Chemical Engineering Thermodynamics

Fulbright Visiting Professor David J. Dixon
Chemical and Biological Engineering Department
South Dakota School of Mines and Technology

WS 2009/2010
Overview

• Introduction
• Chemical Engineering History
• Today’s Chemical Engineering
• Chemical Engineering Thermodynamics Course Overview
Introduction

Dr. David Dixon
Professor of Chemical Engineering
Chemical and Biological Engineering Department
South Dakota School of Mines and Technology

Rapid City, South Dakota, USA
Introduction

Rapid City near Black Hills
Introduction

Rapid City near Black Hills (Paha Sapa, Lakota for “hills that are black”)
Introduction

Rapid City (~60,000)

Looking East

Looking West
Introduction
Introduction
SD School of Mines and Technology (SDSMT.edu)
Introduction

SD School of Mines and Technology (SDSMT.edu)
Introduction

Myself…. 

- BS/MS/PhD Chemical Engineering
- SDSMT/SDSMT/University of Texas at Austin
- Dow Corning Corporation (Process Engineering)
- Overseas military service (Darmstadt)
- Professor SDSMT (16 yrs)
Introduction
Chemical Engineering History

United States:
• J. Willard Gibbs 1st PhD in Engineering in the U.S. (1863)
• L. M. Norton, MIT first ChE course (1888)
• 1st BS program in Chemical Engineering, U Pennsylvania (1892)
• American Institute of Chemical Engineers (AIChE) formed 1908

“The chemical industry had a central position in the changing industrial world of the late 19th century. This industry did not hatch fully grown; it was based on nearly a century’s worth of scientific advances in the universities – particularly German universities.”


Europe:
• Justus von Liebig (1803 – 1873) Giessen
• Göttingen, Heidelberg, and other top universities.
Chemical Engineering History

South Dakota: 1803-4

* "Discovered a Village of Small animals that burrow in the grown... except the ears which is Shorter, his tail like a ground squirrel which they shake & whistle when allarmed. the toe nails long, they have fine fur."

* W. Clark - Friday, September 7, 1804
Today’s Chemical Engineering

Today, the field of chemical engineering is a diverse one, covering areas from biotechnology and nanotechnology to mineral processing.

- Biochemical engineering
- Biomedical engineering
- Biomolecular engineering
- Biotechnology
- Ceramics
- Chemical process modeling
- Chemical Technologist
- Chemical reactor
- Computational fluid dynamics
- Corrosion engineering
- Distillation Design
- Electrochemistry
- Environmental engineering
- Earthquake engineering
- Fluid dynamics
- Food engineering
- Fuel science
- Heat transfer
- Industrial gas
- Mass transfer
- Materials science
- Metallurgy
- Microfluidics
- Mineral Processing
- Nanotechnology
- Natural environment
- Natural gas processing
- Nuclear reprocessing
- Oil exploration
- Oil refinery
- Plastics engineering
- Polymers
- Process control
- Process design
- Process development
- Pulp and paper
- Safety engineering
- Semiconductor device fabrication
- Separation processes (see also: separation of mixture)
  - Crystallization processes
  - Distillation processes
  - Membrane processes
- Textile engineering
- Thermodynamics
- Transport Phenomena
- Unit operations
- Water technology

Additional topics under the title *AlChE’s Technical Divisions and Forums* in American Institute of Chemical Engineers

*Wikipedia, Chemical Engineering*
Today’s Engineering

Darmstadt (BS 3yrs – MS 2yrs)

<table>
<thead>
<tr>
<th>Lectures on chemical engineering subjects</th>
</tr>
</thead>
<tbody>
<tr>
<td>Chemical Engineering Thermodynamics</td>
</tr>
<tr>
<td>Unit Operations</td>
</tr>
<tr>
<td>Advanced Mass Transfer</td>
</tr>
<tr>
<td>Process Systems Engineering (WS)</td>
</tr>
<tr>
<td>Interface Science (WS)</td>
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<td>Fuell Cell Process Engineering (WS)</td>
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<tr>
<td>ADP: Chemical Plant Design Course</td>
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<tr>
<td>Mechanical Process Engineering</td>
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<tr>
<td>Manufacture of Apparatus</td>
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<tr>
<td>Plant Design and Operation</td>
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<tr>
<td>Multiphase Flow</td>
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<tr>
<td>Chemical Reaction Engineering</td>
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<tr>
<td>Nuclear Process Engineering</td>
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<tr>
<td>(Bioengineering)</td>
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<td>Hampe</td>
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<td>Hampe</td>
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<td>Hampe</td>
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<td>Schadler</td>
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<td>Epple</td>
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<td>Vogel</td>
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<tr>
<td>Hampe</td>
</tr>
</tbody>
</table>
# Today’s Chemical Engineering

**USA system (BS 4 yrs)**

- Programming and Numerical solutions to ChE problems
- Material and energy balances
- Fluid flow
- Heat transfer
- Mass transfer
- Unit Operations/separations
- Thermodynamics I and II
- Chemical kinetics and reactor design
- Senior design courses and project
- Process control
- Microbiology
- Global and contemporary issues in ChE

- ChE laboratory experiences
  - Freshman modeling intro
  - Fluid flow
  - Process control intro
  - Heat transfer
  - Separations
  - Elective lab
  - Elective ChE courses
    - Advanced separations
    - Advanced reactor design
    - System dynamics and modeling
    - Polymer engineering
    - Organosilicone chemistry
    - Biochemical engineering
    - Design of experiments for ChEs
    - Coop experiences
    - Undergraduate research
Today’s Chemical Engineering

USA system (BS 4 yrs)
- Professional organizations (AIChE, ACS, other)
Today’s Chemical Engineering

Why study Thermo of mixtures: Motivation
- Example, i.e. SCF measurements, others?
- UO systems (discuss general PFD and where separations fits in plus other things like HT, MT, staged processes, etc)
Today’s Chemical Engineering

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Why study Thermo of mixtures: Motivation
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Figure 2.1 Schematic diagram of the experimental apparatus used by Hannay and Hogarth to obtain solid solubilities in supercritical fluids. The glass tubing (a) is first connected to an air manometer and is then immersed in the constant temperature bath (b).

Supercritical Fluid Extraction (2nd), M. McHugh & V. Krukonis, Elsevier (1994)
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Heat and Material Balance Table

<table>
<thead>
<tr>
<th>Stream ID</th>
<th>FEED</th>
<th>VAPOR</th>
<th>LIQUID</th>
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</thead>
<tbody>
<tr>
<td>Temperature</td>
<td>104.9</td>
<td>114.6</td>
<td>114.6</td>
</tr>
<tr>
<td>Pressure</td>
<td>bar</td>
<td>2.000</td>
<td>2.000</td>
</tr>
<tr>
<td>Vapor Frac</td>
<td></td>
<td>0.000</td>
<td>1.000</td>
</tr>
<tr>
<td>Mole Flow</td>
<td>kmol/hr</td>
<td>10.000</td>
<td>5.000</td>
</tr>
<tr>
<td>Mass Flow</td>
<td>kg/hr</td>
<td>208.207</td>
<td>115.437</td>
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<tr>
<td>Volume Flow</td>
<td>cum/hr</td>
<td>0.243</td>
<td>80.604</td>
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<tr>
<td>Enthalpy</td>
<td>MMkcal/hr</td>
<td>-0.660</td>
<td>-0.283</td>
</tr>
<tr>
<td>Mole Flow</td>
<td>kmol/hr</td>
<td></td>
<td></td>
</tr>
<tr>
<td>WATER</td>
<td>9.000</td>
<td>4.096</td>
<td>4.904</td>
</tr>
<tr>
<td>ETOH</td>
<td>1.000</td>
<td>0.904</td>
<td>0.096</td>
</tr>
</tbody>
</table>
Course Overview

CHEMICAL ENGINEERING THERMODYNAMICS
TU-Darmstadt Winter 2009/2010

Overall Description:
A continuation of the first course in thermodynamics. Emphasis on thermodynamic properties of fluids, flow processes, phase and chemical equilibria.

Prerequisite Knowledge:
- College level calculus and differential equations.
- Application of the First Law of Thermodynamics and other basic concepts (enthalpy, internal energy, volumetric work/shaft work etc) in closed or open systems.
- PVT behavior of pure substances/Equation of State/Generalized Correlations.
- Phase equilibrium of pure substances/the phase rule.

Course Objectives:
- To enhance the knowledge of pure fluid thermodynamics with the emphasis on application and develop a clear understanding and working knowledge of solution thermodynamics and the theories of fluid phase equilibria. A brief introduction will review chemical reaction equilibria, from a process engineering view.

Expected Outcomes: After completion of this course the typical student is expected to be able to:
- Overview of fugacity and fugacity coefficient of pure species and species in solution.
- Perform various VLE calculations (equilibrium composition of liquid and vapor phases, dew/bubble point and L/V ratio) using the Gamma Phi formulation and a variety of its simplifications.
- Use the AspenPlus process simulator to correctly setup and obtain thermodynamic properties for various systems.
- Overview of the chemical equilibrium constant for a specific reaction.
## Course Overview

**Time/Place:** L203/05, W (Mi) 8:00 – 9:30

**Recitation:** To be announced

**Instructor:** Dr. David J. Dixon  
L101/385, +49-6151-16-2364 (w), [dixon@tvt.tu-darmstadt.de](mailto:dixon@tvt.tu-darmstadt.de)  
([david.dixon@sdsmt.edu](mailto:david.dixon@sdsmt.edu))

**Text:** Koretsky, “Engineering and Chemical Thermodynamics”, Wiley, 2004


**WebPage:** [http://webpages.sdsmt.edu/~ddixon/Thermo_TUD.html](http://webpages.sdsmt.edu/~ddixon/Thermo_TUD.html)
Course Overview

<table>
<thead>
<tr>
<th>Item</th>
<th>Points</th>
<th>Tentative grade scale ***:</th>
<th>Points earned</th>
<th>Grade</th>
</tr>
</thead>
<tbody>
<tr>
<td>Exams (3)</td>
<td>60</td>
<td></td>
<td>90</td>
<td>A</td>
</tr>
<tr>
<td>Final Exam*</td>
<td>(20)</td>
<td></td>
<td>80-89</td>
<td>B</td>
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<tr>
<td>Homework**</td>
<td>30</td>
<td></td>
<td>70-79</td>
<td>C</td>
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<tr>
<td>Project</td>
<td>10</td>
<td></td>
<td>60-69</td>
<td>D</td>
</tr>
<tr>
<td>Total</td>
<td>100</td>
<td></td>
<td>&lt;60</td>
<td>F</td>
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</tbody>
</table>

* The Final will be a 2-hour comprehensive exam. All exams will be open textbook and open notes. Of the four exams given, only the top three exam scores will be used in computing the total points and final grade.

** Homework turned in late will be subject to 10% deduction daily. Submitted homework must be clean, readable and logically sound.

*** The final grade will be reflective of a student’s rank in the class as well as the cumulative points earned.

Grading (for this course at TU-Darmstadt):
- Midterm written exam 50%
- Final written exam 50%
- Homework improvement 0.3 pt
Course Overview

Chapter 5
- Thermodynamic Web
- Departure Functions
- Review Equations of state (chapter 4, briefly)

Chapter 6
- Equilibrium (chemical potential)
  * Pure Component
  * Mixtures

Chapter 7
- Fugacity (chemical potential → fugacity → equilibrium calculations)
  * Vapor (overview), liquid, solids
- Activity Coefficients [Fugacity Coefficients (overview)]

Chapter 8
- Phase Equilibrium
  * Diagrams
  * Vapor – Liquid (VLE)
  * Liquid – Liquid (LLE)
  * Solid – Liquid (SLE)

Chapter 9
- Reaction Equilibria
Questions?