

# Syllabus for CHE 2101 Class Number 21702

## Fundamentals of Thermodynamics

Fall, 2008 (2091)

Monday & Wednesday 4:00–5:15 p.m.

Room 1221 BEH

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CourseInfo: <http://courseweb.pitt.edu>

Class notes: <http://puccini.che.pitt.edu/~karlj/Classes/CHE2101/index.html>

FMLC computer accounts: Username: `che2101` Password: `johnson_k`

**Office hours:** MW 1:00 to 3:00 PM, and by appointment

### Philosophy

A working knowledge of thermodynamics and statistical mechanics is critical for solving many classes of problems that occur in both academic and industrial settings. Statistical thermodynamics is important in solving problems in areas as diverse as reaction kinetics, catalysis, biochemical engineering, polymer engineering, drug design, and separations. This class will provide the student with basic thermodynamic tools for solving many classes of problems. It will also help the student gain a working knowledge of classical and statistical thermodynamics specifically as it relates to the calculation of thermophysical properties, phase equilibria, and chemical equilibria.

### Audience

This class is intended for first year chemical engineering graduate students with at least one undergraduate course in classical thermodynamics.

### Scope

This class has 5 areas of study:

1. A review of classical thermodynamics.
2. An introduction to statistical mechanics
3. The calculation of thermophysical properties.
4. The calculation of phase equilibria.
5. The calculation of chemical equilibria.

### Objectives

1. Classical thermodynamics—Be able to calculate heat, work and energy changes for various processes. Topics include:
  - (a) 1st and 2nd laws of thermodynamics.

- (b) Mathematical methods of thermodynamics.
  - (c) Departure functions, process evaluation.
2. Statistical mechanics—Gain a basic understand of statistical mechanics. Be able to use statistical mechanical methods to compute ideal gas and real fluid and solid properties.
- (a) Be able to identify the partition functions for different ensembles.
  - (b) Be able to calculate ideal gas properties for polyatomic molecules.
  - (c) Be able to state the origins and limitations of various equations of state.
  - (d) Be able to use conformal solution theory, group contribution methods.
  - (e) Be able to describe the ideas of pair potentials and forces between molecules.
  - (f) Be able to list the basic ideas of molecular simulation techniques.
3. Thermophysical properties—Be able to identify and use one or more methods to compute a given fluid property.
- (a) Equations of state.
  - (b) Activity coefficient models.
  - (c) Statistical mechanical methods.
4. Phase equilibria—Calculate pure fluid and mixture phase equilibria.
- (a) Pure fluid and mixture properties, excess functions.
  - (b) Identify methods for computing phase equilibrium for pure fluids.
  - (c) Identify methods for computing phase equilibrium for mixtures.
5. Chemical equilibria—Calculate equilibrium concentrations of reactants and products for gas and liquid phase reactions.
- (a) Equilibrium constants, relation to equilibrium composition.
  - (b) Multiple competing reactions, number of independent reactions.
  - (c) Be able to calculate nonideal solution equilibrium compositions.
  - (d) Identify equations for simultaneous phase and chemical equilibria.

## Text

The required text for this class is “Statistical Mechanics for Thermophysical Property Calculations” by R. L. Rowley. This book is out of print but a photocopy should be purchased from the Book Center. The cost is about \$34.00. Several other helpful texts are on reserve in the Engineering Library. See the list below.

## Grading

Grades will be given on a modified straight scale. I will not curve the grades to artificially manipulate the number of As, Bs, etc. I believe that grading on a curve discourages appropriate team work. Points will be given for homework, a research project (to be defined), two mid-term exams, and a final exam. The weighting for each of these is given below.

Homework	30%
Research project	10%
Exams (2)	40%
Final Exam	20%

The final grades will be based on the following scale:

Score	Grade
95-100	A+
90-94	A
85-89	A-
80-84	B+
75-79	B
70-74	B-
65-69	C+
60-64	C
55-59	C-

## Disability Statement

If you have a disability for which you are or may be requesting an accommodation, you are encouraged to contact both your instructor and Disability Resources and Services, 216 William Pitt Union, (412) 648-7890/(412)383-7355 (TTY), as early as possible in the term. DRS will verify your disability and determine reasonable accommodations for this course. Refer to [www.drs.pitt.edu](http://www.drs.pitt.edu) for details.

## Counseling

The University Counseling Center's staff is dedicated to assisting students in their pursuit of personal and academic growth, to helping students gain a better understanding and appreciation of themselves, and to supporting students as they make important decisions about their lives. If you are in need of counseling services, please contact the University Counseling Center at 334 William Pitt Union (412) 648-7930 Refer to [www.counseling.pitt.edu](http://www.counseling.pitt.edu) for details.

## Academic Integrity

See <http://www.pitt.edu/~provost/ai1.html> for the University Guidelines on Academic Integrity. You are encouraged to discuss the homework problems with your classmates, however, **the final work you turn in must be your own**. Copying someone else's work, in any way, is unacceptable. You should not borrow notes, homework, homework solutions, exams, or other materials from students who took this course in previous years. There is a distinction between discussing work, and merely copying someone else's work. The idea here is that you should help each other to understand the problems and the concepts involved; you will learn more if you work on the assignments in groups *and explain the methods to each other*. On the other hand, if you simply copy what someone else has done then you are not increasing your understanding, and you are not being honest. You must put in your own effort on solving the problems. Exams, whether in class or take home, must be strictly each student's individual effort. You must not discuss the exams with anyone but the instructor. Any violation of the Academic Integrity code will be prosecuted to the fullest extent of the code.

## **Homework**

Working problems is the only way to gain detailed understanding of and truly master a topic. Homework is an important part of this class, and hence a major component in the grading. There will be regular homework assignments in this class. You will be expected to turn in homework on time at the beginning of class. Solutions will be either handed out in class or posted on the web. For this reason, no late homework will be accepted. Make up homework sets will be assigned as needed.

## **Exams**

There will be two exams and a final. The exams may be in class or take home and will be determined later. The final exam will be comprehensive.

## COURSE RESERVE LIST

The books listed below are on reserve in the Engineering library. They can be checked out for two hours at a time, and may also be checked out overnight. The first book listed is the one required for this class. However, there is no one single book that contains the material to be covered in this class. I strongly recommend that you have access to your favorite undergraduate thermodynamics text, or one of the thermodynamics texts listed below.

- Rowley, R. L., “Statistical Mechanics for Thermophysical Property Calculations”, TA418.24 R69 1994
- Hill, T. L., “An Introduction to Statistical Thermodynamics”, QD501 .H648
- McQuarrie, D. A., “Statistical Mechanics”, QC174.8 M3
- Chandler, D., “Introduction to Modern Statistical Mechanics”, QC174.8 C47 1987
- Walas, S. M., “Phase Equilibria in Chemical Engineering”, TP156.E65 W34 1985
- Tester, J. W. and Modell, M., “Thermodynamics and Its Applications”, 3rd edition, QD504 T37 199
- Prausnitz, J. M. *et al.* “Molecular Thermodynamics of Fluid-Phase Equilibria”, QD504 .P73 1999
- Poling, B. E. *et al.* “The Properties of Gases and Liquids”, TP242 .P62 2001
- Atkins, P. W. Friedman, R. S., “Molecular Quantum Mechanics”, QD462 A84 1997 (3rd edition) (at the Chemistry Library Reserve desk)

## Class Schedule

Lec.	DATE	DAY	TOPIC	READING*
1	25 Aug	M	Introduction, laws of thermodynamics, notation.	TM:2
2	27 Aug	W	Heat and work.	TM:3,4
-	1 Sept	M	Labor Day—no class.	
3	3 Sept	W	Gibbsian equations, chemical potential.	TM:5.1–5.3
4	8 Sept	M	Mathematical methods, Legendre transforms	TM:5.6,5.7, W:2.1–2.7
5	10 Sept	W	Partial derivative game.	TM:5.8–5.10
6	15 Sept	M	Process evaluation. Residual functions.	W:11.1–11.5, TM:8.5
7	17 Sept	W	Residual functions and example problems.	
8	22 Sept	M	Introduction to statistical mechanics.	R:1.1–1.4
9	24 Sept	W	Quantum mechanics I.	R:1.4–1.5
-	29 Sept	M	<b>Exam 1.</b>	
10	1 Oct	W	Quantum mechanics II.	R:1.4–1.5
11	6 Oct	M	Quantum mechanics III.	R:1.4–1.5
12	8 Oct	W	Statistics and ensembles.	R:2.1–2.3
00	13 Oct	M	No class. Lecture moved to Tuesday	
13	14 Oct	Tu	Ensembles & partition functions.	R:2.4–2.5
14	15 Oct	W	Semi-classical partition function.	R:3.1–3.4
15	20 Oct	M	Properties of ideal gases.	R:3.5–3.6
16	22 Oct	W	Properties of ideal gases, examples.	
17	27 Oct	M	Example calculations.	TM:16, R:3, W:10.1–10.4
18	29 Oct	W	Chemical equilibria: ideal & real fluids.	TM:17, W:10.5
-	3 Nov	M	<b>Exam 2.</b>	
19	5 Nov	W	Pair potentials and nonideal behavior. van der Waals partition function.	R:5, W:1.2, 1.7 R:6, W:1.4
20	10 Nov	M	Conformal solution theory.	TM:8.3, W:1.5–1.6
21	12 Nov	W	Conformal solution theory, pure fluids & mixtures.	R:11.1–11.2, W:1.3
22	17 Nov	M	(AIChE) Ideal solutions & partial molar quantities.	TM:9.1–9.3
23	19 Nov	W	(AIChE) Partial molar properties & fugacity.	TM: 9.6–9.8; R:11.3–11.5
24	24 Nov	M	Local composition models.	R:9.1–9.2
-	26 Nov	W	Thanksgiving Recess.	
25	1 Dec	M	Crystalline solids.	R:4.1–4.2
26	3 Dec	W	Surface adsorption.	R:4.3
27	8 Dec	M	Molecular simulations. (Note: class in 1239 BEH)	R: 7,8
-	10 Dec	W	<b>Final Exam.</b>	

\*Abbreviations in the READING column refer to books listed on the course reserve list. They are keyed according to author as follows: R = Rowley; C = Chandler; W = Walas; TM = Tester & Modell. The notation TM:2, for example, means chapter 2 in Tester & Modell's "Thermodynamics and Its Applications".