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 \(\rightarrow\) 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
  • \(\text{CO}_2\) Emissions from vehicles
  • Stationary Source Emission Abatement
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- Bioartificial Pancreas
- Protein Expression
- Make Polystyrene Peanuts from Raw Materials
- Drug Delivery

Session 1: content
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
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**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
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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