It is your responsibility to be aware of all announcements that may be made in class during this semester. If warranted by circumstances, the instructor may modify course policies during the semester.

**CLASS**
CHEM–5396–001 Advanced Physical Chemistry

**ROOM**
FOSC 313

**TIME**
TBA

**INSTRUCTOR**
W. Horstemke

Office: 313 FS, Phone: 214–768–4241

e-mail: whorsthe@mail.smu.edu

web page: http://faculty.smu.edu/whorsthe

**OFFICE HOURS**
by appointment

**TEXT**

**HOMEWORK**
Three homework assignments. Homework may be discussed, but all written work must be prepared independently.

**TERM PAPER**
A short term paper on a topic concerning the Belousov-Zhabotinsky reaction, the chlorite-iodide malonic acid reaction or chlorine dioxide-iodine-malonic acid reaction. You may choose a different topic, subject to instructor approval. The term paper may be submitted electronically (pdf format only) or in hard copy. A tentative title of the term paper is due by October 16, 2013, a preliminary outline by November 6, 2013. The term paper is due by Monday, December 9, 2013.

**TESTS & FINAL**
None

**COURSE GRADE**
The final course grade will be based on the score of the three homework assignments, each 20%, and the term paper, 40%.

The SMU Undergraduate Bulletin stipulates that “A student may receive a grade of Incomplete (I) if the majority of the course requirements have been completed with passing grades but for some justifiable reason, acceptable to the instructor, the student is unable to complete the full requirements of the course. In accordance with University policy, at the time an Incomplete is given the instructor must stipulate in writing to the student and to the University Registrar the requirements and completion date that are to be met and the grade that will be given if the requirements are not met by the completion date. The maximum period of time allowed to clear the Incomplete grade for an undergraduate course is 12 months.”

A grade of Incomplete (I) will be assigned only if you have completed two homework assignments and the term paper or all three homework assignments, resulting in an overall grade of at least a C−.
No work other than the homework and the term paper can be considered for the final grade.

Policies

1. Disability Accommodations: Students needing academic accommodations for a disability must first be registered with Disability Accommodations & Success Strategies (DASS) to verify the disability and to establish eligibility for accommodations. Students may call 214-768-1470 or visit http://www.smu.edu/alec/dass.asp to begin the process. Once registered, students should then schedule an appointment with the professor as soon as possible, but no later than two weeks before the first test, to make appropriate arrangements.

2. Religious Observance: Religiously observant students wishing to be absent on holidays that require missing class should notify the instructor in writing at the beginning of the semester, and should discuss, in advance, acceptable ways of making up any work missed because of the absence. The last day to request excused absence for observance of a religious holiday is Wednesday, September 11, 2013.

3. Excused Absences for University Extracurricular Activities: Students participating in an officially sanctioned, scheduled University extracurricular activity will be given the opportunity to make up class assignments or other graded assignments missed as a result of their participation. It is the responsibility of the student to make arrangements with the instructor prior to any missed scheduled examination or other missed assignment for making up the work.

4. Policy on Academic Dishonesty: All work undertaken and submitted in this course is governed by the University's Honor Code. Students who violate University rules on academic dishonesty (the SMU Honor Code) are subject to disciplinary penalties, including the possibility of failure in the course and/or dismissal from the University. Since such dishonesty harms the individual, all students, and the integrity of the University, policies on academic dishonesty will be strictly enforced. You agree to abide by the SMU Honor Code, though there may not be a specific pledge on a test or final.

Course Outline

1. Review of elementary kinetics
2. Transport processes: Molecules in motion
3. History of nonlinear chemical phenomena
4. Well-stirred reactors I (bistability): One-variable pool chemical models – Schlögl I and II models; Verhulst model
5. Well-stirred reactors II (oscillations): Two-variable pool chemical models – Lotka-Volterra model, Brusselator
7. Well-stirred reactors IV (models of oscillating reactions): Oregonator model of the Belousov-Zhabotinsky reaction; Lengyel-Epstein model of the chlorite-iodide malonic acid reaction and chlorine dioxide-iodine-malonic acid reaction

8. Reaction-diffusion systems: Turing instability; front propagation

9. Stochastic kinetics: Effects of internal fluctuations and external noise

**OBJECTIVES**

You should be able to use the methods of chemical kinetics and nonlinear chemical dynamics to determine the spatial and temporal behavior of reacting and diffusing systems.

1. You should be able to formulate rate equations for a given mechanism and solve them.

2. You should be able to determine properties related to transport in gases and liquids.

3. You should be able to determine the steady states and their stability for well-stirred reacting systems with one or two species.

4. You should be able to determine the steady states and their stability for reacting and diffusing systems with one or two species.

5. You should be able to calculate simple characteristics of the probability distribution of well-stirred systems with one species subject to internal fluctuations or external noise.