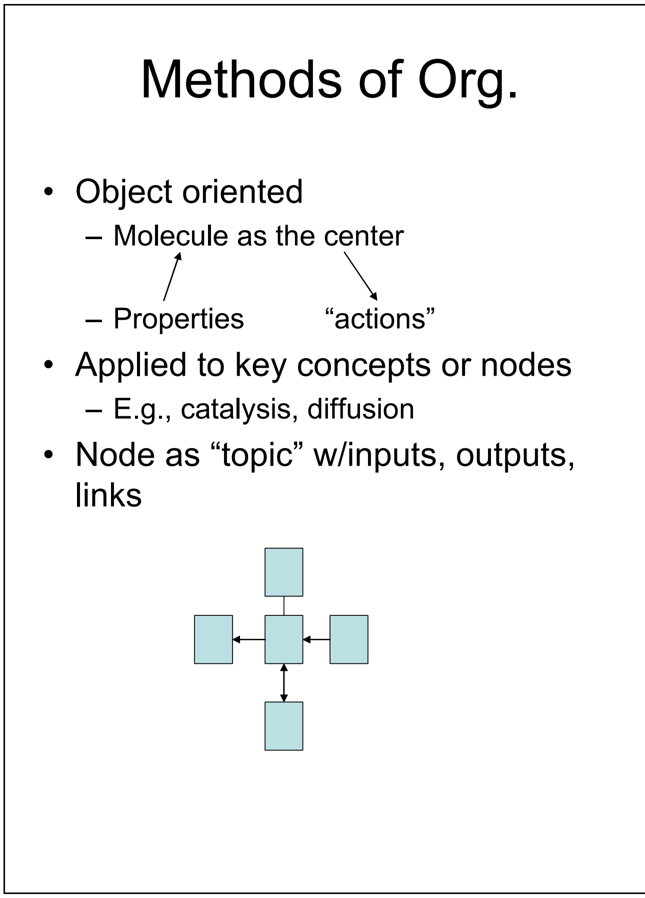
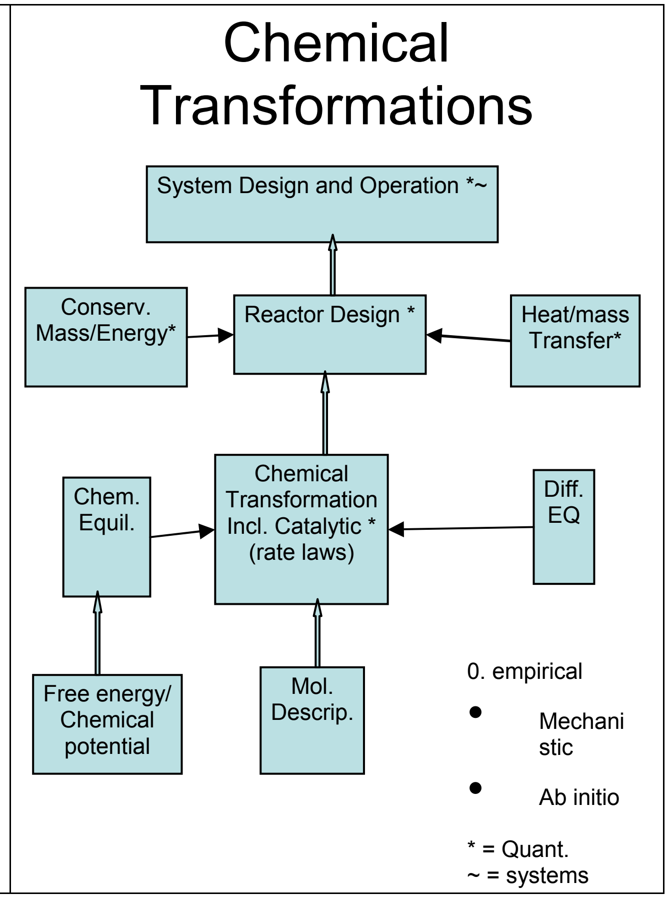
Session 2: connections among the organizing principles
Wednesday morning, 2003 April 9

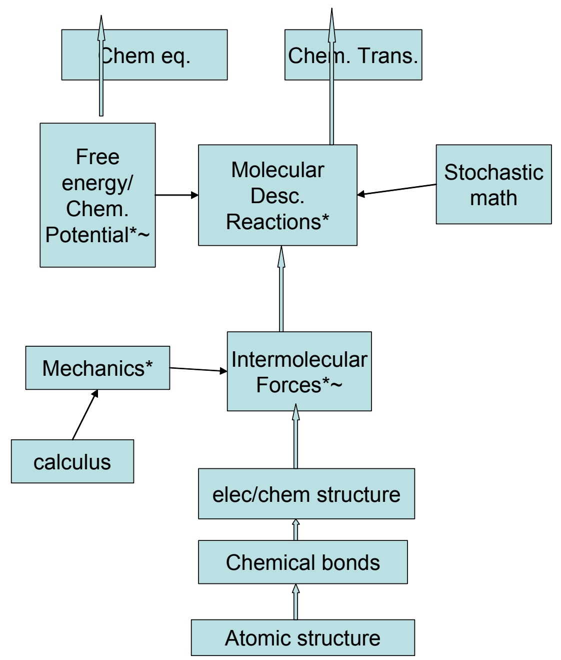
Workshop participants remained in their four working groups from Session 1, each charged to identify points at which their organizing principle connected with the others.

Group 1 (Molecular Transformations)

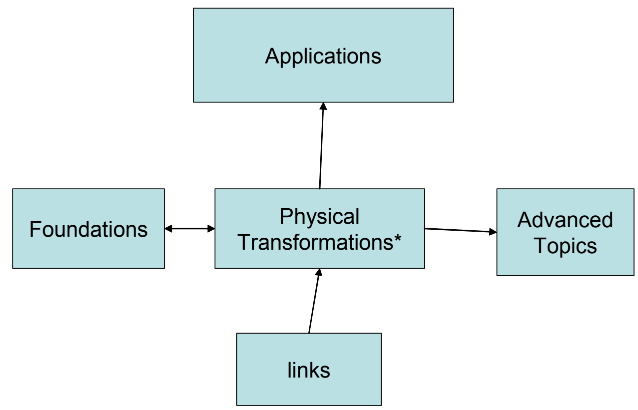




Chemical Transformations (con't)



Chemical Transformations (con't)



* Phase change, micell formation, self assembly, adsorption

Foundations

- Chemical Structure
  - Bonding
  - Higher order (3-D)
  - Chirality
- Equilibrium
- Free Energy
- Entropy
- Inter/Intra molecular forces
- Nomenclature
- Atomic structure
- Conservation principles
- Molecular dynamics

Advanced Topics

- Reactor design
- Staged operations
- Separations
- transport

Applications

- Metallurgy
- Thin film deposition
- Material processing
- Protein folding
- Personal care products

Links

- Multiscale
  - Molecular → continuum
    - [stat mech]
    - Driving forces
  - Quant
    - Algebra, cale., diff eq, stochastic
  - Systems
    - Reactor design
    - Unit ops

Group 2 (Quantitative Analysis)

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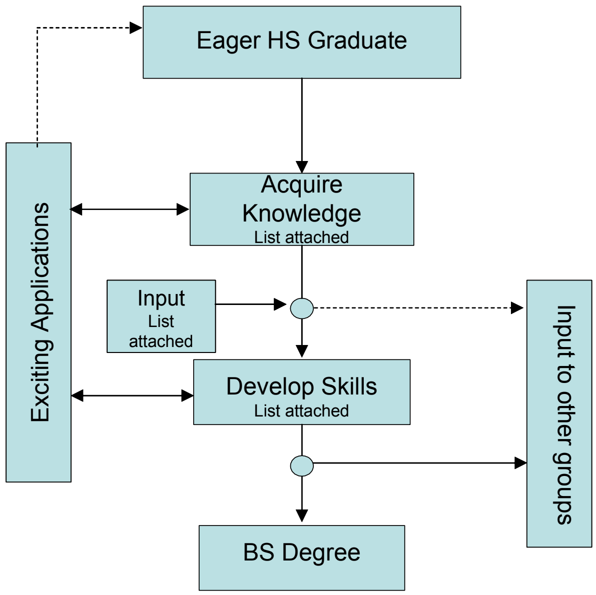


Knowledge

- Diff. Eqns.
- Calculus
- Probability/statistics
- Linear algebra
- Numerical methods

Inputs

- Physics
- Biology
- Chemistry
- HS Grad. Skills
- Population balances
- Conservation laws
- Material properties
- Quantum mechanics
- Continuum concepts
- Molecular dynamics

Skills

- Math. Descriptions of physical phenomena
- Computer-based skills
- Economic analysis
- Scaling/order of magnitude analysis
- Process exploration
  - Sensitivity/uncertainty
  - "What if" explorations
  - Optimization

Group 3 (Multiscale Analysis)

Ramon Cerro, Mike Prudich, Dick Turton
Mike Dudukovic, Raj Rajagopalan, Fred Weber
Peter Kilpatrick, Mike Thien, Ted Weisner

Molecular Transformations

Connections	Organizing and Motivating Themes	Physical	Chemical	Biological	Dependencies
Systems integration of scales	Sub-molecular		-Quantum chemistry (DFT, energy/ quantum)		-Translation of science/physical laws into math -Sensitivities Analysis -Rational assumptions – incomplete or excess information -Order of Magnitude analysis -Dimensional analysis -Stochastic and probabilistic processes -Engineering math
	Molecular	-Quantum/ Molecular dynamics		-Biochemical rxn mechanisms -Molecular biology -Molecular immunology	
	Nano/Molecular aggregate	-Interfacial transport -Statistical thermo, DLVO -Adsorption -Nucleation theory -Colloidal interactions -Molecular assemblies	-Catalyst development	-Secondary, tertiary, quaternary protein structure -Protein folding, aggregation, vesicles, signal transduction, enzymology	
	Micro/Continuum	-Fluid mechanics -Thermodynamics -Transport -Crystallization -Phase separations, -MEMS, Micro-fluidics	-Reaction engineering	-Cell physiology -Cell culture and fermentation	
	Macro	-Mass & energy balances -Control volumes -CFD -Control -Separations/unit ops	-Reactor design -Scale-up	-Bioreactor & bioprocess design -Bioseparations-macro -Systems biology	
	Super-macro		Atmospheric chemistry and dispersion		

← Plant/Product Design →

Group 4 (Synthesis/Systems)

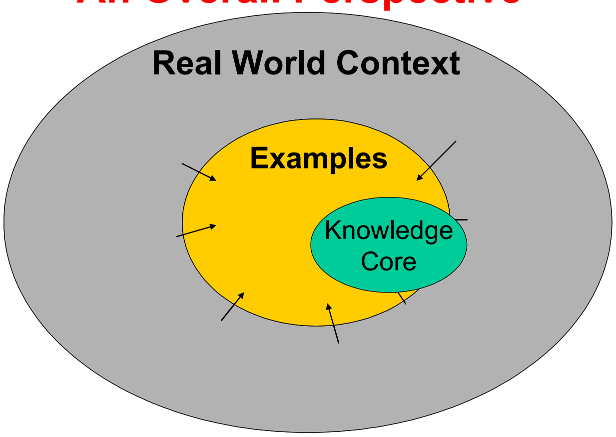
Group 4 - Synthesis/Systems

Wayne Bequette
Tom Edgar
Christos Georgakis
Cammy Kao
David Hackleman
Kenneth Hall
Greg McRae
Jim Rawlings
Bill Olbricht

Five Key Questions

- How does one communicate the excitement of Chemical Engineering to students?
- Can a systems perspective be used to teach Intro to Chemical Engineering?
- Design should not be a “capstone” course?
- How to provide faculty with systems examples?
- How to strengthen links to experiment?

An Overall Perspective



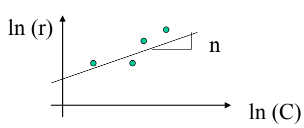
Systems Core Knowledge

- Mathematical modeling and simulation
- Optimization
- Design strategies (iterative/combinatoric)
- Statistics/Data Analysis/Acquisition/DOE
- Feedback
- Dynamics (Time and Frequency)
- Finance/Business
- and new knowledge

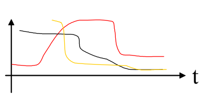
Linkages/Opportunities

Traditional Approach

$r = kC^n$



Using Modern Systems Approach



$r_i = k_i C_j C_k$ $\min_{c,t} ||c_i - c_{obs}||$

New knowledge

How to do estimation for 100’s of molecules?

Introduction to ChE

Examples provide context to:

- Present a compelling roadmap four 4 years
  - e.g. Why do I need to learn Thermodynamics...
- Show the need for understanding fundamentals
  - Bio, Math, Thermo, Kinetics
- To appreciate and be comfortable with limits of understanding
  - Provides the motivation for continuous learning
  - A framework for assumptions / approximations
  - Problem solving requires iterations
  - External factors (regulation, market needs)

Linkage Example: Desalination	Connections/Dependencies
– Market needs (Water shortage) – Knowledge Needed (linkages) • Salt solutions (Thermodynamics, activities) • Evaporation (Heat/Mass transfer) • Corrosion (Materials science) • Salt disposal (Environmental) • Energy use (Economics) • Process choice (Alternatives, economics) • Piping and distribution (Fluid dynamics) – Business Context • Innovation	• Chemical Engineering IS Systems Engineering • Introduce systems quantitative ideas into other courses, especially Biology • Creating examples that show the connections/dependencies • Identify "new" knowledge needed tackle systems examples

Discussion following Small Group Reports

- Group 1 Report –
  - "system design and operation" added
- Each Organizing Principle addresses all of ChE
- Optimistic about curriculum development
- This is a new paradigm – scales and connections
- The connections illustrate what a modern ChE can do
- ChEs should be taught to think differently
- "Multiscale" concepts are ~20 years old, but now we're seeing the possibility to use them in an organized way
- We teach the components at present, but do not integrate well (usually only at macro-level)
- A new appreciation of co-teaching; e.g. two instructors who emphasize different scales
- Teach to complement

General reflections on Session 2

- Is quantitative analysis even needed as an organizing principle?