

10.40 Chemical Engineering Thermodynamics: a Multiscale Approach for the 21st Century

- Brief review of 1st and 2nd laws and empirical EOS property models
- Calculus of thermodynamics and the fundamental eqn of thermodynamics
- Classical approach to equilibrium and stability criteria
- Mixture thermodynamics formalisms
- Basic principles of Statistical Mechanics
- Connections between molecular level effects and macroscopic properties
- Constitutive property models and their application to phase equilibrium and stability
- Computer methods will be used for both classical problems (e.g. cubic EOS use) and molecular simulations (e.g. MC and MD methods)
- Applications to multicomponent, multiphase systems in phase and chemical equilibria
 - phase partitioning in polymer solutions and complex reacting mixtures
 - phase stability and spinodal decomposition
- Applications for providing Sustainable Energy
 - carbon dioxide separation and sequestration for stabilizing climate
 - alternative energy from methane gas hydrates and geothermal systems
 - process heat and power integration
 - advanced power convertors

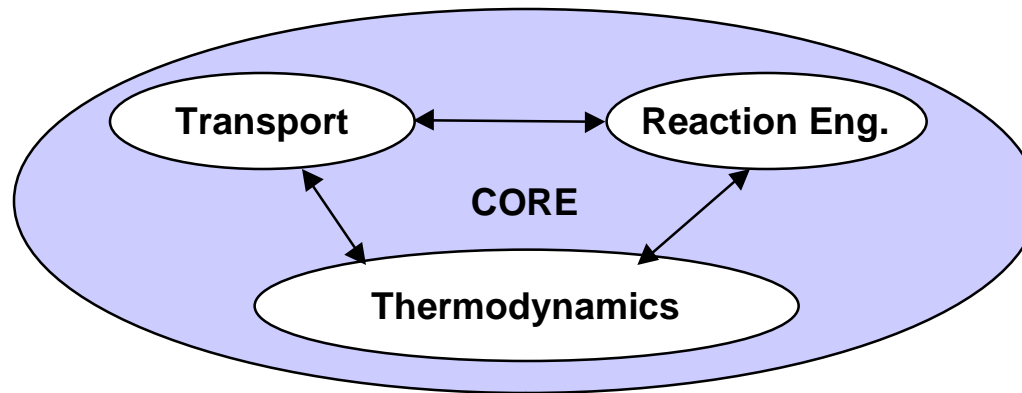
10.40 Chemical Engineering Thermodynamics: Fall 2000 4-0-8 MTWTh

- Instructors -- Professors J. Tester and B. Trout
- Teaching Assistants -- Matthew Reagan and Michael Timko
- Completely revised content merging elements of the old 10.40 and 10.42
- Incorporates both classical and molecular concepts
- Emphasis on applying fundamentals to problem solving
- Meets formally for 4 class periods per week 9 to 10 am MTWTh

10.40 Chemical Engineering Thermodynamics: Your first assignment for Wed 9/6/00

- read chapters 1-3 of *our text*, *Thermodynamics and Its Applications, 3rd ed*
- *optional* - you might find it helpful to revisit your undergraduate thermodynamics and physical chemistry textbooks, for example,
 - Smith and Van Ness, 5th ed. Chapters 1-5, 8-10
 - Kyle, 2nd ed (1992) Chapters 1-4, 5.1-5.5, 8, 9, and 15
 - Sandler, 2nd ed Chapters 1-4, parts of 6 and 7
 - Castellan, *Physical Chemistry*
 - Alberty and Silbey, *Physical Chemistry*
 - Atkins, *Physical Chemistry*
- look over the problems at the end of Chapter 3 in our text, for example problems 3.9 and 3.10

Old Versions of 10.40 And 10.42 pre-21st Century

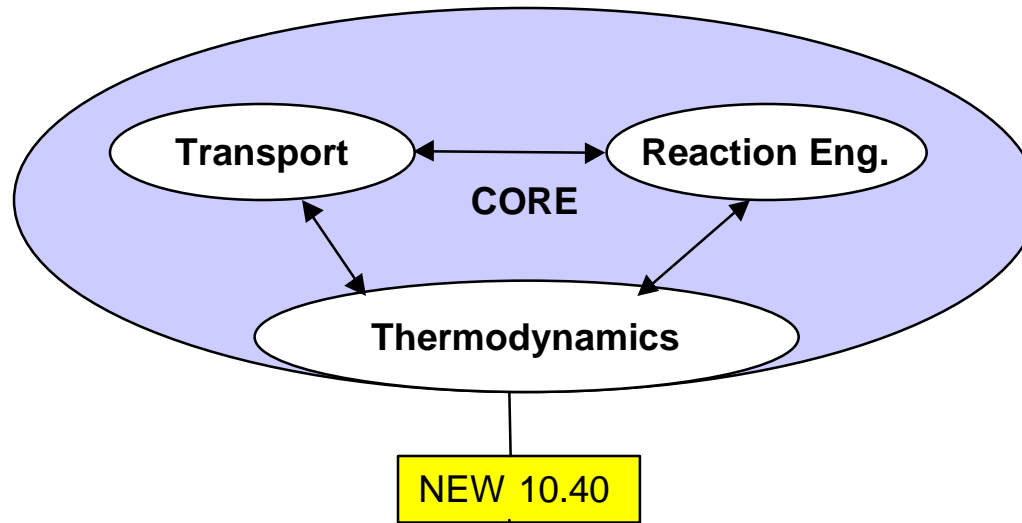


10.40 (Fall)
Chem. Eng. Thermodynamics

- Focus on applying fundamentals to solve problems
- Brief review of 1st & 2nd Laws
- Calculus of thermodynamics via Gibbs fundamental equation
- Equilibrium and stability criteria
- Constitutive property models
 - PVTN EOS (empirical)
 - Connection to molecular effects
 - Activity coefficient models
- Applications
 - Mixtures
 - Phase and chemical equilibria
 - Pinch and availability analysis

10.42 (Spring)
Advanced Thermodynamics

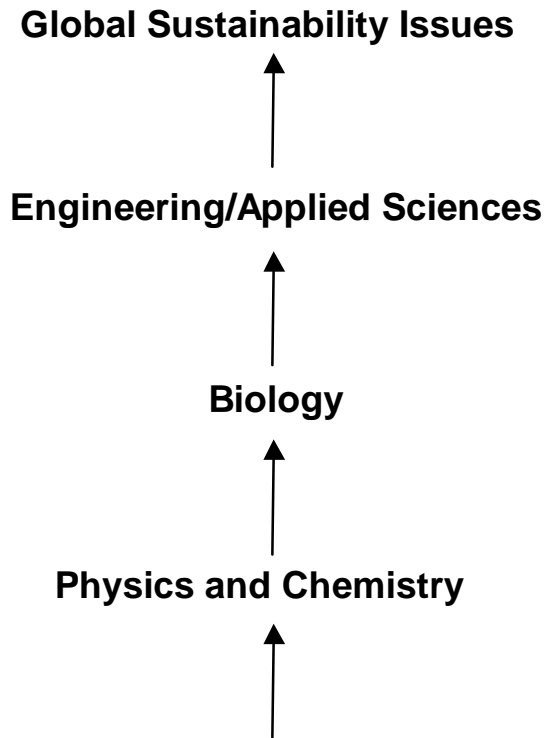
- Emphasis on modeling properties in non-ideal systems
- Molecular to macroscopic scales
- General treatment of classical statistical mechanics
- Virial EOS & corresponding states
- VdW & McMillan-Mayer theory
- Lattice & Flory-Huggins models
- Local composition models
- Quasi-chemical models
- Electrolytes
- Phase stability and critical phenomena
- Spinodal decomposition
- Electromagnetic and potential fields
- Surface thermodynamics



- Focus on applying fundamentals to solve problems
- Brief review of 1st & 2nd Laws
- Calculus of thermodynamics via Gibbs fundamental equation
- Equilibrium and stability criteria
- Constitutive property models
 - PVTN EOS (empirical)
 - Connection to molecular effects
 - Activity coefficient models
- Applications
 - Mixtures
 - Phase and chemical equilibria
 - Pinch and availability analysis
- Emphasis on modeling properties in non-ideal systems
- Molecular to macroscopic scales
- General treatment of classical statistical mechanics
- Virial EOS & corresponding states
- VdW & McMillan-Mayer theory
- Lattice & Flory-Huggins models
- Local composition and quasi-chemical models
- Phase stability and critical phenomena
- Spinodal decomposition

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→ From Molecules to Machines From Potentials to Phases to Processes →



Mathematics:

- Multivariable Calculus
- ODE/PDE
- Vectors/Matrices

