Session 3: definition of the curriculum
Thursday afternoon, 2003 June 12

Workshop participants were divided into six groups to define the curriculum content. Three groups worked on the three organizing principles, a fourth examined laboratories, a fifth considered supporting courses, and a sixth identified the gaps - what remains to be done. Their reports are given here:

Group 1 (Molecular Transformations)

Sophomore

- Simple Calculations
    - Heat capacity, latent heats
    - Some bio things
    - equations of state
- Classifications of molecules/groups and properties
    - correlations
    - intermolecular forces
    - biomolecules
    - biological binding energies

Sophomore/Junior

- Phase transitions
- Transport properties
    - Polymer/protein conformation issues
    - Mixture properties
- Chemical Equilibrium
- Reaction Rate Theory
    - Diffusion-limited
- Molecular biology

Special Topics

- Self assembly
- Interfacial Phenomena
- Nucleation/growth
- Material properties

Needs

- Parallel examples between Molecular/Multiscale/Systems/labs
- Texts should include the appropriate molecular theory
    - e.g. include kinetics in Reaction Engineering.
- Include self-instruction

Group 2 (Multiscale Analysis)

Topic?

- Application of <u>conservation laws</u> at different length and time scales
  - Outcomes of physical processes depend on scales
  - Scaling up or down
- Year 1
  - Introduction of scaling laws
  - Dimensional analysis

Year 1	Year 2	Year 3	Year 4
Scaling laws Dimensional Analysis ↓ Intro Course	Nano-tech ↓ Assemblies Colloids Interfacial Homogeneous Reactor Eng. Could be: • Cell • Atmosphere • μ reactors	Continuum Descriptions Heterogeneous systems Assemblies (Advanced) • Flow • Diffusion • Thermal effects • Colloidal phenomena	Product design (uses multiscale info)

Group 3 (Systems Analysis and Synthesis)

Intro to Systems - Sophomore

- Conservation Laws for simple dynamic/static [mostly] systems
- Statistics and Data Analysis
- Numerical simulation tools
- Experimental Design (including the sensors)
- Plant viewpoint (the product)
- Exposure to complexity, dynamics, uncertainty
- Degrees of freedom

Systems Meets the Molecule – Junior

- Stochastic
- Molecule level reaction as a system
- Design: from molecule to product
- Catalyst deactivation (steady-state feedback?)
- Systems at all scales
- Data analysis/lab
    - Uncertainty, reconciliation
- Simulation as an enabling technology
    - Simulation result as a driver to experiment
- System evolution
- Optimization principles
- Examples: separation, microelectronics

Systems and the Marketplace – Senior

- multi-scale systems
    - resolution at time and length scales
- dynamic analysis and feedback
- use of constitutive equations, etc., for analysis and design
- process and product design (see Session 1, Group 4)
- lab experience
- 'softer' skills
- business skills, entrepreneurship

Interactions with other parts of the curriculum

- math requirements: matrix analysis and ODEs
- molecular dynamics ($F = ma$)
- Monte Carlo (randomness)
    - sensitivity
    - statistics
    - uncertainty propagation (μ vs. σ^2/covariance)
- CFD
- molecular and multiscale
    - are there design elements?
    - how much understanding of software manuals?

- Where are
  - reaction engineering?
  - separations?
  - physical property prediction (pure component properties as functions of T)?

<u>Miscellaneous recommendations, beyond the topic</u>

- Assessment
  - hire experts to measure retention vs time
  - use alumni surveys
  - meet again in 2020s to assess curriculum
  - what are job opportunities in 2020s?
- Dissemination
  - do as ‘conference style’

Group 4 (Laboratory Experience)

What is the topic?

Undergraduate Laboratory

- Real, Virtual, and/or Remote

Objectives/Goals

- Teamwork
- Communication skills
- Dealing with "real" problems/data
- Open-ended problem solving
- Experimental Design
- Integration of course/module material into and via lab
- Safety
- Environmental & regulatory issues

What are the particular needs?

- Develop specific labs/projects (real, virtual, and/or remote)
- Industry input (problem statements)
- "Complete" project (addresses all goals/issues)
- Propose methods for administrative systems/maintenance

How do we measure?

- What do we measure?
    - attainment of goals
- Outside evaluators
- Academic "swapping" of evaluators
- Performance assessments (have the students actually do something)
- "Seek professional help"

Incentives?

- I-Lab sharing system
- Fund development of laboratory experiences
- Reform of reward system
- Recognize contributions as being critically important
- Provide release time for curriculum developers
- TA support/Post-docs

SUPER-LAB

- Come up with *x* projects
- Each project must contain all of the objectives/goals
- Should serve as suitable templates for future projects
- Must contain the major/core curriculum
- Competition
- Cycle through different sector topics (e.g. food, microelectronics, biotech)

MODULAR LAB

- Remote labs/virtual labs combination
- Come up with *y* projects
- Flexibility
- Targeted objectives
- Industry input
- "Industrial remote labs"
- National distribution & collection
- Interactive

Group 5 (Supporting Courses)

Main Points

- Physics: include biophysics, solid state; eliminate relativity
- Chemistry: keep existing except organic synthesis; add analytical/quantitative techniques; delete thermo from physical chemistry, add quantum
- 2 Bio classes:
    - Biochemistry
    - Molecular & cellular Bio
- Computer Science: Excel & visual basic & a math package

Physics	Statics/Dynamics
Chemistry	~~Statistics~~
Biology	~~Circuits~~
Math	~~Economics~~
Computer Science	Management/Business
Materials Science	~~Second language~~
English/Communications	Ethics
Humanities	

Recitation section(s) to supply context for differential equations, chemistry, physics, statistics, biochemistry.

<u>OR</u>

Context supplied by vertically-integrated lab or project.

Supplementary and Supporting Material

<u>Math</u>
• Calculus through ODEs • (minimize analytical integration, derivativation, proofs, series) • Increase emphasis on vectors & tensors • Numerical methods • Linear algebra • Statistics (Design of experiments) • ANOVA, basic metrics, parametric studies

<u>Comp. Science</u>	
~~C++~~ Excel Math package	~~Fortran~~ Visual Basic

Physics	
Electricity and magnetism	~~Astronomy~~
Forces	~~Fluid mechanics~~
RLC circuits	Sound
Waves	Solid State
Optics ~~(lenses)~~	Biophysics
~~Relativity~~	Physics of macromolecules
Quantum Physics	Self assembly
Mechanics	~~Spectroscopy~~
Statistics	Plasmas

Chemistry	
Stoichiometry	Analytical/Quantitative technique
Acid/base	van der Waals
Solution chemistry	Dipole
Atomic structure	Induced dipole
Molecular orbitals	Ionic/ Covalent
Periodic table	Plasmas
Electronegativity	Stereochemistry
Ionization potential	Electrochemistry
Reactivity	Nomenclature
Colloids/dispersions/gels	Molecular reactivity.
~~Thermo~~	Reaction mechanism
Crystal structure	Transition states
Distribution functions	Schrodinger equation.
Quantum mechanics	Hamiltonian
Statistical mechanics.	Solution equilibrium
Monte Carlo	Spectroscopy
Molecular dynamics	Kinetics
Quantum calculations	Mean free path
Radicals	Kinetic theory of gases

Organic Chemistry	
Basic reaction mechanisms	Bonding
Polymers/polymerization	Acid/Base catalysis

Biology	
Biochemistry	Molecular and cell biology

Materials Science
• Multiscale: relate molecular structure to macroscopic properties • Chemistry of materials • Dispersions, colloids

Group 6 (Gaps)

Workshop 1 – Common Themes

- Biology is a foundation science
- Agreement that the need for change goes beyond biology
  - Diversity of employment
  - Public perception
  - Recognition of molecular-level understanding
  - Competition for best students
- Need to engage enabling sciences in change
- Infuse curriculum with contemporary examples that integrate principles of chemical engineering
- Chemical engineering involves analysis, design, and synthesis

Common Themes continued

- Need to articulate to freshmen the intellectual challenges and professional opportunities
- Chemical engineering includes multi-scale descriptions of materials and phenomena
- Agreement on the desired attributes of the chemical engineering graduate
  - Experience in labs
  - Communication skills
  - Problem solving skills
  - Etc …
- Curriculum should be designed for flexibility

Building Blocks – Areas of Agreement

- The enabling sciences are:
  - biology
  - chemistry
  - physics
  - math
- There is a core set of chemical engineering principles
- Molecular level design is a new core principle
- Chemical engineering contains both product & process design
- There is a need for 1st year chemical engineering experience

New Technologies

- Nanotechnology
- Microchemical systems
- Fast science
- New materials
  - Organic LEDs, new coatings, …
- Improvements in processing engineering and science
- Energy production and storage
- Biological science and engineering: food, medical, genetic engineering, …
- Environment
- Information technology – handling large amounts of information

What Chemical Engineers Do

- Use molecular sciences and engineering to create, design and operate products and processes that meet societal needs

Example Problems

- Customize, design, and produce an organic LED to reflect only certain colors
- Design and production of bio-organic computing chips of the future
- Control batch reactors, e.g. deal with large set of data to manageable system

Potential Gaps

- Freshman year experience
- IT
- Ensure coverage of skills and attributes
  - Communication, critical thinking, dealing with uncertainty, fearlessness…
- Do we have a sufficiently broad set of examples to capture modern chemical engineering
- Is there an adequate balance between biology and chemistry as enabling science

Bridges/Problems

- Find the right balance for teaching molecular sciences in chemical engineering vs. biology and chemistry
  - From biology and chemistry – what enables us to create, analyze and manipulate molecules/systems
- Do we have sufficient repetition of key ideas?
- Have we limited our objectives sufficiently to ensure learning can take place?

Actual Gaps

- Phase changes
- Constitutive equations
- Basic experimental skills