational Progress [1] and has been developed for classroom use by Dr. Barbara Walvoord, Director of the *Kaneb Center for Teaching and Learning* at Notre Dame. Course or module development using PTA consists of the following steps:

1. Define desired student learning outcomes, expressed in terms of the *primary traits* that students should embody upon completion of the module or course. (“Upon completion of this module, students should be able to”)
2. Define a scoring rubric that measures student performance to the desired learning outcomes. (“Upon completion of this module, students should be able to . . . , as measured by”) The rubric should be quantitative.
3. Readings, tutorials, and other teaching components are developed within the framework of the stated learning outcomes, and the rubric-based assessment methodology. Scoring rubrics are developed for individual assignments, and these rubrics are in turn linked to the primary course goals.
4. As students complete their assignments, the scoring rubric is used to assess the work. Collected data not only provides individual students with targeted feedback on areas for improvement, but also provides the professor with an accurate picture of which concepts are clear to the class as a whole and where there are problems.

Figure 2 presents the learning outcomes for the chemical reactor control module of the first-year engineering systems course (EG111-112). In reviewing these diverse outcomes with an eye towards assessment, it is clear that a variety of “instruments” is needed to measure student learning. Having the students work on traditional problem sets that have well-defined answers could test some outcomes, such as the ability to set up mass balance equations. Other outcomes, such as those involving communication skills, require careful analysis and judgment by the grader to determine a score.

- 1. Concepts of conservation of mass and chemical species for a reacting system:** A student should be able to:
 - use the principle of conservation of mass as applied to a fixed control volume to describe the rate of change of total mass and individual chemical species in for a well-stirred chemical reactor, with inflows and outflows in terms of a first-order ordinary differential equation
 - use basic concepts of chemistry to describe equilibrium or changing concentrations of chemical species for this well-mixed reactor.

- 2. Modeling of dynamic systems:** A student should be able to:
 - understand the difference between transient and steady-state behavior of a simple dynamic system or process
 - develop the appropriate equations to use Euler's method to solve numerically a simple system of first order differential equations
 - be able to describe how power is transmitted in mechanical devices using torque, rotating shafts and gears
 - be able to design and develop a simple gear train to provide a required torque and shaft speed

- 3. Application of MATLAB:** A student should be able to:
 - use MATLAB to solve a system of first order differential equations using Euler's method
 - be able to interpret the instructions in a MATLAB procedure that uses nested loops and conditionals
 - modify a MATLAB procedure in order to alter output or program behavior in order to adapt the procedure to a specific case or condition

- 4. Introduction to dynamic system control:** A student should be able to:
 - qualitatively describe the concept of feedback and its use in the control of a dynamic system or process
 - differentiate between a system with feedback control and one without
 - use the concepts of proportional and integral control to control a simple dynamic process
 - integrate sensors and actuators into a simple microprocessor to control a dynamic system

- 5. Development of written communicating skills:** The students should be able to:
 - prepare an engineering project report that demonstrates that they have gained a sound understanding of the fundamental issues listed above details the design, testing and evaluation of a process controller
 - describe the difference between simulation of a process and physical measurements associated with the actual process and be able to explain the sources of those differences

Figure 2. Learning Objectives for the feedback controlled acid neutralization reactor

Even more problematic to assess are skills where the student is expected to master a *process*, such as learning an efficient design methodology or optimization strategy. The difficulty here is that in order to assess the efficiency of a student design process, we need an accurate and reliable record of the sequence of actions that occurred during design. In some courses, faculty require students to submit design notebooks or logs, but these are often incomplete and don't lend themselves to quantitative scoring. In earlier work [6] [7] we have developed a set of tools and techniques for automatically capturing and analyzing computer-based design processes transparently as designers work with CAD tools and simulators. We propose to apply and extend these techniques to evaluate the efficiency with which students design their PI controllers. In the

following section, we discuss the proposed architecture of the web-based learning module and its relationship to PTA.

Architecture of the Web-Based “Virtual Learning Center”

As discussed in the previous section, the key feature of PTA is that it systematically integrates the assessment strategy with development and presentation of a learning module. In this section, we give a brief overview of the components of the proposed web-based “virtual learning center”.

Today, there are a number of “e-learning” environments available on the market for developing online course materials. Typically, these environments provide an infrastructure for integrating readings, quizzes, bulletin boards and chat rooms with a student database. Notre Dame has adopted one of the most popular of these, WebCT, which was originally developed at the University of British Columbia. We will implement the virtual learning center within the WebCT framework and focus our development efforts in two areas: 1. development of content for lectures, readings, and quizzes in standard online formats and 2. development of a simulation-based tutorial on the design of a pH controller that tracks and analyzes the design process.

One of the key technical contributions of our work will be the development of the Java simulators and a design tutorial that is based on these. The tutorial will lead students through a sequence of activities that start with elementary conservation of mass concepts in the reactor and continue through controlling the flow of base into the reactor to maintain the pH at a given set point. At each step in the tutorial, students will be assessed and given feedback, possibly being required to repeat activities, before continuing. We envision the following sequence as the main steps in the tutorial:

1. overall mass balance of liquid flowing in and out of tank
2. mass-balance with non-reactive species
3. mass-balance with reactive species
4. PI control to maintain pH

While each of the simulation activities serves a unique purpose highlighting different aspects of the design process for the students, they will all be implemented around a common software core. Used successfully in other projects at Notre Dame, this approach greatly reduces software development time and improves reliability. The simulation architecture and its relationship to WebCT, with the software components is described below.

Simulation engine. Central each of the applets is an identical simulation engine. The simulation engine is a Java class that implements an Euler solver for the mass-balance equations for a generic continuous-stirred tank reactor system. The simulation engine accepts simulation input parameters and produces output data in a standard format.

GUI and Assessment Front-End. Each simulation example has a custom front-end that implements the graphical user-interface (GUI) and that calculates statistics relevant to that demonstration by capturing a trace of the students’ interactions with the simulator. Examples of assessment rubrics that may be calculated could include the total amount of time that students spent on the examples or the number of trials that it took for students to find an acceptable design.

WebCT Student Database Interface. This model translates the assessment statistics generated by the front-end into a format acceptable to WebCT. If a different database were used, this is the only module that would have to change.

Status

To date, we have developed and tested a number of simulation tool, along with laboratory apparatus, in conjunction with this project. Below, we give a brief overview of these tools.

CSTR-PI Matlab Simulation

For the Spring 2002 offering of the Introduction to Engineering Systems course, we developed a Matlab implementation of the pH controller that showed good agreement with the physical apparatus in the Learning Center. It uses Euler's Method to iteratively update the state of the CSTR/PI controller system at each time step. The underlying model is the set of mass-balance differential equations for the species HA, A⁻, and OH⁻ flowing in and/or out of the reactor, or being produced or consumed in the reactor. A full implementation of the simulator is available on the course web site at http://www.nd.edu/~engintro/Lectures/cstr_pi_pro.m

Computer Architecture Online Tutorial

For the Fall 2001 offering of the Introduction to Engineering Systems course, we developed a Java-based online tutorial on fundamentals of computer architecture that introduced students to the inner working of the Lego Mindstorms RCX processor, the same processor that they used in implementing their pH controllers in the Learning Center. As we propose here, the computer architecture tutorial leads students through a sequence of activities of increasing complexity, with interspersed readings, quizzes and surveys. While this simulator did not integrate the assessment mechanisms in the proposed research, there are some similarities in both the design of the software, with each of the exercises implemented around a common software core. Over 250 first-year students completed the online computer architecture tutorial, and we have extensive feedback from students on its strengths and weaknesses, which will greatly help in the development of the proposed project. The complete tutorial is publicly available at <http://www.nd.edu/~jvasim/APPLETS/RCXSIMULATOR/Directions.htm>

Acid Neutralization Experiment

A working version of the acid neutralization experiment has been developed and used by over 600 students. Figure 3 shows a photograph of the set up. The reactor total volume is 0.75 l and be adjusted down to about 0.3 l by using the screw-driven mechanism. In its current version both the acid and base are gravity fed and the outflow is thus determined by the in-flows once the reactor is full. The acid is an aqueous .1 M Acetic acid solution. The base is about 0.2 M NaOH in water. Typical flow rates are 1-10 ml/minute. Control is achieved by a mechanical valve mechanism that is driven with the computer/interface of LegoMindstorms. The interface "brick" can be programmed in "not quite C" and will log the pH as a function of time and provide control action in accord to its programming.

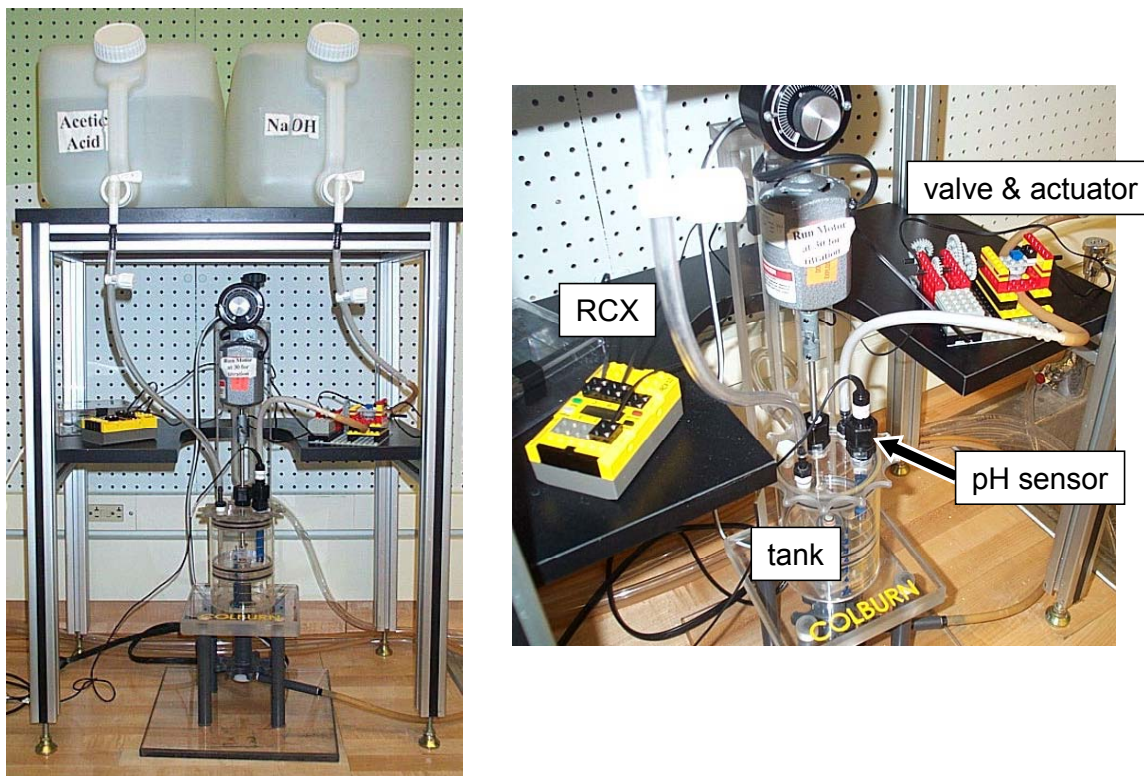


Figure 3. The acid neutralization reactor.

Particle-Based Simulations of the Acid-Base Reaction

One of the more difficult concepts for students to grasp in relation to this project is the concept of chemical equilibrium (and dynamic equilibrium in general). To help students gain better insight into this phenomenon, we have developed several particle-based demonstrations/simulations of a slowed-down chemical reaction using Matlab. Figure 4 illustrates one example. In this example, colored balls represent particles of each of the reagents involved in the reaction. By clicking on the buttons, users can “drop in” quantities of the species and observe through the interactions of the particles how the system achieves equilibrium. A second window illustrates the concentrations of the species over time.

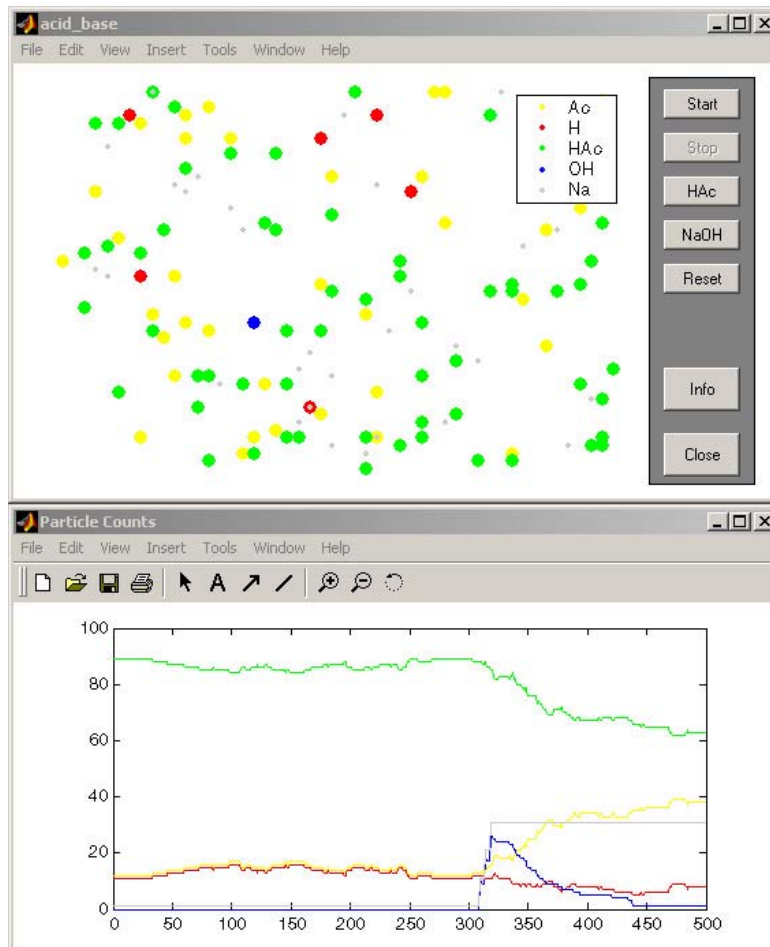


Figure 4. Particle-based simulation of acid/base system.

Simulation of PID Control Dynamics with a Virtual Ball and Beam

A disadvantage of teaching control concepts in a chemical reactor is that it is difficult to visualize the dynamics. To further illustrate the behavior of a PID controller, we use a Matlab simulation of a ball and beam system.³ Here, students may set different values for the control coefficients, and observe how the system seeks to position the ball at a set position along the beam by adjusting the beam angle. The simulation also has a manual mode wherein students can “grab” the end of the beam with the mouse and attempt to control the system themselves.

³ Developed by Dr. Jeffrey Kantor, Department of Chemical Engineering, University of Notre Dame

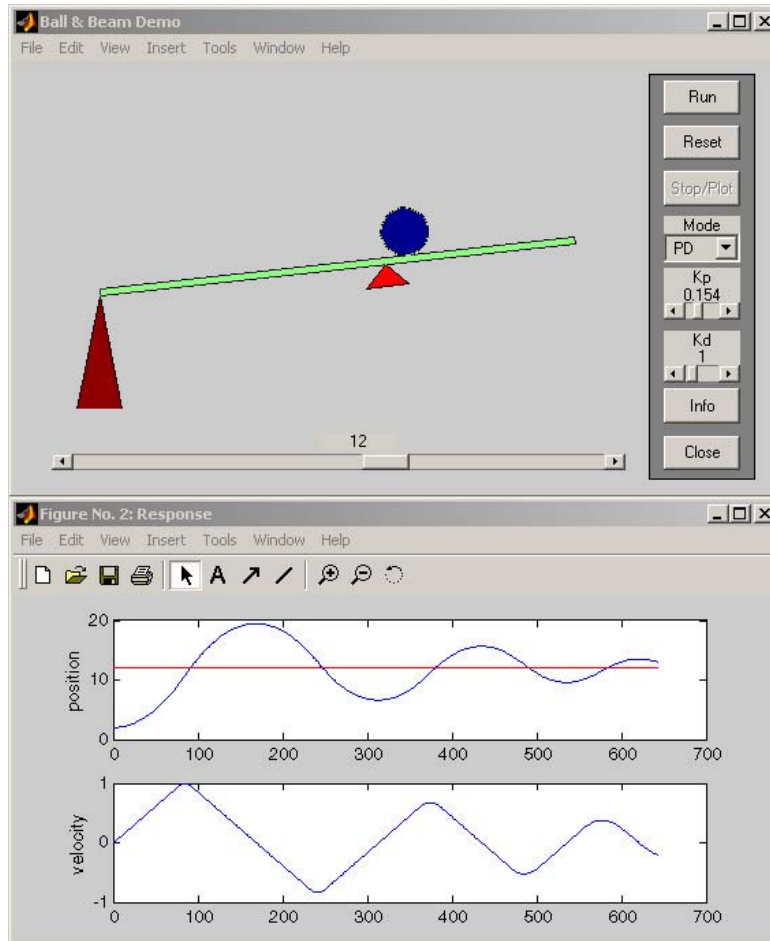


Figure 5. Ball and beam controller simulation.

Over the next year, we will be developing web versions of these Matlab prototypes as Java applets.

References

1. Lloyd-Jones, R. (1972) "Primary trait scoring in the evaluation of writing: Describing, measuring, judging", ed. C. Cooper and L. Odell, National Council of Teachers of English, Urbana, IL pp33-66.
2. Brockman, J. B., T. E. Fuja, and S. M. Batill, (2002) "A Multidisciplinary Course Sequence for First-Year Engineering Students," in *Proceedings of the 2002 ASEE Annual Conference*, Montreal, Canada.
3. Felder, R. M., and R. W. Rousseau (2000) "Elementary Principles of Chemical Processes" John Wiley and Sons, Inc.
4. Russell, T. W. F. and M. M. Denn (1998) "Introduction to Chemical Engineering Analysis" (draft edition), John Wiley and Sons, Inc. Original published edition is 1972

5. Wright, R. A., B. E. Smith and C. Kravaris (1998) "Online Identification and Nonlinear Control of pH Processes", *Industrial and Engineering Chemistry Research* **37**, 2446-2461.
6. Brockman, J. B. (1996) "Evaluation of student design processes," in *Technology-Based Re-Engineering Engineering Education*, *Proceedings of Frontiers in Education FIE'96 26th Annual Conference*, Salt Lake City, UT, USA, pp. 189-93.
7. Johnson, E. W. and J. B. Brockman, (1998) "Measurement and analysis of sequential design processes," *ACM Transactions on Design Automation of Electronic Systems*, vol. 3, no. 1, pp. 1-20.

JAY B. BROCKMAN

Associate Professor, Department of Computer Science and Engineering, Concurrent Associate Professor, Department of Electrical Engineering, University of Notre Dame. Dr. Brockman is currently a Visiting Associate at the Center for Advanced Computing Research at the California Institute of Technology. His research interests include computer architecture, VLSI systems, and multidisciplinary design and optimization.

JUCAIN E. BUTLER

Senior Research Technician, Department of Computer Science and Engineering, University of Notre Dame. Mr. Butler's research and teaching interests include virtual labs, web-based learning tools, and engineering education.

MARK J. MCCREADY

Professor and Department Chair, Department of Chemical Engineering, University of Notre Dame. Dr. McCready's research and teaching interests include complex fluids and flows, and minimizing the environmental impact of chemical manufacturing processes.