Session 1: knowledge, skills, attributes, and examples
Tuesday afternoon, 2003 April 8

Workshop participants were divided into four working groups, each charged to explore the implications of a particular organizing principle. The groups were to specify the knowledge a B.S. graduate should have and the skills required to use this knowledge. Furthermore, the groups were to consider the attributes desired in a B.S. graduate, beyond 'having the knowledge' and 'executing the skills'. Finally, groups were encouraged to think of examples that could be used to illustrate subject matter and cultivate attributes.

Group 1 (Molecular Transformations)

- Chemical Structure
- Phase (Transformation)
  - Intra
  - Inter
- Orientation/Conformational
- Bulk to Surface
- Reversible
- Dipole (Electronic)
- Polymer Extension
- Component Assembly
- Molecular Assembly
  - Atomic
  - Self
- Polymer Assembly
- Direct vs. Indirect Network & Complexity
- Inorganic/Organic/Bio

- Knowledge – Groups of Thoughts
  - Chemical Structure
  - Inter/Intra molecular forces
    - Short/long range
  - Driving forces
    - Entropy
  - Molecular description of reaction
  - Equilibrium concepts
    - Free energy
  - Water is special
  - Electronic structure
  - Analytical methods?
  - Scale up to continuum
  - Differentiation
  - Integration
  - Geometry

    - Differential Equations
    - Stochastic math
    - Catalysis
    - Mechanics/dynamics
    - Waves/Particles
    - Biological info flow
    - Reaction network (interfaces with systems principle)

- Skills
    - Molecular info → EOS
        - Macroscopic behavior
        - Transport properties
    - Calculate thermodynamic properties
    - Order of magnitude estimates for ranking importance
    - Spatial perception
    - Awareness of all time scales
    - Data/error analysis/interpretation
    - Reaction analysis
    - Reactor design
    - Process selection
    - Effective communication
    - Model building
    - Lab skills
    - Critical thinking
    - Knowledge of available information

- Attributes
    - Knows how to learn
    - Thinks critically
    - Desires life-long learning
    - Receptive to new ideas
    - Understands and works with uncertainty and sensitivity
    - Seeks appropriate connections with other fields
    - Thinks like a molecule

- Application Examples
    - Water Desalination
    - Design for Self Assembly
        - Polymer coating
        - Nanotechnology
        - Hybrid systems
    - Design of Membranes
        - Next generation beer bottles
        - Fuel cells
    - CO_2 Emissions from vehicles
    - Stationary Source Emission Abatement

- Bioartificial Pancreas
- Protein Expression
- Make Polystyrene Peanuts from Raw Materials
- Drug Delivery

Group 2 (Quantitative Analysis)

- Knowledge
  - Numerical Methods
  - Differential Equations
  - Calculus
  - Probability/Statistics
  - Conservation Laws
  - Population Distributions

- Skills
  - Translate Physical Descriptions into Math-based Equations
    - Applying conservation laws
    - Knowing when to use what model
    - Knowing when to neglect things
  - Model testing and validation
  - "What if" explorations
  - Sensitivity/uncertainty analysis
  - Scaling analysis
  - Order of magnitude analysis
  - Economic analysis
  - Computer-based skills
  - Use of analogies

- Attributes
  - Makes rational assumptions
  - Communicates qualitative concepts
  - Determines important parameters
  - Applies skill set to open-ended and novel problems
  - Determination of properties within equations using measured data
  - ~~Computer implementation~~
  - ~~Regression analysis~~

- Applications/Examples
  - Develop understanding of physical process
  - Blood flow in body
  - Formulating and solving balance equations
    - Mass
    - Energy
    - Momentum
    - Population
  - Using a model to:
    - Determine most important physics
    - Make a prediction
    - Scale-up
  - Analysis/compare experiment w/model predictions
  - Handling "messy" data

- Teach quantitative skills through examples
- Product, process, and experimental design
- Mass and energy balance of CSTR
- Plot Arrhenius data from experimental data
- Trouble-shooting
- Quality control
- Economic & market analysis

- Miscellaneous
    - What constitutes a reasonable solution to a problem?
    - Is this really problem-solving?
    - Environmental impact
    - Governmental regulations
    - Extent of numerical vs. software skills
    - McMaster problem-solving skill set

Group 3 (Multiscale Analysis)

- Framework:
    - Different phenomenological scales: e.g.:
        - Length
        - Time
        - Environment
        - Economic
    - In problems from varying enabling sciences:
        - Physical
        - Chemical
        - Biological
- Goals:
    1. Define problem and work solution to appropriate scale(s).
    2. Develop an appropriate "model" to solve problem.
- Means:
    1. Knowledge of phenomena at different scales
    2. Recognition that multi-scales are ubiquitous
    3. Heuristics to choose scales at which to analyze – Occam's razor
    4. Key assumptions
    5. Matching and integration of scales

- Knowledge (not yet in curriculum explicitly)
    1. Molecular dynamics
    2. Stochastic processes (random walks)
    3. Quantum mechanics
    4. Interactions and packings of atoms/molecules
    5. Biological sciences
    6. Geometrical similarities (scaling)

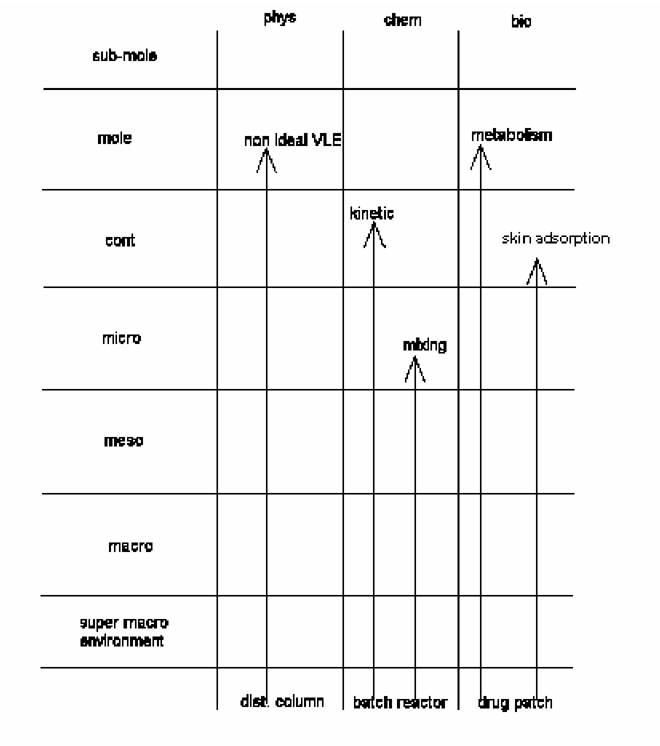
- Skills (not yet explicitly covered) (also in previous Means bullet)
    1. Simplification of mathematical models
    2. Probability and statistics

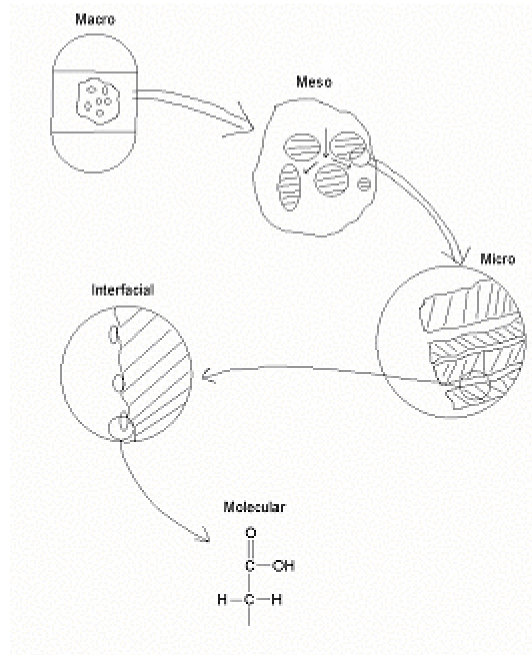
- Attributes
    1. Prudent risk-taking
    2. Keeping it simple
    3. Where does ChE fit in globally?

- Future applications
    1. Lab on a chip
    2. Miniaturization of ChE
    3. Nano drugs

- Examples
    1. Design of Distillation Column → Molecular modeling of Non-ideal phase equilibria

2. Chromatographic Separation of Proteins – all scales
3. Catalytic and/or multiphase reactor design
4. Drug Patch design





Group 4 (Systems Approach/Synthesis)

- Applications Examples (Organizing Framework and Context)
    - Hydrogen from biomass
    - Climate change
    - Viral infections
    - Atomic Layer Deposition
    - Controlled particle formation
    - +15 Others

- Attributes of Example(s) (and Systems Viewpoint)
    - Need to feel comfortable with
        - Incomplete information
        - Multiple (often conflicting objectives)
        - Multiple solutions (and multiple paths to solution)
        - Iterative problem solving
        - Incorporation of uncertainty
        - Managing complexity
        - Risk taking
        - Rapid generation and pruning of alternatives
    - Social Responsibility (Broadly)
    - Driven to add value

- Skills Needed
    - How to treat and analyze data
        - Multivariate analysis
        - What data to acquire?
    - Integrate Knowledge
        - From chemistry/biology/physics/mathematics
        - Other fields
    - Team work
    - Time (and resource) management
    - Active learning
    - Critical thinking

- Knowledge
    - Basic Systems Analysis Tools
        - Mathematical modeling and simulation
        - Feedback and recycle
        - Optimization
        - Control
        - Dynamic systems
    - Financial Analysis
    - Statistics and Experimental Design

- Challenges and Discussion

  - Lots of overlap with topics/examples from other groups; systems concepts are everywhere
    - How to integrate?
    - Where in the curriculum?
  - Need for broader faculty participation
    - How?

- Supplementary Application Examples (generate excitement for ChE as a profession - pick an area where ChEs work, and pick a major example)
  - metabolic systems
  - drug delivery
  - artificial organs
  - semiconductor unit processes
  - aerosols, carbon nanotubes, etc.
  - reaction /diffusion system
  - heterogeneous system
  - defense against chemical warfare
  - protein and cell catalysts
  - synthetic biology - biosensors, tissues
  - substitute for MTBE
  - buy a chemical company
  -
- Supplementary Notes
  - all examples integrated into curriculum
  - use shared instruction
  - relate educational goals to students
  - use systems approach to frame the ChE curriculum
  - the students need to know they must add value!
  - students must have the ability to relate to normal humans
  - we must educate the faculty

Group reports – Audience Feedback

Group 1 (Molecular Transformations)

- Include some quantum mechanics

Group 2 (Quantitative Analysis)

- Add optimization w/r/t handling "messy data"
- Get students to recognize what's being neglected for later evaluation

Group 4 (Systems Approach/Synthesis)

- Bioinformatics could contribute to systems teaching
  - Similarly, ChE systems could inform bio systems
- Need interesting applications to teach systems
- Want core tools to present systems, not dispersed to other areas

General Discussion

- Sum of this material greatly exceeds a B.S. degree
- We must make decisions and choices to form a curriculum
- How to make materials transferable so that multi-faculty can teach?
- This is a challenge, but worthwhile to pursue
- Great principles; mismatch with present curriculum → opportunity and lots of work
- Examples cut across organizing principles
- Examples can cut across – so there is lots of opportunity
- This material reminds of research; therefore more interesting to teach
- Remember that students must be interested, too
- Can't control what other departments offer in service courses → a constraint
- Service departments may be able (and willing) to modularize
- The example of med school – teach in short, intense blocks
- How to come up with textbooks?
- Textbooks may become virtual – modifiable, adaptable – assembled from modules ad hoc
- Design/synthesis problem presented early, motivating subject matter study, before returning to design
- Will radical curriculum reorganization affect the hiring process?
- the curriculum should change, because industry has changed

Reflections on Session 1 Work - gathered Wednesday morning, 2003 April 9

- Outcome – how to implement?
- Flexible – according to department needs and mission
- This curriculum is not so radical, yet
- Plan to engender acceptance?
  - e.g. trial runs at particular schools?
- Describe at AIChE?
  - Discuss at Cape Cod Workshop
- There is indeed curriculum variability at present
- Need follow-on workshops to promote new curriculum, convert faculty to the new materials
  - 10 years required?
- Should we propose incremental or sweeping revision?

- Industry stakeholders – should they review changes?
- Discuss with lots of industry segments; each WS participant could do this now.
- Early, frequent, diverse discussions will help
- WS I too premature to communicate. WS II may be better
- WS I key – bio, molecular design is new principle.
    - Some faculty ambivalent.
- Striking result of WS I – consensus that all ChE students should study biology
    - Now convinced that bio IS important
    - Fidelity of message is IMPORTANT
- SUGGEST POWERPOINT SLIDES for use in communicating
- Satellite link in Cape Cod workshop?
    - As means to inspire others
- AIChE forum – standalone, or keynote
    - In San Francisco meeting? (Nov)
    - Sunday afternoon time slot
    - Have large segment of WS participants at meeting with AIChE
- Amundsen report said to have made a difference – can we do as well?
- Tirrell report focuses on research – some connection with our work