155:511 Advanced Chemical Engineering Thermodynamics **Fall 2016**

Instructor: Prof. Yee C. Chiew
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Meeting place/time: SEC-117, Busch; Thursday, 5:00pm – 8:00pm

Required textbook:
J. J. de Pablo and J. D. Schieber, "Molecular Engineering Thermodynamics," Cambridge University Press, 2014.

Suggested textbooks:
Koretsky, M. D., "Engineering and Chemical Thermodynamics," 2nd edition, Wiley, 2012.
Smith, van Ness and Abbott, "Introduction to Chemical Engineering Thermodynamics," McGraw-Hill, 7th edition, 2005.
Dill, K. A. and Bromberg, S., "Molecular Driving Forces – Statistical Thermodynamiacs in Biology, Chemistry, Physics, and Nanoscience," 2nd edition, Garland Science, 2011.

A course website is available on Sakai.rutgers.edu. Information about the course will be communicated and course materials will be distributed through the course website. Make sure to access the Sakai course website to download course materials.

Course Outline:
This course presents the foundational principles and laws of thermodynamics and an introduction to statistical mechanics. Emphasis will be placed on modeling the thermodynamic properties of gaseous, liquids, and solids and fluid phase equilibria. Molecular thermodynamics will be employed to interpret and estimate material properties. Quantitative thermodynamic models for a great variety of systems relevant to a broad range of practical applications will be discussed.

Students successfully completing this course will learn the principles of thermodynamics and apply molecular thermodynamic models to estimate the thermodynamic properties and phase equilibria encountered in chemical and biochemical engineering.

Homework
Homework problems will be assigned. Students are expected to complete and hand in all assigned homework problems on due dates. Selected homework problems will be graded.

Assessment: Homework and Project 40%, Exams (2) 60%

Course contents:

	Topic	Chapters
1	Foundations of thermodynamics, postulates of thermodynamics, thermodynamic potentials, Legendre transforms, fundamental equations, extremum principles, thermodynamic relations	Chapters 1 – 3
2	Phase equilibrium, thermodynamic stability, thermodynamic phase diagrams	Chapter 4
3	Applications of laws of thermodynamics to processes and engineering systems, power cycles and refrigeration cycles	Chapter 5
4	Introduction to statistical mechanics – canonical and grand canonical ensembles, statistical mechanics of ideal gases, Langmuir adsorption; intermolecular interactions, molecular simulations	Chapter 6 – 7
5	Gaseous fugacity, fugacity coefficient, vapor-liquid equilibrium, Lewis fugacity mixing rule, solute solubility in compressed gases	Chapter 8
6	Liquid fugacity, activity coefficient, theories of solutions, molecular models for activity coefficients and excess Gibbs energy	Chapter 9
7	Selected topics	Chapter 10 – 12

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- obtain all data or results by ethical means and report them accurately without suppressing any results inconsistent with his or her interpretation or conclusions
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