Session 1: instructional modules
Wednesday afternoon, 2003 June 11

PRESENTATIONS

Presentations by Sureshkumar, Edgar, and Westmoreland described current and proposed instructional modules that cut across boundaries in the present curriculum. Titles and abstracts are listed here; the presentations are contained in separate files.

Providing Multiscale Engineering Experience to Undergraduates

R. Sureshkumar
Washington University

The overall behavior of real systems is governed by the mutual interactions of physico-chemical and biological processes that take place over a wide range of length and time scales. For example the successful design of a drug delivery system requires considerations involving drug dissolution at the microscale, diffusion and transport of the drug over the blood stream at the macroscale and the affinity of the drug to reach the intended target organs defined by its properties at the molecular scale. The time scales involved also vary from hours or days it takes for the drug to dissolve, to minutes it takes to transport the drug to the target organ and seconds it takes it to react or interact with the cells.

Multiscale engineering, i.e., engineering of systems in which the properties or performance of the final product or process depend on phenomena that occur at different length and time scales, has emerged as a paradigm for engineering practice for the 21st century. The research and development sector has been placing overwhelming emphasis on interfacing engineering and computer science to biology and nanoscale physics and chemistry. This has sparked research aimed at the integration of physico-chemical and biological phenomena that occur at *nano* (e.g. molecular interactions, genetic mapping), *micro* (e.g. biopolymer physics, supra-molecular structures), *macro* (e.g. human body, pharmaceutical production, plant scale engineering) and *global* (e.g. fate of chemicals produced, environmental impact) scales to develop, novel therapeutic agents for hitherto incurable diseases and high performance materials for resilient structures, and to improve existing technologies by enhancing productivity and energy efficiency while minimizing environmental impact.

The success of emerging and future technologies and their potential to improve our quality of life depends largely on the creation of a workforce that is well equipped to tackle the challenges of modern engineering practice requiring the utilization of cross-disciplinary expertise in highly collaborative environments. The solution of modern engineering problems requires the establishment of faithful models that link seemingly uncorrelated phenomena that occur at disparate length and time scales. How can we equip our students to tackle such problems? This presentation will try to identify challenges confronting the introduction of multiscale engineering analysis and design into the core curriculum. Solutions will also be proposed.

Batch Processing Module

T.F. Edgar
University of Texas

Batch processing is widely used to manufacture specialty chemicals, metals, electronic materials, ceramics, polymers, food and agricultural materials, biochemicals and pharmaceuticals, multiphase materials/blends, coatings, and composites - an extremely broad range of processes and products. Batch processing is a topic that is currently under-emphasized in most chemical engineering courses and textbooks.

In batch processing, a sequence of one or more steps, either in a single vessel or in multiple vessels, is performed in a defined order, yielding a finished product (usually a complex molecule or material) of a specific quantity. Because the volume of product is normally small, large production runs are achieved by repeating the process on a predetermined schedule. The key challenge for batch plants is to consistently manufacture each product in accordance with its specifications while maximizing the utilization of available equipment. Typically it is not possible to use blending operations in order to obtain the desired product quality, so product quality specifications must be satisfied by each batch.

This module is intended to provide an introduction to batch process operations. Content to be covered intersects with process design/operations, process control, process safety, reaction engineering, and biochemical engineering. This module also emphasizes applications in non-traditional industries rather than chemical/petrochemical sectors. First we introduce the operational practices and control system design for batch plants, which differ markedly from continuous plants. Batch control systems operate at various levels:

- batch sequencing and logic control
- control during the batch
- run-to-run control
- batch production management scheduling

Batch operations include a number of unique features that are distinct from continuous processing. Sequencing of control steps that follow the recipe involves, for example: mixing of ingredients, heating, waiting for a reaction to complete, cooling, or discharging the resulting product. In addition to discrete logic for the control steps, logic is needed for safety interlocks to protect personnel, equipment, and the environment from unsafe conditions. Detection of when the batch operations should be terminated (end point) may be performed by inferential measurements of product quality, if direct measurement is not feasible.

Recipe modifications from one run to the next are common in specialty chemicals manufacture. Typical examples are modifying the reaction time, feed stoichiometry, or reactor temperature. When such modifications are done at the beginning of a run (rather than during a run), the control strategy is called batch-to-batch or run-to-run-control. Run-to-run control is frequently motivated by the lack of on-line measurements of the product quality during a batch run (the product can be analyzed by laboratory samples at the end of the run). Run-to-run control is commonly employed in the semiconductor industry.

Batch process modeling also offers a rich variety of alternatives to be considered by the instructor. Bioreactors can be operated in batch or semi-batch modes. Many polymer or crystallization systems are described by population balances. Also batch processes do not operate at steady-state, hence there is a need to cover fundamental models for batch reactors and distillation columns because linearized models are not feasible. In the area of semiconductor manufacturing, there are many types of equipment that carry out such operations such as etch, lithography, and deposition that are of interest to chemical engineers.

A Course to Tie Chemical and Molecular Principles into Chemical Engineering

Phillip R. Westmoreland
University of Massachusetts Amherst

At its heart, chemical engineering is centered around applying chemical principles to practice. Increasingly, these are molecular principles. Undergraduate chemical engineering students routinely take six or more chemistry courses, but often they do not learn how these principles are part of engineering. Because molecular biology and biochemistry are seldom parts of the core ChE curriculum, students seldom see how chemistry is the underpinning of modern life sciences. Graduate students meet the same limitations. One way to re-center the profession around chemistry is to remark on these principles throughout the curriculum, but a new chemical engineering course is necessary to establish this linkage firmly.

I will describe a course developed at the University of Massachusetts with the central idea of understanding and exploiting the chemical principles of engineering. The course provides both continuum and molecular perspectives using theoretically based correlations and molecularly based modeling, including statistical mechanics, computational quantum chemistry, and molecular simulations. It has been taught both as a UG/G and as a graduate course.

WORKING GROUPS

After the presentations, workshop participants were divided into six working groups, charged to develop instructional modules suitable for freshmen, sophomores, juniors, seniors, laboratory, and cross-year experience. Their reports are given here.

Group 1 (a module for freshmen)

Characteristics that Modules should have

a. Attributes
    - Quantitative: include data collection and/or analysis
    - Societal relevance/ethical issues
    - Lab/lecture(s)
    - Encompass variety of concepts
    - Transferable
    - Chemistry
    - Scalability
    - Economics

b. Outcomes desired
    - Perspective of profession and possibilities/concepts that will be developed later
    - Chance to do something new
    - Faculty involvement in recruiting
    - Teamwork
    - Links to other disciplines

c. Examples
    - CO_2/global warming
    - H_2O purification
    - Fuel cells
    - Sensors
    - Food processing
    - Sunscreen
    - Drug delivery
    - Dialysis

d. Mechanisms
    - Inside ChE
    - Service courses
    - Time scale/faculty involvement
    - Uses “best” presenters

A Developed Example

TITLE: Water Purification
CONCEPT: Semester-long Module with Subsets

Example topics
- Desalination
- Physical/chemical treatment
- Oil spills

- Disinfection

Provide

- Context
- Objectives
- Metrics
- Multiple scales
- Other impacts

Include

- Physico/chemical principles - σ, ρ, Δp, ΔH, pH
- Process/Hardware choices
- Economics
- Environmental issues
- Safety

One example: solution chemistry; pH measurement; CO_2/H_2O chemistry
applied to hard water treatment

Discussion

- Module could be variable-length: a full semester or subsets. It could actually transport the topic to a freshman chemistry course
- Is this too complex a topic for freshmen?
    - need to keep at appropriate level
- What will the students' memory be 2 years later, versus the stated 'desired outcomes'?
    - The concepts will be reinforced in later years.

Group 2 (two modules for sophomores)

1. Molecular/Multiscale
    - Concepts: 1st Law/2nd Law
    - Molecular Basis of Energy/Entropy
    - Qualitative Molecular Bonding/Forces

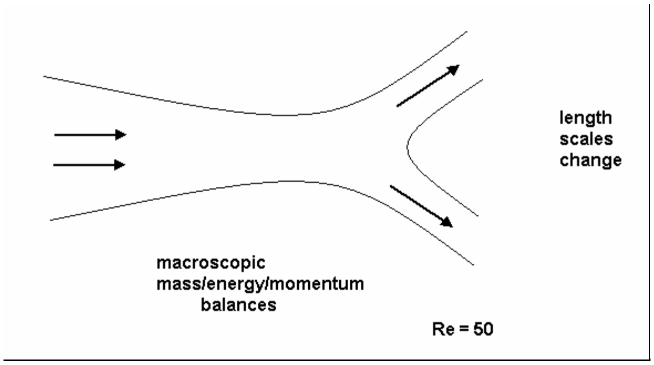
2. Systems/Lab
    - Build Model for an experimental dynamic system
    - Collect and Analyze Laboratory Data
    - Build Numerical Simulation
        - Differential equation.
        - MATLAB (?)
        - Parameter Estimation (from messy data, including uncertainty estimates)
    - Construct Equipment/Sensor
    - Presentation/Teamwork experience
    - Different Groups do different experiments.

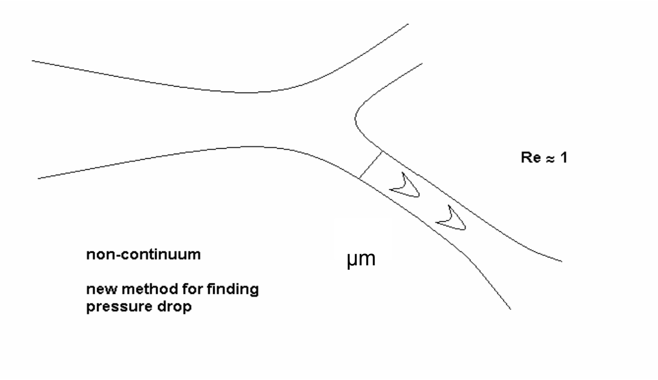
Discussion

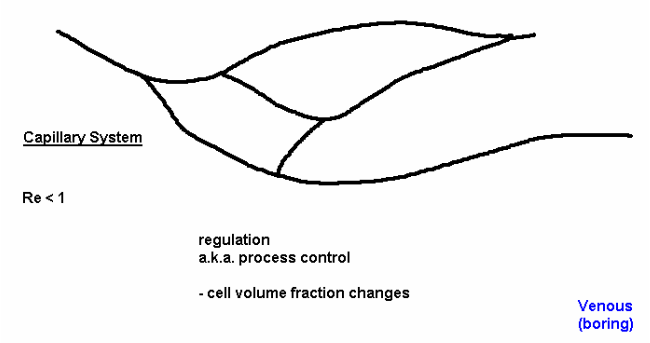
- Can sophomores actually build things?
    - Use simple (non-breakable) materials.
- One person used LEGO for a lab project.
- The systems module would include a transient component – one accumulation term.
- It's intended as a 1-semester course.
- Choose the appropriate level of model difficulty.
- The goal is to provide the whole picture to a sophomore – a complete exercise in modeling and data fitting

Group 3 (a module for juniors)
Multiscale Systems Analysis of Human Circulation:
Chemical Engineering Principles and Applications

<u>Cycle 1</u>
Ventricle → pressure, incompressibility
Aorta → laminar flow in a tube
Composition and material properties of blood → pressure drop, shear stress, work; Re=10^3;







<u>Cycle 1a</u>
Pulmonary

- O_2 carrying
- Henry's "constant"
- Mass transfer
- Air flow - bronchiole system
- Gas exchange – composition
- hemoglobin
- CO

<u>Cycle 2</u>
Blood goes to specific organs

- Kidney – separation
- Liver – plug flow *reactor* with enzyme kinetics
- Brain – brain/blood barrier

- Muscle – energy metabolism

<u>Cycle 3</u>
System Modeling
Applications –

1. Drug delivery
2. Alcohol metabolism
3. Snake venom

Predicting time response (Pharmacokinetics)

<u>Cycle 4</u>
Flow Separation

- Shear stress effects on cells
- Molecular biochemistry
- Mechanicosignal transduction
- Plaques

Aneurysm – flow disturbance

- Stents
- Grafts
- Biocompatibility

Issues:

- Is this a vehicle for <u>introducing</u> or <u>applying</u> principles?
- Limited or unlimited?
- One module or more?
- Example of using a system to build a narrative

Discussion

- Consider blood flow in other organisms, as well – the brontosaurus for change of scale
- What would the biomedical engineering profession present on such a topic?
  - less quantitative
  - they are becoming increasingly quantitative.
- Emphasize the question of how to position this module: for example, does it introduce fluid mechanics to the students, or does it depend on a previous presentation of fluids?

Group 4 (a module for seniors)

Senior Project Plan

Semester 1 - two courses in parallel (1-2 faculty)

- Static Design & Optimization
- Process Dynamics & Synthesis

Semester II - Long-term Project (multi-faculty teaching)

- Process/Product Design alternatives:
    1. Product Design, the Process to make the Product
    2. Two case studies – Process & Product

There is a need for "fully worked out case studies"

Product and Process Design Project

- Economics
- Safety
- Marketing
- Environmental impact (green engineering)
- Life Cycle Analysis
- Optimization
- Molecular Modeling/insight
- ABET a-k, current issues
- Sensitivity ("what if…" analysis)
- Dynamics
- Globalization
- Industrial interaction
- Multi-institution
- Multi-disciplinary
- Multi-faculty
- Real industrial problems
- Technology specific [bio, electronic, environmental, etc]

Sample Case Studies

- Functional coatings
- Lab on a chip
- Intracellular product
- Water decomposition cycles
- H_2 storage

Group 5 (a module for laboratory experience)

Undergraduate Laboratory

"Super Lab": Labs involving teams across years (freshmen → senior)
- Utilize material from "core": molecular, multi-scale, systems
- Multiple modules involving the same concepts (different industry sectors) (enzymes, food, microreactors, …)
- Introduce competitive spirit (?)
- Presentation, communication, writing skills
- Replace, or integrated with design?

Modular labs
- Remote laboratories accessed over the internet/intranet (I lab)
- Virtual experiments
- Easily integrated into courses
- Nationally distributed
- Illustrative of concepts

Examples
- Fluid flow
- Heat exchange
- Crystallization (phase behavior, in general)
- Reaction
- Mass transfer

Discussion
- Suggest a lab for developing troubleshooting skills

Group 6 (a module for Cross-year Experience)

Proposed #1

Multi-level (Freshman-Senior) and multi-disciplinary design experience

- Empowers lower level students to contribute
- Each level must have some knowledge or skill of value to the group
- Realistic/industrially relevant projects w/scope that allows multi-level analysis
- Limit size of teams
- Need a plan to evaluate or grade the students
- Need to assess the educational pedagogy

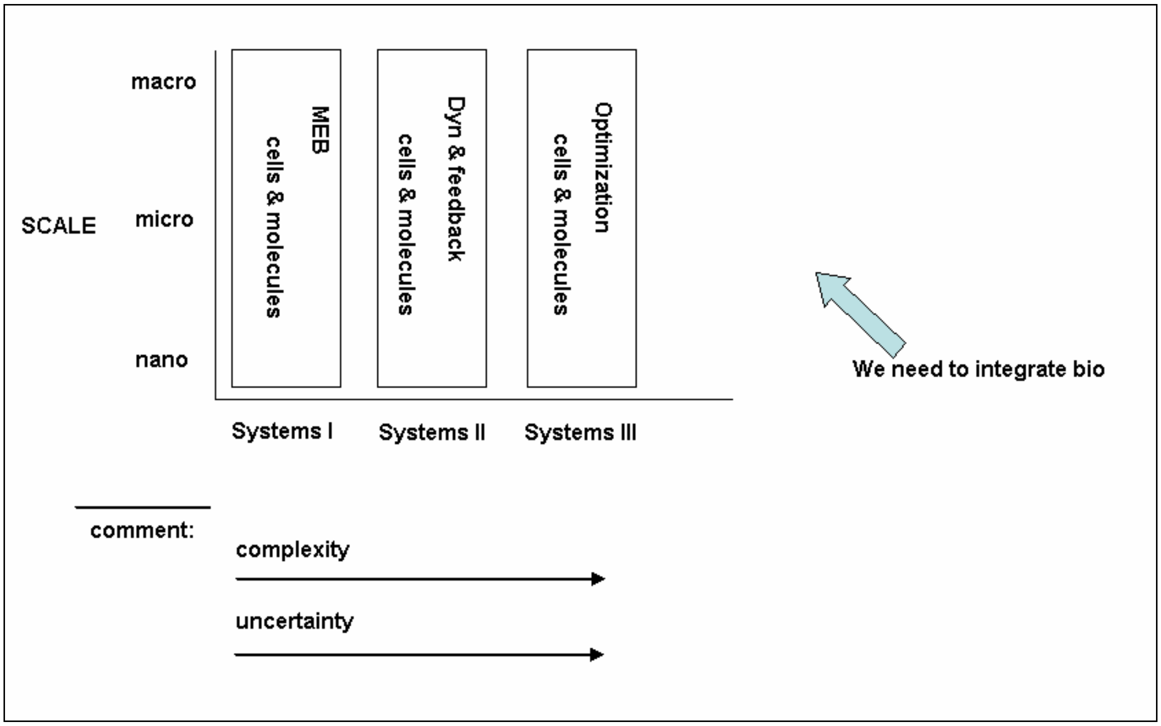
Proposed #2

Multi-dimensional system approach

- Dimensions: economic impact, safety, health, environment
- System dynamics connected to content area or application
- Chem-Bio Systems I (Material and Energy Balances)
- Chem-Bio Systems II (Dynamics & Feedback)
- Chem-Bio Systems III (Optimization)

Examples

- Nano materials
- Cell as a chemical plant
- Virus that mutates
- Artificial kidney
- Liver
- The earth



Discussion

- Various ways to structure the multi-class partnership. For example, have juniors and freshmen be partners; they then become senior-sophomore partners in the following year. A single design project may cover two years, therefore.
- Such a scheme could be deployed as a short project, a full semester, or a year +.
- Such a scheme could also be used as a design component in each year's technical courses.

Supplementary Notes from Group 6, extending the report given above

1. Introducing biological engineering into ChE (threaded curriculum)
    - First course asks students about the analogy between chemical plant and cell
    - Second course introduces thermodynamics into its topics
2. In lab, justify threaded curriculum by examining a chromo - sophomores through seniors do the lab
3. Vertically integrated team design projects (situated learning)
4. Course sequence on chemical and biological systems - main objective is to teach core concepts:
    - steady vs. transient
    - batch vs. continuous
    - open vs. closed loop
    - data vs. prediction/model
    - certain vs. uncertain
5. Make the design project the same for a given class of students - revisited year after year
6. Get freshmen hooked on chemical engineering. Look at the earth as a system with multiscale phenomena and then longitudinally move into more depth in their analysis. We can check their understanding of the concepts as they progress.
7. Honors thesis. Perhaps get ideas from this and break it into fresh ideas…
8. Use fuel cell as thread. Topics can change, but what is missing is depth. So repeating may yield depth in understanding.
9. Student competition problems. Have a multiyear design of both product and the corresponding process.
10. Extend this idea to the multilevel analysis of a phenomenon. Perhaps Jr-Sr collaboration.
11. Each freshman is mentored by a junior, and then continued to the next year. Thus every student is involved in 2 projects for 2 years.
12. Beer-brewing experiment for sophomores and seniors - many chemical and biological elements
13. Service learning project with the outside community

Comments/assumptions

- students need realistic projects to motivate them
- we are missing multi-disciplinary approaches
- have some prior experience with non-engineers contributing
- industry needs engineers with the ability to work on teams, on problems that are ill-defined, who can speak to the impact (economic, environmental, societal)

  - How can we embed the core knowledge of concepts and phenomena into the design or experiment-based learning opportunities?
  - The experiment-based learning project must allow faculty to check the students' understanding of underlying concepts. Difficult to separate individual and team contributions
  - Should the Fr-Sr idea allows the development of student portfolios where they can keep track of things learned?
  - Why can't students learn on their own from a web module? Need to measure the student's performance based on faculty expectations, perhaps without teaching
  - students need very interesting things to learn to motivate them and maintain positive attitude

Discussion on Session

- After seeing these examples, the content of course units is now becoming clearer.
- This looks like a LOT of work to develop these new course units.
- Extraordinary, fantastic group creativity
- How to ensure that everything important will actually have a place in the curriculum?
- Do the industry people agree?
  - Shell – their themes of teamwork, messy data, communications are being included
  - Merck – these modules are NOT dropping fundamentals, they are giving students the practice in applying them. The student arriving in industry, being shown a problem won't have to be told whether it's a transport or a thermo problem, but will be accustomed to analyzing systems and solving problems.
  - Pfizer – these proposals seem to focus on applications
- These modules will require a high workload and lots of money. Would it be better to phase in gradually?
- These modules did not feature much about molecules – but see the lab module.
- Ultimately, of course, we need to ensure complete coverage of subject area.