FRONTIERS OF CHEMICAL ENGINEERING:

THE SYSTEMS APPROACH

T.F. Edgar[1] and J.B. Rawlings[2]

[1]*University of Texas, Department of Chemical Engineering, Austin, Texas 78712*

[2]*University of Wisconsin, Department of Chemical and Biological Engineering,*

Madison, WI, 53706

Abstract: A dramatic shift in chemical engineering undergraduate education has been proposed based on NSF-funded, discipline-wide workshops that took place in 2003. This has led to a broad consensus regarding foundations for chemical engineering undergraduate education in the future based on the organizing principles of (1) molecular transformations; (2) multiscale analysis, and (3) the systems approach. The third area is the focus of this paper, as it relates to systems and control and the increasing importance of biological systems in chemical engineering as well as the development of new educational materials.

Keywords: biological systems, process control, chemical engineering curriculum, educational materials.

1. INTRODUCTION

Chemical engineering skills are critical to such sectors as microelectronics, medicine, biotechnology, and new materials. While demands for well-trained engineers in these areas have continued to grow, undergraduate educational programs have not kept pace, especially in these new areas. The curriculum will need to change if chemical engineers are to play a leading role in meeting the workforce needs in emerging technologies based on molecular transformations. Current teaching materials and textbooks do not reflect recent advances that have taken place in the underlying sciences of chemistry and biology.

In 2003, three NSF-funded workshops were held to assess the chemical engineering curriculum. Faculty from more than 53 universities and industry representatives from 5 companies reached strong consensus that there is a need for significant change. The participants reached broad consensus on basic principles for chemical engineering undergraduate education in the future; these principles address fundamental knowledge, skills and attributes of graduates, and methods of engagement with students. See http://web.mit.edu/che-curriculum for full proceedings of these workshops. A key driver for curriculum reform was to address the increasingly central role of biology in the traditional industries that hire chemical engineers and the need to prepare students for versatile, multifaceted careers.

Workshop participants defined the scope of what chemical engineers do and described the elements of an undergraduate chemical engineering education without relying on the conventional categories of the traditional curriculum. Three organizing principles emerged. First, chemical engineers seek to understand, manipulate, and control the molecular basis of matter, and the molecular-level processes – physical, chemical, and biological – that underlie observed phenomena in nature and technology. Molecular transformation is a unified treatment of phenomena at this level.

Second, chemical engineers are effective because they combine macroscopic engineering tools with molecular understanding. Multiscale analysis covers the tools appropriate to a given length scale (molecular dynamics, continuum equations, macroscopic averages), an appreciation for the ways in which phenomena occur at different scales (e.g., in a packed bed reactor, ranging from kinetic mechanism to heat duty), and an understanding of how phenomena at one scale affect another (e.g., molecular structure affects macroscopic properties). This also deals with connection of transient and steady-state processes.

Third, realistic chemical engineering problems (that is, the dynamic behavior of batch and continuous processes and systems in nature, technology, and society) feature multiple interacting components and draw important information from fields outside chemical engineering. The analysis of such problems depends on coordinating a variety of tools. Systems analysis and synthesis is the organizing principle that leads to the ability to manipulate systems to achieve desired behavior or performance. Furthermore, chemical engineers design and create products and processes, so that there is a strong component of synthesis, as well.

In short, the chemical engineer leverages knowledge of molecular processes across multiple length scales to synthesize and manipulate complex systems that encompass both processes and products. In this paper we focus on the systems approach and its strong connection to education of students in the subjects of process modeling and control.

1.1. Desirable Attributes of Graduates and the Systems Approach

Engineers are fundamentally problem solvers, seeking to achieve some objective of design or performance among technical, social, economic, regulatory, and environmental constraints. The chemical engineer brings particular insight to problems in which the molecular nature of matter is important. Educators cannot teach students everything that might be encountered; instead the aim is to equip graduates so they grasp fundamentals and engineering tools, enabling them to specialize or diversify as opportunity and initiative allow. The systems component of the curriculum should:

(1) Cultivate professional attributes, such as willingness to make estimates and assumptions, readiness to face open-ended problems and noisy data, and ability to visualize the solution.
(2) Hone the professional skills of problem solving; estimating uncertainty; using computational tools; economic analysis; and the ability to plan, execute, and interpret experiments.
(3) Integrate knowledge and information to aid in solution of chemical engineering problems.

2. THE SYSTEMS APPROACH IN THE CHEMICAL ENGINEERING CURRICULUM

The systems component of the curriculum ensures that chemical engineering graduates should be able to:

(1) create and understand mathematical descriptions of physical phenomena,
(2) scale variables and perform order-of-magnitude analysis,
(3) structure and solve complex problems,
(4) manage large amounts of messy data, including missing data and information,
(5) resolve complex and sometimes contradictory issues of process design: sensitivity of solutions to assumptions, uncertainty in data, what if questions, process optimization.

The systems approach is a fundamental concept that is explicitly addressed only in a few chemical engineering courses. The concept of analyzing a collection of components and processes as an overall system, rather than as individual components, is critical for frontier areas of chemical and biological engineering, as well as traditional areas.

The systems component of the curriculum is the part that trains the students in the tools for synthesis, analysis and design of chemical and biological processes, units and collections thereof. Systems education teaches the students how to convert scientific facts and principles of chemical and biological systems into engineering decisions. The knowledge base of systems consists of methods for dynamic and steady-state simulation at multiple length and time scales, statistical analysis of data, sensitivity analysis, optimization, parameter estimation and system identification, design and analysis of feedback, methods for online monitoring and diagnosis, and methods for design of products and processes.

New educational materials that enable instructors to integrate the systems concepts into the curriculum at each stage of the undergraduate educational program are needed. This integration is a new and essential component. As the students learn new scientific concepts, the systems tools that enable specific scientific knowledge to be harnessed for engineering purposes can be presented in parallel. This purposeful and tight integration marks one significant change to the traditional curriculum. The changing scientific principles of interest, which include both newly emerging concepts in molecular biochemistry and cellular biology as well as the expanding tools of molecular modeling, require a concomitant change and expansion of the systems tools currently used. The four years of the curriculum can be structured as shown below.

The Freshman Systems Experience

- Plant-wide and product viewpoints
- Exposure to multi-faceted, real-world problems
- Degrees-of-freedom analysis
- Computer programming concepts and simple computer applications

The Engineering Systems Experience (Sophomore Year)

- Conservation laws for simple dynamic and steady-state systems
- Simple models for an experimental dynamic system (chemically reacting system)
- Acquisition and analysis of noisy, complex, dynamic laboratory data
- Numerical simulation for simple models (single ODE)
- Parameter estimation for simple models (one or two parameters estimated from one or two dynamic sensor measurements)
- Equipment construction and sensor design

Methods for Molecular Systems (Junior Year)

- Random variables, probability and statistics
- Stochastic systems and molecular level reactions as systems
- Stochastic kinetic models and Monte Carlo models
- Simulation as an enabling technology
- Optimization principles for design, parameter estimation, and decision making
- General principles of experimental design for static and dynamic systems
- Use of models in predicting and understanding system behavior (analysis) and subsequent use of models in shaping system behavior (synthesis)
- Systems biology: sequence to function: in metabolic networks, gene expression networks, integrated gene-metabolic networks
- Examples from microelectronics, catalysis, systems biology

Systems Integration and the Marketplace (Senior Year)

- Multi-scale systems, separation and resolution of time and length scales
- Design and analysis of feedback control systems
- Frequency response and analysis of spectroscopic data
- Monitoring and fault detection
- Energy and mass integration, design for environment and process efficiency, network targeting concepts
- Process operations: planning, scheduling, and the supply chain
- The design experience: economics and business skills, safety, marketing, environmental impact, life cycle analysis, ethics, intellectual property, globalization, social and national needs

A significant portion of the new teaching materials can be developed as case studies and modules that can be integrated into each year of the curriculum. Eventually new textbooks will be produced, but other forms of dissemination are also effective. For example, modules in the systems area can be distributed electronically and take advantage of computer simulation and animation to illustrate the concepts.

Case studies and modules supporting the concepts could include the following real-world engineering applications, some in non-traditional areas of chemical engineering:

- Desalination of sea water
- Hydrogen from biomass
- Synthesis of specialty polymers
- Global climate change
- Regional air quality analysis
- Production, separation, and purification of natural products and recombinant proteins
- Reconstruction of cellular networks. Design of cells and biomolecules.
- Insulin regulation
- Pharmacokinetic and pharmacodynamic models
- Biomedical control systems
- Drug patch design
- The human body as a chemical process

- Environmental cycles (water, carbon, nitrogen, etc.)
- Chemical plant design and operation (refining, plastic, power plant, pharmaceutical, etc.)
- Cell design (human, animal, plant, etc.), DNA replication, RNA transcription, translation, regulation of metabolic pathways
- Product design (need, conception, product engineering, process manufacturing, disposal, life cycle analysis)
- Batch processing for semiconductor manufacturing
- Particulate processes (cell dynamics, aerosols in drug inhalers, smog, crystallization, dispersions, emulsions)

3. IMPLEMENTATION OF THE NEW CURRICULUM

The preceding view that the systems approach is a critical component in chemical engienering is not shared by all faculty. At the first Frontiers Workshop, after the first breakout sessions, different groups reported a long and varied list of proposed changes to the curriculum. Notably, a few groups reported that the subject of process control was high on the "hit list". While process control was not perceived as the only option for elimination, it was disconcerting to see it in such an egregious position. Apparently the value of process control to academic chemical engineers is apparently not as high as many in the control community believe it should be.

In a related article, Cussler et al. (2002) declared that a number of fields like thermodynamics, reaction engineering, transport, and control can be relegated to the scrap heap of "mature technologies" that will not have much future impact in the gain in knowledge. They proposed dropping courses on control and optimization but added several disclaimers: "First, we accept without question the importance of process optimization to commodity chemicals. Secondly, we recognize that process control has a key role in ensuring the success of those other cornerstones of competitive advantage in specialty product manufacture; safety, consistency and quality. Our third hesitation stems from our unwillingness to sacrifice any of our technical core to less-quantitative business ideas. Still, we recognize that a large part of our future is going to be in areas where different skills are needed". This article has sparked spirited discussions in many departments who are considering curriculum change.

Industrial chemical engineers seem to have little doubt that process control is important to keeping modern chemical plants operating, a view that was articulated by several industrial attendees at the Frontiers Workshops. Perhaps the disconnect between the two positions is how the typical faculty member views where employment opportunities will reside in the future, say in 2020. If chemical engineers are not involved in making value-added "stuff" at a desired quality level, the contribution of chemical engineering to the national economy will undoubtedly be greatly reduced.

Perhaps the current emphasis of the typical process control course that heavily focuses on Laplace transforms, analytical solutions to linear differential equations, linear algebra, frequency response, and multiple methods to tune a PID controller needs to change. Computer simulation should not take a back seat to theoretical analysis. In fact the availability (since 1998) of computer-based tools such as Simulink in MATLAB or Control Station (www.controlstation.com) has completely changed the way in which process control can be taught.

3.1 New Educational Materials in Process Control

It is clear that a system viewpoint is very important for dealing with biological processes and biotechnology. Unsteady-state behavior and feedback control are important concepts in living systems, and any organism that is at steady-state is dead (arguing for an understanding of dynamic process models).

The topics I cover when I teach process control include dynamic behavior (with about one lecture on Laplace transforms and analytical solutions to ODEs), physical and empirical modeling, computer simulation, measurement and control hardware technology, basic feedback and feedforward control concepts, and advanced control strategies. Many of these topics can be presented to reflect applications in biochemical or materials engineering. More emphasis could be placed on modeling, optimization, and data analysis/statistics in a revised course. Unfortunately existing textbooks (including one I have co-authored) mostly use examples from continuous processes in petrochemical plants (vs. batch specialty products). Therefore it is valuable to introduce different examples to emphasize principles that are relevant to non-traditional applications.

Three process control textbooks contain a number of examples and exercises that illustrate applications of process control to biological engineering as follows:

(1) Ogunnaike and Ray (1995): drug delivery, blood pressure control, bioreactors
(2) Bequette (2003): biochemical reactor, pharmacokinetic models, drug delivery, blood glucose control, blood pressure control
(3) Seborg, Edgar, and Mellichamp (2004): fed-batch bioreactor, drug delivery

Below is an example of an open-ended homework problem recently assigned in the process control course at the University of Texas that helps the student understand the difficulty of control in a biomedical application. The problem statement is as follows:
Diabetes Mellitus is characterized by insufficiency of the pancreas to produce enough insulin to regulate the blood sugar level. In Type I Diabetes the pancreas produces no insulin, and the patient is totally dependent on insulin from an external source to be infused at a rate to maintain blood sugar levels at normal levels. Hyperglycemia occurs when blood glucose level rises much higher than the norm (>8 mmol/L) for prolonged periods of time; hypoglycemia occurs when the blood sugar level falls below values of 3 mmol/L. Both situations can be deleterious to the individual's health. Hyperglycemia can lead to blindness, kidney failure, and other complications on a long-term basis. The effects of hypoglycemia are more critical on a short-term basis, leading to loss of consciousness and coma within a few hours. The normal range of blood sugar in a healthy patient should staty between 3.8-5.6 mmol/L, the target range for a controller regulating blood sugar.

A Type I Diabetic needs your help to maintain her blood sugar within an acceptable range (3 mmol/L < glucose < 8 mmol/L). She has just eaten a large meal (a disturbance) that you estimate will release glucose according to $D(t) = 0.5\ e^{-0.05t}$, where t is in minutes and D(t) is in mmol/L-min. She has a subcutaneous insulin pump that can release insulin up to 115 mU/min (mU = 10^{-3} Unit of Insulin). The flowrate of insulin is the manipulated variable.

A model of her blood glucose level is given by (Lynch and Bequette, 2002; Bequette, 2002):

dG/dt = -P1 * (G - G_basal) - (X - X_basal) * G + D;
dX/dt = -P2 * (X - X_basal) + P3 * (I - I_basal);
dI/dt = -n * I + U / V1;

where P1, P2, P3, V1, n are constants. G, X, and I are values for glucose concentration in the blood (mmol/L, insulin concentration in the body (mU/L), and plasma insulin concentration, respectively. Basal values refer to the initial values for each one. G_basal = 4.5 mmol/L and X_basal = I_basal = 15 mU/L. D is the rate of glucose release into the blood (mmol/L-min) as the disturbance. U is the flowrate of insulin (mU/min) as the manipulated variable.

This model is implemented in a MATLAB function 'blood_glucose.m'. You can calculate the glucose response by calling an integrator in MATLAB, such as ode45. Appropriately label any graphs that you produce.

(a) What will happen to her blood glucose level if the pump is shut off initially?
See Figure 1 for the solution.

(b) What will happen to her blood glucose level if the pump injects at a constant rate of 15 mU/min?
See Figure 2 for the solution.

(c) Is there a constant infusion rate of insulin that will help her stay within an acceptable glucose range (3mmol/L < G < 8mmol/L) for the next 400 minutes?

By trial and error, the students can determine that a constant rate strategy will not work, which leads to the need to develop more elaborate control strategies. Student reaction to this example was quite positive, especially because some of them had diabetic relatives. About one-third of the class is taking a "bio"-emphasis in their course selection for the B.S. Ch.E. degree, but even for students in the traditional curriculum this type of problem is quite understandable. Developing new educational materials such as proposed in the NSF workshops will certainly add to the base of interesting control applications. In addition, a CACHE task force on Biosystems, chaired by Frank Doyle, will be developing educational materials in this area.

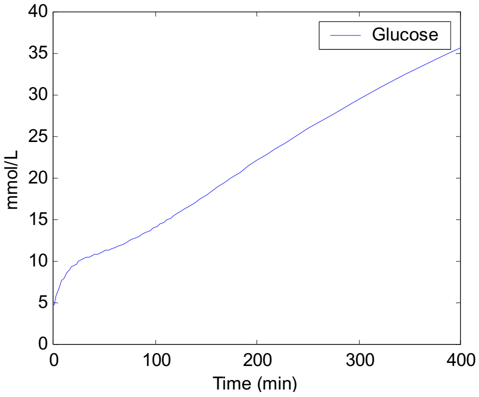

Fig. 1. Effect of No Insulin Flow on Glucose After Meal Disturbance.

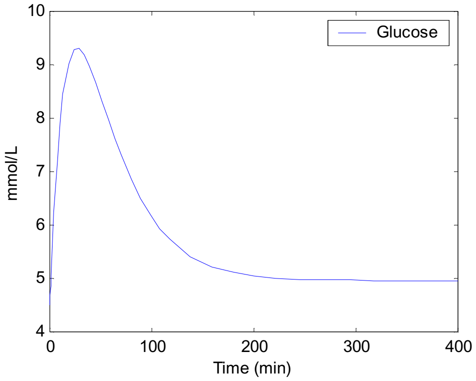

Fig 2. Glucose Dynamic Behavior with Constant Insulin Flow After Meal Disturbance.

CONCLUSIONS

Most educators agree that a systems viewpoint is valuable for chemical engineering graduates. Dynamics, feedback, and stability are intellectual underpinnings required for understanding many new and complex systems of interest to chemical engineers. Control, like design, can be taught in a way so that students must integrate knowledge from other core ChE courses in process modeling and analysis of process behavior. There are not many courses in the curriculum that fulfill these needs. New educational materials should be developed to augment the limited number of examples and exercises in existing textbooks.

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