

## 10.40 CHEMICAL ENGINEERING THERMODYNAMICS : A MULTISCALE APPROACH

Fall 2000

Instructors – Bernhardt Trout and Jefferson Tester

### Description

The focus of this graduate core subject is on developing your ability to solve a variety of challenging thermodynamics problems by applying relatively simple principles and concepts to new and often unusual situations. While the material covered is largely centered on classical thermodynamics, numerous connections will be made to molecular-level effects using statistical mechanics. We are assuming that you have completed at least one prior thermodynamics and physical chemistry course. Consequently, the review of 1st and 2nd Law fundamentals will be brief and somewhat theoretical. Emphasis in coverage will be placed on techniques of calculating various derived thermodynamic quantities, open system, transient 1st and 2nd Law problems, estimating conversion efficiencies for heat to work conversions, mixture thermodynamics, macroscopic and molecular constitutive property models for non-ideal fluids and their connection to equations of state, and to fugacity and activity coefficients, phase and chemical equilibria, and critical phenomena and stability with numerous examples. Linkages to how intermolecular sizes and forces determine the properties of non-ideal fluids will be explored using molecular simulation methods. The course syllabus/outline that follows provides details.

### Textbook

*Thermodynamics and Its Applications*, by J.W. Tester and M. Modell,  
3<sup>rd</sup> ed., Prentice-Hall, Upper Saddle River, New Jersey (1997)

### Additional Readings

*Statistical Mechanics*, by D.A. McQuarrie, Harper and Row, New York, New York  
(1976)

*Thermodynamics and an Introduction to Thermostatistics*, by H.B Callen, 2<sup>nd</sup> ed., Wiley,  
New York, New York (1985)

*Introduction to Modern Statistical Mechanics*, by D. Chandler, Oxford, New York,  
New York (1982)

*Applied Statistical Mechanics*, by T.M. Reed and K.E. Gubbins, Butterworth-Heinemann,  
Boston (1973)

## Prerequisites

1 course in physical chemistry and undergraduate thermodynamics and 1 year of calculus through partial derivatives of multivariable functions and ordinary differential equations

## Coverage and Recommended Preparation

Please note that topics listed in syllabus indicate corresponding chapters in the textbook and that approximate class times devoted to each topic are also given. During the first two weeks of the course, the conceptual material in Chapters 1 through 4 and part of Chapter 5 is reviewed fairly quickly as we are assuming that students have covered these topics in their undergraduate engineering thermodynamics and physical chemistry courses. Class assignments in this part of the course are designed to apply 1<sup>st</sup> and 2<sup>nd</sup> Law fundamentals and derived property partial derivative manipulation techniques to the solution of graduate-level engineering problems.

To illustrate the type of problems that will be assigned, three examples taken from the text are given below:

---

1. *1<sup>st</sup> -Law Example Problem (3.10)*
  2. *2<sup>nd</sup> -Law Example Problem (4.11)*
  3. *Multivariable calculus example problem (5.4)*
- 

Regarding the normal variations in coverage that occur in undergraduate thermodynamic subjects, we recommend that incoming students should be familiar with the concepts and level of problems that are found in these popular undergraduate chemical engineering and physical chemistry textbooks as outlined below:

1. *Introduction to Chemical Engineering Thermodynamics*, 5<sup>th</sup> ed.,  
by J.M. Smith, H.C. Van Ness, and M.M. Abbott. McGraw-Hill (1996)  
Chapters 1-5, 8, 9, and 10
2. *Chemical and Engineering Thermodynamics*, 2<sup>nd</sup> ed.,  
by S.I. Sandler, Wiley (1989).  
Chapters 1-4, 6.1-6.6, and 7.1-7.4

3. *Chemical and Process Thermodynamics*, 2<sup>nd</sup> ed.,  
by B.G. Kyle, Prentice-Hall (1992)  
Chapters 1-4, 5.1-5.5, 8, 9, and 15
4. *Physical Chemistry*, 4<sup>th</sup> ed.,  
By P. W. Atkins, Freeman (1990)
5. *Physical Chemistry*, 1<sup>st</sup> ed.,  
by R. A. Alberty and R. J. Silbey, Wiley (1992)

The depth of undergraduate prerequisite material would be comparable to MIT's undergraduate subjects 10.213 and 5.60.

Like 10.50 and 10.65, we assume that students have a practical working knowledge of solving ordinary differential equations and of partial derivative operations in multivariable calculus. Students are assumed to own or have access to a programmable calculator for use in solving homework and examination problems. A working knowledge of FORTRAN, C, or a comparable language, experience with MAPLE, MATHEMATICA, MAT LAB and similar software packages, and familiarity with MIT's Athena and more generally with IBM-PC or MAC platforms will be helpful. Some experience with vector, matrix and determinant notations and operations will be useful in the latter part of the course as well.

### **Closing Remarks**

Students might find it helpful to look over Chapters 1-4 of the text and associated problems at the end of Chapters 3 and 4 before the first class. In this way, you can calibrate your own background and undergraduate preparation against the technical level, problem complexity, and depth of coverage of 10.40.

If you have further questions please feel free to call us at 617-253-3401 (Tester) and 617-258-5021 (Trout), send an e-mail to [testerel@mit.edu](mailto:testerel@mit.edu) or [trout@mit.edu](mailto:trout@mit.edu), or stop by our offices during orientation.

Jefferson W. Tester  
Bernhardt Trout