Syllabus - **CHE 317 - Chemical Dynamics**

Fall Semester — 4 semester hours credit
Class: Hederman Science Building, Room 312 — MWF 11:00 - 11:50 AM
Laboratory: Hederman Science Building, Room 405 — M or W 1:30 - 4:30 PM

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Instructional Materials:
The required text is *Physical Chemistry, 2nd edition* by Thomas Engel and Philip Reid. In addition to this text you will need a scientific calculator. General procedures for individual laboratory experiments will be distributed as well as many of the class notes.

Prerequisites:
Differential and integral calculus, general physics, and CHE 241. The latter may be taken as a co-requisite.

Disclaimer:
Although I expect to conduct the course according to the following, I reserve the right to make modifications if circumstances dictate.

Course description: A study of the thermodynamics and kinetics of chemical processes.

Rationale:
Physics is the fundamental science, while chemistry is the central science. Thus, this first course in physical chemistry is a study of the fundamentals of the central science. It not only presents the underpinnings for much of the chemistry which a student has already encountered, it provides a foundation in physical chemistry for all future chemical study. Development of problem solving and critical thinking skills are stressed.

Attendance:
Your attendance at all class meetings is expected. Please refer to the *Mississippi College Undergraduate Bulletin* for a discussion of the university's attendance policy. Absences are recorded on the grade report at the end of the semester. If a regular class meeting is missed, it is the student's responsibility to obtain any assignments or instructions that were given by the instructor. Missing a class is **not** an excuse for not preparing for the next class meeting or not having an assignment ready on time. **Do not miss a scheduled test!** In the event of an extreme emergency and an excused absence, a make-up test will be given. The test must be made up prior to the graded tests being returned to the class. Make-up tests are usually different from the regular test and may be more difficult. If the student cannot return to class until after the tests have been returned, the grade on the final exam may be substituted for the missing grade.

Methods of Instruction: Class will consist primarily of lectures and working problems.

Academic integrity:
Mississippi College students are expected to be honest. Please refer to the *Mississippi College Undergraduate Bulletin* for a discussion of honesty. Also refer to the *Mississippi College Tomahawk* or to University Policy 2.19.

Course and Lab Overview:
The course covers material presented in chapters 1-10 of the textbook. The laboratory provides the opportunity to measure physical and chemical constants related to the theory studied in class. In addition to demonstrating established principles and reinforcing and expanding one's understanding of the basic concepts, the lab should help to develop research aptitudes by providing experience with the types of experiments and instrumentation that can yield new results in a given field. In addition, statistics will be emphasized in determining how precisely a given physical or chemical constant was measured. In short, the aim is to train not lab techs, but research scientists.

Brief Course Outline:
I. Mathematical Review
II. Equations of State
III. Critical Behavior of Fluids
IV. Partition Functions
V. First Law of Thermodynamics
VI Second Law of Thermodynamics
VII. Third Law of Thermodynamics
VIII. Free Energy
IX. Phase Equilibria
X. Chemical Equilibria
XI. Kinetic Theory of Gasses
XII. Chemical Kinetics

Grading:
Two or three tests will be given during the semester, each with a value of 100 points. These tests will most likely be given after the study of the first law, after the study of phase equilibria, and after the study of chemical kinetics. Unannounced pop tests are occasionally given, the total number of pop test points and points from homework assignments will be approximately 50. Pop tests that are missed are <u>not</u> made up. The final exam is comprehensive and is worth 200 points. Laboratory participation, laboratory computer assignments, and lab reports together total 125 points. The course grade is determined by dividing your grand total by the total possible points. Final letter grades are determined on an 11-point scale. Please refer to the *Mississippi College Undergraduate Bulletin* for a discussion of the university's grading system and how quality points are assigned.

Required Practices:
You are expected to read the appropriate sections of your text and work any problems assigned before coming to class. Periodically throughout the semester special problem sets will be distributed which must be completed for a grade. These grades will be added to quiz grades as discussed above. Also, as previously mentioned, you will need a good scientific calculator and be fairly proficient with it.

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Learning Objectives: (*This is not an exhaustive list.*)

1) Learn to use differential and integral calculus in chemical and physical problems.
2) Learn how to expand a function as a power series.
3) Learn how to regress experimental data with a calculator and with a spreadsheet to find the line of best fit and the correlation coefficient.
4) Learn how to numerically integrate experimental data.
5) Learn how to find roots of equations numerically.
6) Learn how to determine partial derivatives.
7) Learn how to find the total differential of a function of several variables.
8) Learn the difference between exact and inexact differentials and how these relate to thermodynamic functions.
9) Learn how to compute state functions from various equations of state, particularly for gases.
10) Learn about the virial equation and learn how to compute second virial coefficients.
11) Learn about the critical temperature, the critical pressure, and critical volume of fluids and how the behavior of different fluids are related through the Law of Corresponding States.
12) Learn how to compute molecular partition functions for different substances and learn how these can be used to compute bulk thermodynamic properties.
13) Learn how heat and work are related through the First Law of Thermodynamics.
14) Learn what the heat capacity of a substance is, how the heat capacity of a substance is related to the vibrational modes of the molecules which compose a substance, and learn the difference between the heat capacity at constant volume and the heat capacity at constant pressure.
15) Learn the true definition of entropy, how entropy is related to the Second Law of Thermodynamics, and how entropy is related to disorder and randomness.
16) Learn how to calculate heat, work, internal energy, enthalpy, and entropy for different chemical and physical processes.
17) Learn how to solve partial differential equations related to the First and Second Laws of Thermodynamics.
18) Learn how the Third Law of Thermodynamics defines both a zero point for entropy measurements and an absolute zero temperature.
19) Learn what is meant by free energy, how it is related to energy and entropy and to the spontaneity of a process.
20) Learn how the Gibbs free energy is related to the chemical potential of a pure substance and how the chemical potential relates to phase equilibria.
21) Learn how to approximate the activities of species in a chemical reaction and how these activities are related to the equilibrium constant.

22) Learn how the Gibbs free energy of a process is related to the equilibrium constant.
23) Learn how to solve for the extent of a reaction using the equilibrium constant.
24) From the kinetic theory of gases, learn how to compute the most probable speed, the average speed, and the root-mean-square speed of molecules of a gas.
25) Learn what is meant by the order and the half-life of a reaction.
26) Learn how to derive and use the integrated rate laws for simple kinetic reactions.
27) Learn how mechanistic reactions are related to the overall stoichiometric reaction.
28) Learn the difference between a transition state and a reaction intermediate.
29) Learn how a catalyst speeds up a reaction by lowering the activation energy.
30) Learn how to compute activation barriers by measuring how rate coefficients vary with temperature.