Nonlinear Dynamics Lab

May 10, 2013

Report due May 17, 2013

The work on this task-sheet should be written up in a very brief (about one type-written page) report. The equation numbers refer to equations in the paper C.R. Gray, *An analysis of the Belousov–Zhabotinskii reaction*, Rose–Hulman Undergraduate Mathematics Journal **3**(1), 2002.

You should assume the parameter values stated in the paper, in particular, $f = 3/2$.

1. Consider the reduced FKN mechanism for the BZ reaction, given as equation (8–9) in the paper by Gray. Get an analytic approximation for the period of the oscillation using the "relaxation oscillation" analysis presented in class.

   (You may use any kind of analytical or numerical integration scheme when convenient.)

2. *Alternative task:* Solve the Oregonator system (5–7) numerically and measure the period of oscillation.

3. Very briefly compare the results from 1 and 2, where you should refer to the complementary result from one of your classmates.

4. Write a brief description of the laboratory experiment, listing the chemicals used, their concentrations, and the procedure. Measure the period of oscillations in the stirred case and describe the patterns in the unstirred case.

Note: In the lab, we will see a Ferroin-catalyzed version of the BZ reaction, different from the FKN mechanism described in Gray, where the main reaction pathways include

$$2\,\mathrm{Br^-} + \mathrm{BrO_3^-} + 3\,\mathrm{H^+} + 3\,\mathrm{H_2Mal} \longrightarrow 3\,\mathrm{HBrMal} + 3\,\mathrm{H_2O} \tag{1}$$

$$\mathrm{BrO_3^-} + 4\,\mathrm{Ferroin^{2+}} + \mathrm{H_2Mal} + 5\,\mathrm{H^+} \longrightarrow 4\,\mathrm{Ferriin^{3+}} + \mathrm{HBrMal} + 3\,\mathrm{H_2O} \tag{2}$$

$$4\,\mathrm{Ferriin^{3+}} + \mathrm{HBrMal} + 2\,\mathrm{H_2O} \longrightarrow 4\,\mathrm{Ferroin^{2+}} + \mathrm{HCOOH} + 2\,\mathrm{CO_2} + 5\,\mathrm{H^+} + \mathrm{Br^-} \tag{3}$$

However, these reactions are insufficient to explain oscillatory behavior. Extending the reaction set to fully describe the observed dynamics is a nontrivial task, but could be a very rewarding Guided Research/Thesis project for anyone interested in the mathematical aspects of chemistry.