CHBE 451/551 Applied Statistical Thermodynamics – 2020 W2

Course Description: In this course, we will build the fundamental concepts of thermodynamics from both classical and statistical mechanics perspectives. We will learn to apply these concepts using molecular simulation. Fundamental equation of thermodynamics and various other laws will be derived using statistical thermodynamic theory, providing molecular interpretation to basic concepts such as energy and entropy. These methods will be applied to the analysis of various systems and processes using Monte Carlo and molecular dynamics simulations. Current research questions in engineering will be addressed using simplified physical models.

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Lectures:

M 10:00-11:20am Room:
W 10:00-11:20am Room:

Recommended textbooks:

- *Molecular Thermodynamics of Fluid-Phase Equilibria* by J.M. Prausnitz, Prentice Hall, 1999. Ch. 1-6.
- *Thermodynamics and Statistical Mechanics - An Integrated Approach* by M. Scott Shell, Cambridge Press, 2015.
- *Computer Simulation of Liquids* by M.P. Allen and D.J. Tildesley, Oxford University Press, 2017.

Course Website: Course website can be accessed at www.canvas.ubc.ca. A campus wide login is required to access this website.

Prerequisites: Exposure to basic undergraduate thermodynamics, multivariate calculus and elementary probability and statistics. Basic experience with programming (in any language).

Grades: Your performance will be evaluated through 2 midterm exams (50%), a term project (30%), and participation (20%). **MIDTERM DATES: February 8 & March 15.**

CHBE 451:. The undergraduate student will be given an option to turn in suggested problems for each assignment. The student will be expected to reproduce part of a published work of choice for the term project.

CHBE 551: The graduate student will be given a fundamentally more complex midterm. The term project will consist of applying the methods learned to a new research question of their interest.

Course Learning Outcomes: Upon successful completion of this course, students will be able to

- identify and define thermodynamics problems in engineering applications
- obtain a molecular understanding of thermophysical properties of condensed systems
- apply thermodynamic principles to gases, solutions, solids and reaction systems
- gain understanding of modern simulation techniques
- set up, program, and utilize molecular simulation and visualization tools
- understand the limitations and sources of error of molecular simulation
- set up and solve simplified problems using molecular theories relevant to research in modern chemical and biological engineering

Academic Integrity: The academic enterprise is founded on honesty, civility, and integrity. As members of this enterprise, all students are expected to know, understand, and follow the codes of conduct regarding academic integrity. At the most basic level, this means submitting only original work done by you and acknowledging all sources of information or ideas and attributing them to others as required. This also means you should not cheat, copy, or mislead others about what is your work. Violations of academic integrity (i.e., misconduct) lead to the breakdown of the academic enterprise, and therefore serious consequences arise and harsh sanctions are imposed. For example, incidences of plagiarism or cheating may result in a mark of zero on the assignment or exam and more serious consequences may apply if the matter is referred to the President's Advisory Committee on Student Discipline. Careful records are kept in order to monitor and prevent recurrences. Link to the relevant Calendar section:
http://www.calendar.ubc.ca/vancouver/index.cfm?tree=3,286,0,0.

Topics to be covered:

- Thermodynamics of phase-equilibria
    - Phase and Chemical Equilibria
    - Thermodynamic properties from PVT data
    - Intermolecular forces
    - Calculating the fugacity of gas mixtures
    - Calculating the activity of liquid mixtures

- Statistical Mechanical Ensembles
    - Postulates of statistical thermodynamics
    - Ensemble averages
    - Statistical perspective of the laws of thermodynamics
    - Fluctuations

- Molecular simulations
    - Force fields and intermolecular force
    - Metropolis Monte Carlo method
    - Molecular dynamics method with LAMMPS software
    - VMD visualization software