**PORTLAND STATE UNIVERSITY**

**DEPARTMENT OF CHEMISTRY** **Winter, 2007**

CHEMISTRY 410/510: ADVANCED TOPICS IN PHYSICAL CHEMISTRY

**Course Title:** ***Nonlinear Dynamics and Chaos from Chemical, Physical and Biological Systems*** [Physical Chemistry Graduate Course: offered under the official PSU title of *'Advanced Topic in Physical Chemistry'*] This course is cross-referenced as Chem 410 for those undergraduate students who might want to take the course.

Prerequisites: An adequate mathematics background (working knowledge of ODE's preferable but not essential), Chem 440, Chem 441 (or equivalent). For students from other departments, consult with the professor first before registering for the course (see contact details below).

Instructor: **Reuben H. Simoyi** (SB2 372, phone 5-3895, rsimoyi@pdx.edu)

Office Hours: Monday, Wednesday; 2:30 - 3:30 PM (Final office hours to be set after first week of classes).

Timetable: Two 75-minute lectures per week on **Mondays and Wednesdays; 1500 – 1615**. Final timetable will be set after first week of classes. These times may end up being retained, or they may be altered, depending on students' schedules.

Venue: **SB1 304**

Textbook: 'An Introduction to Nonlinear Chemical Dynamics' by I. R. Epstein and J. A. Pojman; Oxford University Press (1998), ISBN # 0-19-509670-3 (recommended).

Other Texts: 'Chaos and Nonlinear Dynamics' R. C. Hilborn, Oxford University Press (1994), ISBN # 0-19-508816-6; 'Chemical Oscillations and Instabilities' P. Gray and S. Scott, Oxford University Press ISBN # 0-19-855864-3; 'Chemical Chaos', S. Scott, Oxford University Press, ISBN # 0-19-855658-6.

## Introduction

*Preamble:* The existence of chaos had been postulated by the great French mathematician, Poincare', but it was Lorenz who suggested its existence in dissipative dynamical systems, starting with hydrodynamic fluid flow. Lorenz proved that chaos can exist in systems with three or more coupled ordinary differential equations. Feigenbaum also proved that chaos can exist in discrete onto mappings via the period-doubling sequence. What was most important is that simple mathematical models can generate chaotic behavior and that these simple models could be used to describe very complex real systems. Chaos is the name given to intrinsic randomness, which is random behavior arising from deterministic systems. Chemical chaos in particular has been restricted to the behavior of chemical oscillatory systems. With the help of a suitable bifurcation parameter, e.g. temperature, flow rate or concentrations, the continuous oscillatory system can be studied by applying discrete recursive formulae and symbolic dynamics. Chaotic behavior can also be observed in many physically unrelated systems.

Chaotic behavior as applied to nonlinear systems should be characterized by positive Lyapunov exponents, continuous Fourier spectra and strange attractors with fractal structures.

This course will attempt to take the student from the basic mechanistic understanding of clock reaction behavior, to the generation of complex oscillatory dynamics and the link to chaotic behavior.

**General Syllabus.**

**I**

*Introduction:* far from equilibrium behavior, feedback loops, clock behavior, autocatalysis. Simple models, the Lotka-Volterra scheme, the Brusselator model, bistability, flow diagrams, reaction-diffusion schemes.

**II**

*Chemical Kinetics:* Mechanisms, the Belousov-Zhabotinsky reaction, stability analysis, the Jacobian, eigenvalues and eigenvectors, multivariable systems, attractors, phase diagrams, oscillatory dynamics, the FKN mechanism.

**III**

*Experimental techniques:* Systematic design of chemical oscillators, batch and flow reactors, the CSTR environment and design, (the chlorite-iodide system is used as an example for most of this section).

**IV**

*Biological oscillators:* cell cycles, neural oscillators and networks, bursting.

**V**

*Modeling:* Computational tools, stiff ODE's, semi-implicit methods, Euler, Taylor, Runge Kutta techniques.

**VI**

*Chemical chaos:* complex oscillations, mixed-mode oscillations, Farey arithmetic, one-dimensional maps, period doubling in the BZ system, map iterations, symbolic dynamics, characterizing chaos, Lyapunov exponents, strange attractors, (controlling chaos), universality, Faigenbaum numbers.

**VII**

*Chaotic dynamics:* (this section will deal with non-chemical systems that show chaotic dynamics). The RLC circuit and its route to chaos and bifurcation diagram; biological population growth; the Lorenz model for convecting fluid.

**VIII**

*Waves and patterns:* Stability analysis, $IO_3^-/H_3AsO_3$ system; propagator-controller system, wave initiation, curvature, spirals.

**IX**

*Convective instabilities:* multicomponent and double-diffusive convection, Marangoni convection, electric field effects, Rayleigh-Benard convection, Benard-Marangoni convection, Navier-Stokes equations. Turing patterns, the CIMA reaction and the chlorite-thiourea reaction.

Each section should take 3- 4 lectures. Some sections, such as IV and VIII will not be handled in too much detail so that class will spend more time on the introductory aspects of the course which are covered in sections I and II. The class needs a good base from which to build upon. There is really no true text book which will cover topics in this course to the level the professor would prefer, but the *Epstein and Pojman* book is as close as any other text, which is why it is the recommended text. Most lecture material will be pulled out of recent literature publications. Guest professors may pop up for some items listed in sections II and V.

I hope students will have a lot of fun in this course while still learning a lot. It is a very fascinating topic and one can really get lost in it. This subject is a little like golf: once you get into it, you become addicted.

***PS***

The professor wrote the following poem (Sonnet minus 10 lines!) during his stint as a postdoctoral fellow at the University of Texas after discovering the Universal Sequence (**U-sequence**) of *Metropolis, Stein and Stein* in the BZ system:

**"The U-sequence is now really quite tame**
**With Simoyi, Wolf and Swinney, they've put it to shame**
**With an 'R' here and an 'L' here, that's the name of the game**
**And if you want to reverse bifurcate, it is still all the same"**

- R. Simoyi

- based on the work published in *Phys. Rev. Lett. Vol 49, pp245 - 8 (R. Simoyi. A. Wolf and H. Swinney)*