Session 3 - Status of the Academic Theme Areas

The academic participants met in five groups, three representing the organizing principles of Molecular Transformations, Multiscale Analysis, and Systems, and two others representing curriculum components of the Laboratory, and the First-Year Experience. Each group was to assess the state of development in its area.

Molecular Transformations

<u>Developed Approach – Work to Date</u>

- Analyze physical / chemical / biological process
- Use this to develop new products and processes
- Integrate throughout curriculum
- e.g. structure-property relations (statistical mechanics)

<u>Present</u>

- What about classic plant operation?
- Distinguishing character of Chemical Engineering is molecular transformations
- Reason for current syllabi
- Rely on other Organizing Principles for other topics
- Is the terminology "molecular transformations" good – does it express what we want it to? Does it show a problem focus? Does it contribute to the engineer's understanding of plant operations?
- * Strong need for eng.

<u>Basic concepts</u>

- molecular basis of thermodynamics
- entropy
- equilibrium
- conservation systems
- quantization
- activated processes
- mixing
- ideal/non-ideal
- $e^{-\beta Ei}$
- mass-energy balances
- electrostatics physics

<u>Physical Molecular Transformations</u>

(1) – highest priority, (2) – middle priority, (3) lowest priority

- (1) statistical mechanics
- (1) Quantitative structure-property relationships
- (1) structure/ property relationships

- (1) constitutive equations (molecular basis of)
- (1) equations of state for gas, liquid, solid phases
- (1) interaction forces/ quantum mechanics/ hydrophobic-hydrophilic
- (1) kinetic theory of gases (concept)
- (2) surface adsorption
- (2) assembly of molecular structures, micellization, conformation, co-polymers
- (3) solid state crystal structures
- (3) kinetics of phase transitions

<u>Chemical Molecular Transformations</u>
(1) – highest priority, (2) – middle priority, (3) lowest priority

- (1) Organic chemistry
- (1) Quantitative structure-activity relationships
- (1) Rates, TST, etc.
- (1) Acid – base
- (1) Catalysis
- (2) Surface chemistry/ catalysis
- (2) Quantum mechanics. – molecular orbital chemistry, etc.
- (2) Reactivity
- (2) polymerization
- (3) chirality

<u>Biological Molecular Transformations</u>
(1) – highest priority, (2) – middle priority, (3) lowest priority

- (1) basic biochemistry
- (1) biological quantitative structure-activity relationships
- (1) enzymatic catalysis (bio/chem.)
- (2) recognition/ binding
- (2) metabolic eng./ dynamics
- (2) systems biology (systems)
- (2) protein structure 1,3 3, 4
- (3) protein folding/ denaturation
- (3) ion channels
- (3) molecular motors
- (3) drug design
- (3) cryopreservation
- (3) fermentation
- (3) directed evolution
- (3) combinatorial chemistry
- (3) bio/ chemo informatics
- (3) sensors

<u>Curriculum Structure</u>
Present material from all areas in each year, but with increasing complexity. For example,

Freshman

- mass-energy systems
    - Examples that feature molecular content
        - Fuels
        - 6H potential
        - Molecular simulation
        - Ultrafiltration of bio-fluids

Sophomore

- Physical molecular transformation
    - Continuum & statistical thermodynamics, integrated and including non-ideal behavior
    - Unimolecular → bimolecular
    - Quantitative structure-property relationships
    - Interaction forces
- Some activated processes/ kinetics
    - Kinetic theory of gases, as needed, timed w/multiscale
- Qualitative understanding

Junior

- More complex continuum and statistical thermo
- Bimolecular → multiple body
- Rates and TST
- Molecular origin of constitutive equations
    - Many-body
- Hydrophobic/philic

Senior

- Biological quantitative structure-activity relationships
- Catalysis
- hydrophobicity

Multi-scale Analysis (and Design)

from basics to processes to profits...

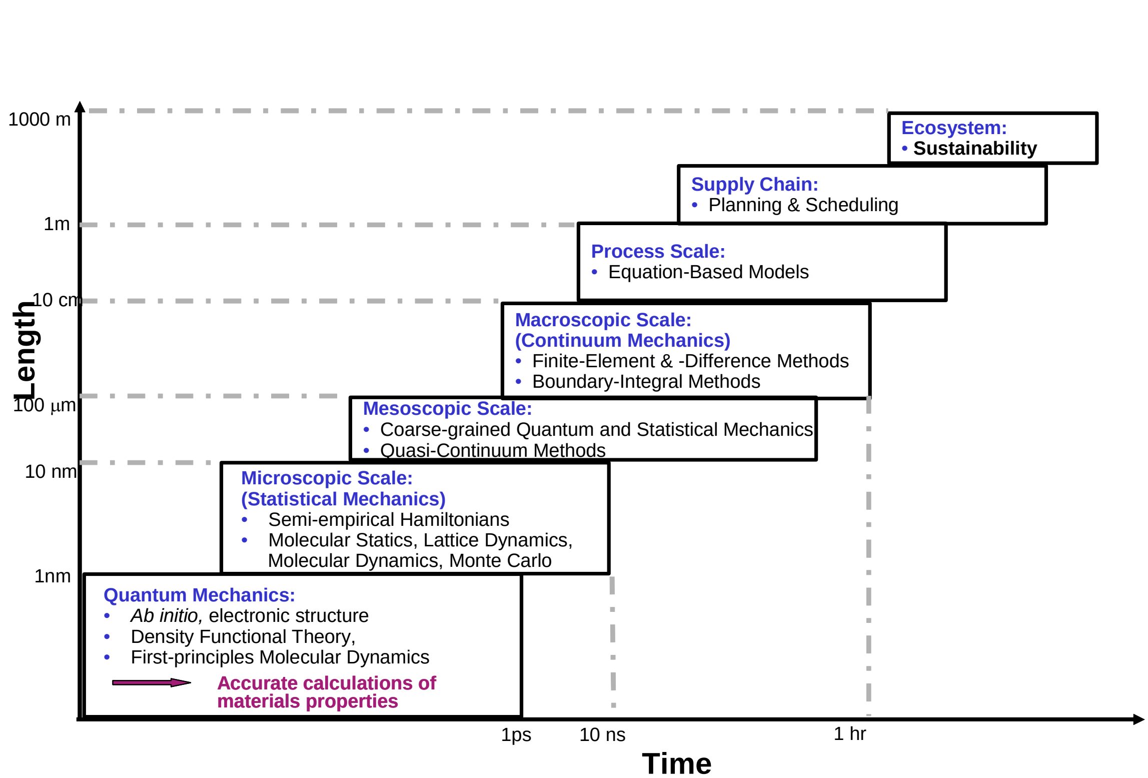
John Ekerdt
Cammy Kao
Helen Lou
Greg McRae
Bill Olbricht (Chairman)

Outline of Presentation

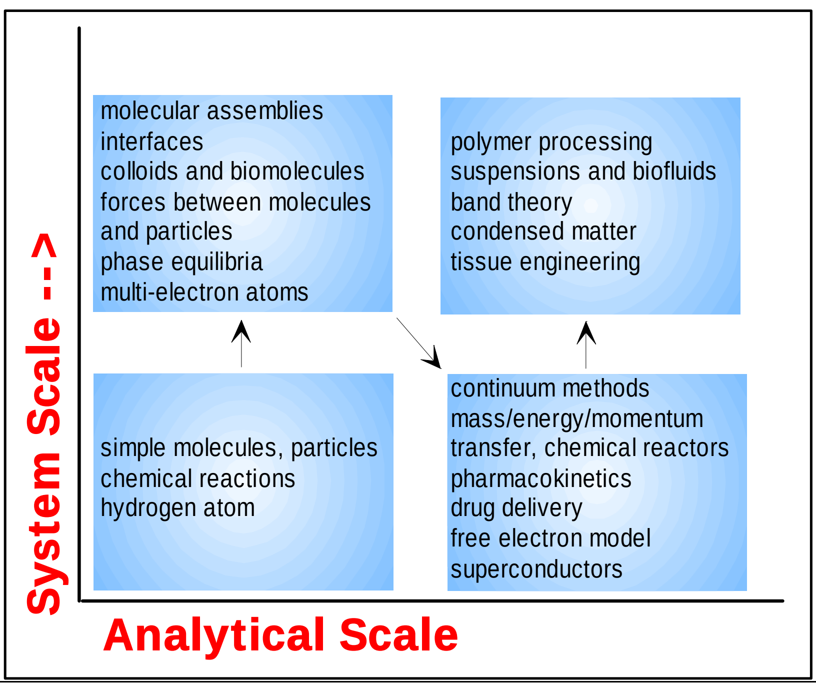
- What is multiscale?
- Curriculum implications
- Need for examples
- Forward plan

Key Objective: Integrate design and multi-scale concepts from day one, <u>not a capstone course.</u>

Multiscale Phenomena for Chemical / Materials Processing

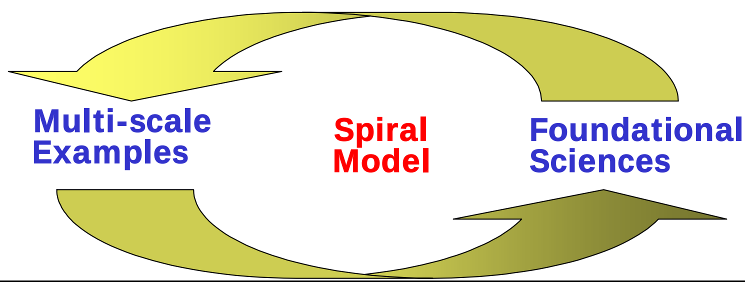


Multi-scale Concepts

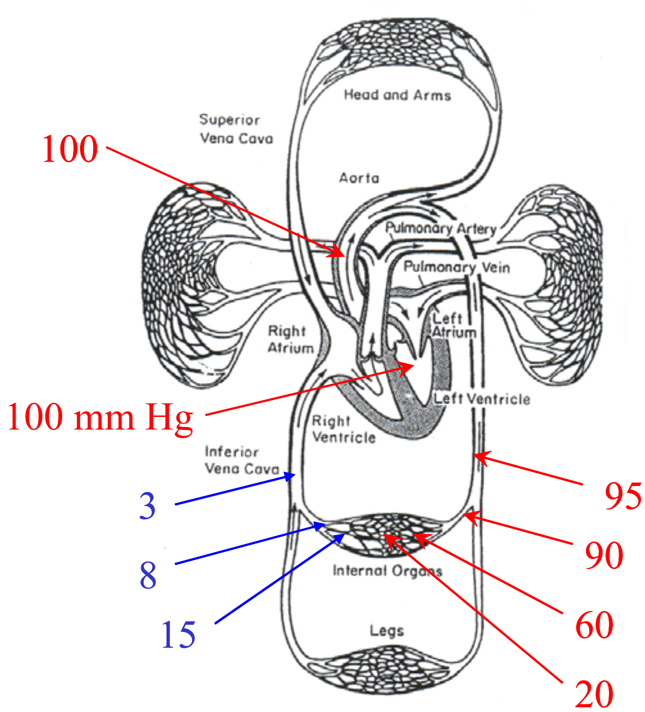


Examples of Multi-Scale Systems

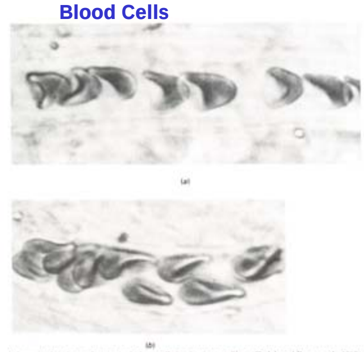
- Blood flow in the human body
- Water purification
- Production of monoclonal antibodies
- Ethylene Oxide
- Atmospheric transport/transformations



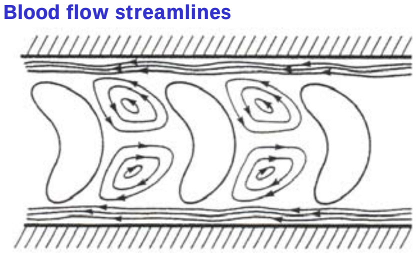
Blood Flow in the Human Body



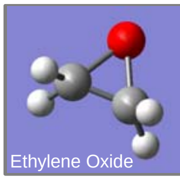
Blood Cells



Blood flow streamlines



Motivating Problem – *Improving old processes*



- World capacity 22 billion lbs/year
- Very low margins
- > 50 year old process

C_2H_4O →
- Ethylene Glycols →
  - Coolants (29%)
  - Polyesters (32%)
- Surfactants (13%)
- Glycol ethers (7%)
- Ethanolamines (6%)
- Other (13%)

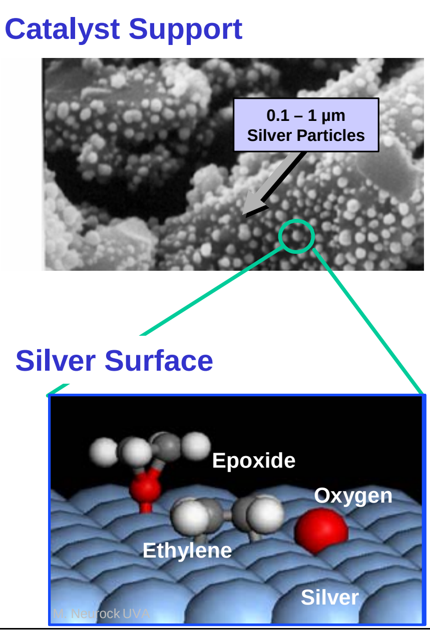
Win-Win Design – *Do not make CO_2*

$$C_2H_4 + \frac{1}{2}O_2 \rightarrow \underbrace{C_2H_4O}_{\text{Product}}$$

$$C_2H_4 + 3O_2 \rightarrow \underbrace{2CO_2}_{\text{Climate Problem}} + 2H_2O$$

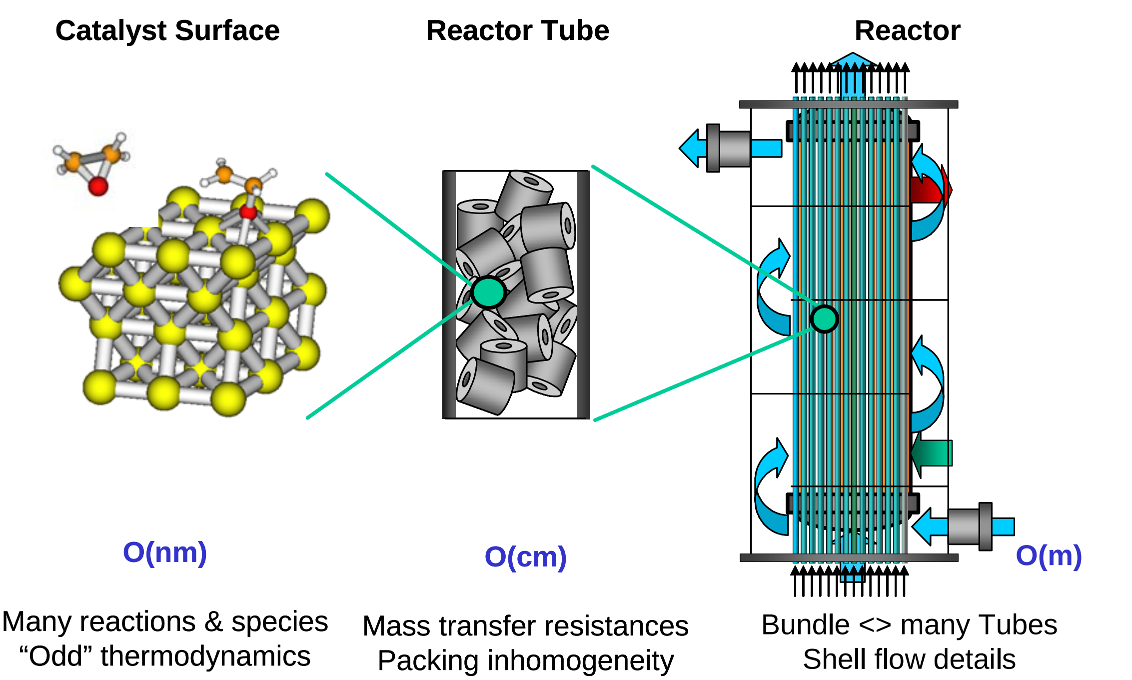
Improving yield / selectivity can improve both profit and reduce climatic impacts

What's New – *Multiscale Engineering*



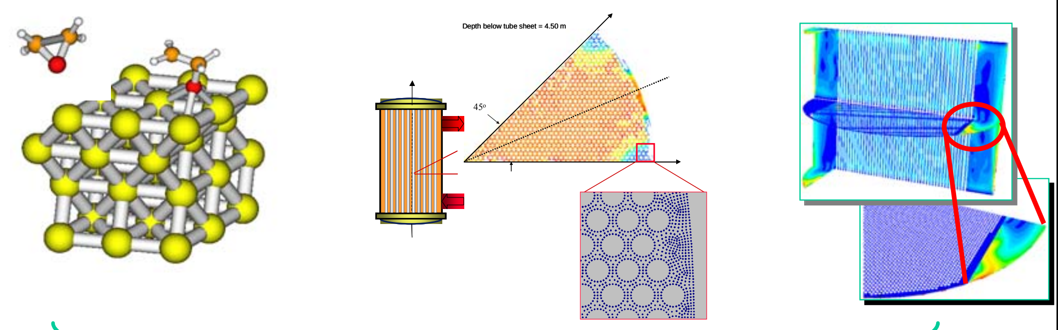
- Use science-based models built on molecular level understanding, experiments and plant data
- Employ problem solving environments that seamlessly integrates the needed tools
- Explicitly deal with uncertainties to manage risk and resource allocation
- Understand the economic value of productivity improvements

Multiscale Engineering – *Seamless Integration*



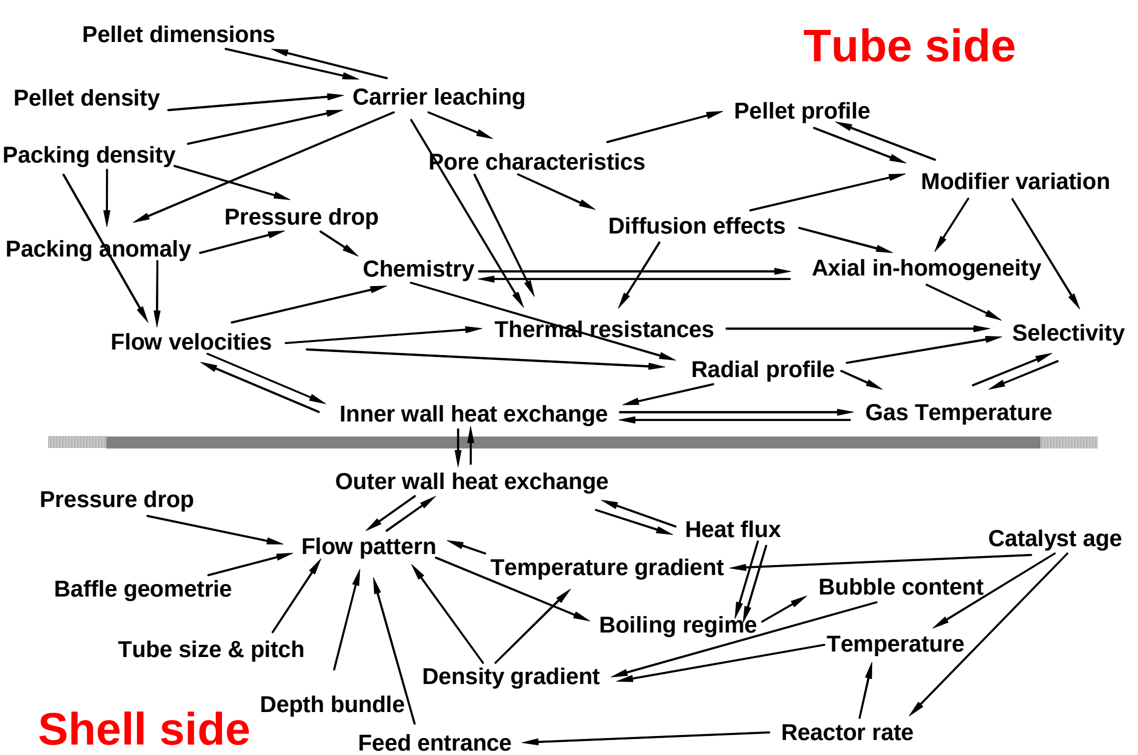
Integration of Multiscale Tools

Experimental Data and Quantum Chemistry (Gaussian,…) ⟷ CFD Models of Reactive Flow (Fluent, StarCD,..) ⟷ Design Optimization (gPROMS, Aspen,…)

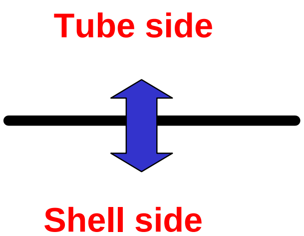


Seamless Integration of Tools and Scales

Problem Solving Issues – *A professional viewpoint*



Same Problem but evolving levels of detail with regard to scales – *Spiral Model*



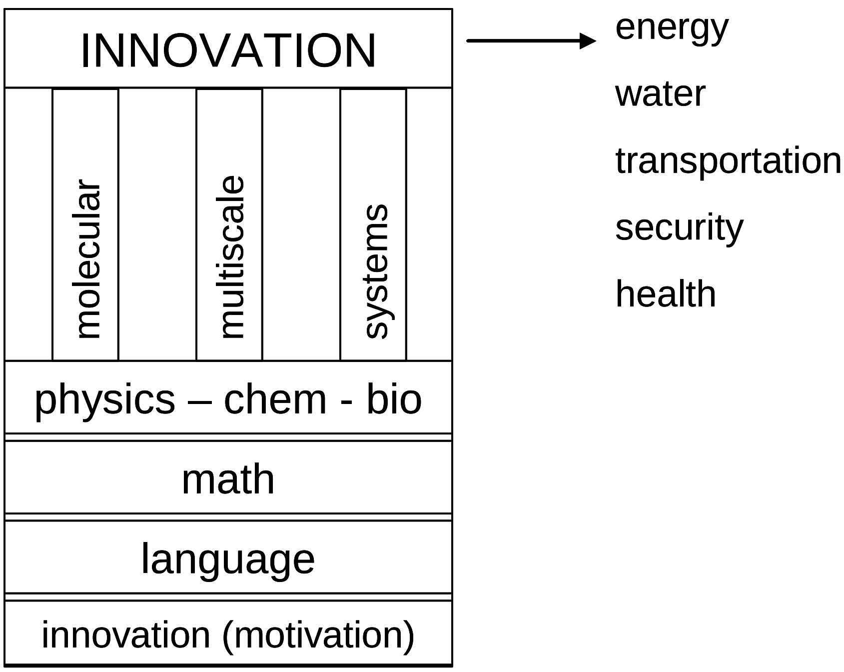
Year Level of Treatment

1. Overall heat transfer coefficient
   (Introduction to scaling, Dimensional Analysis)
2. Boundary layer and multiphase flow
   (B/L thickness, Phase equilibria)
3. Catalytic heat generation
   (Surface kinetics, pore transport, reactor)
4. Integration with whole reactor/plant
   (Unit/Process modeling)

Where are we now and next steps

- Help us with the development of examples that can cross traditional disciplinary boundaries
- Address question of how to use examples to enliven or restructure traditional curriculum
- Development of multi-scale analysis tools themselves
- Begin the formation of teams to do the work

Systems
The curriculum begins with a student's desire to innovate, and culminates in a graduate who is able to innovate, and thus contribute to societal needs. Thus innovation is a bridge between the technical tools and application areas.



Outlining a curriculum:

<u>Sophomore Year</u>
1. Rename Material and Energy Balances to "Introduction to Chemical and Biological Systems"
   - bring biologicql and chemical examples to an equal footing
   - simple dynamic behavior
   - Six modules @2 weeks for 12 weeks total
2. Additional topics
   - sensitivity and uncertainty
   - data acquisition and analysis
   - parameter estimation

<u>Junior Year</u>
(No existing systems course, but there are systems concepts in other courses, such as reaction and separation systems)
1. System modeling and analysis tools
   - deterministic
   - stochastic
   - data-driven
   - integration
2. Other topics

Senior Year

1. Product and Process Design
    - many modules and contemporary case studies
    - emphasis on innovation
    - global marketplace
2. Control and Operations
    - dynamics and feedback
    - planning and scheduling
    - monitoring and detection
3. Other Topics

Comments from the audience:

- Put molecular systems in Junior Year
- Put separation systems in Junior Year

First-year Experience

What Can ChE Programs Offer in the First Year?

- Some required to offer
- Common first year
- Some not allowed to offer required course in first year

What Should the First Year Experience Accomplish?

- Informed choice
- Retention /recruiting for those who don't know the excitement of ChE
- Self-assess learning styles
- Teamwork (exercises)
- Ethics
- Design? (conceptual/open-ended, uncertainty, ambiguity, economics, trade-off)
- Professional development skills
- Problem-solving

but NOT

- Details of ChE Science
- Complexity

Who Takes the First-Year Course?

- Require all engineers to take courses of this type
- Optional (lower credit?) (motivated, self-selected)
- Non-engineers to expose to technology?

Goals

- Building confidence
- Motivating and justifying further study

Pedagogy

- How many credits?
- Natural to do with case studies
- Active learning
- Design problems
- Quantitative (but not detailed, in-depth models)
- Structured milestones

What Should be in the Course?

- What are ChE roles in the "big problems" of the future?
- What are the achievements of the past?
- What does a ChE do day-to-day?
    - range of jobs, career opportunitites
- Ethics (through case studies)
- Design experience (active learning)
- Problem-solving
- Join a learning community
- Illustrate the Organizing Principles in case/design studies

- Communication and team skill building
- NOT scientific or engineering science details, or complex design criteria

<u>Logistics</u>

- A real course
- Put a good instructor in it
- Senior/TA support - select properly
    - more TAs
    - seek volunteers
    - help to professional development
    - help to reinforce their own understanding of curriculum content
- Significant human resource investment
- Could accomplish many goals in range of 1-3 credits
- Need materials (text, cases/design problems)

Three Levels of Labs

- Classical Labs
  - Purpose is Demonstration of Concepts
- Projects Lab
  - Purpose is to emphasize professional skills (e.g. oral and written communication, teaming skills)
  - Very expensive
- Laboratory components in a lecture class
  - Web labs
    - Expensive
    - Need to share facilities
  - In-class demos
  - Video-taped experiments

Summary

- Classical Labs
  - Nothing beats a hands-on experiment
  - Messy data, “real” problems
- Projects Lab
  - Probably the most ideal, but too much of a drain on resources to do every year
  - However, strongly suggested at least one course
- Things I can do in class
  - Cheaper
  - Easier to implement and “squeeze” into a class
  - Less instructive

➢ One purpose of a laboratory is to gain experience with things that go wrong.

Examples

- Traditional / “Continuum” scale demos
  - Many examples
  - Need to collect and organize
- Molecular
  - Low pressure reactors
  - Strong need for more examples
- The Laboratory in the Freshman Experience
  - Meets four needs
    - Recruitment
    - Retention
    - Gives engineering experience (seeing the big picture)
    - Some fundamentals
  - This dictates need for “everyday” items and experiences
- Having students build equipment for laboratory work is desirable, but costly.