Chemistry 4010 Fall 2019
Test 1

Time allowed: 2 hours

Marks: 51

Handwritten notes are allowed. No printed or mechanically reproduced materials of any kind are permitted.

Software allowed: text editor, XPPAUT, calculator. If any other software is found to be in use during this exam, you will receive a grade of zero.

Answers are to be written in the exam booklets provided. If your answer involves the use of software, make sure to describe the calculation and to provide a reasonable sketch of any graphical results.

1. Sketch trajectories in a two-dimensional phase space near each of the following types of equilibrium points: [2 marks each] **6 marks**
   (a) stable node
   (b) unstable node
   (c) saddle point
2. Sketch the bifurcation diagram for a transcritical bifurcation. Be sure to distinguish stable and unstable equilibria, perhaps using solid vs dashed lines, and provide a legend to indicate which line type is which. [3 marks] **3 marks**
3. Explain, using both text and diagrams, the difference between a supercritical and a subcritical Andronov-Hopf bifurcation. [6 marks] **6 marks**

4. The following is a simple mass-action model for a population that reproduces sexually: **20 marks**

$$\mathrm{X} + \mathrm{Y} \xrightarrow{k_x} 2\,\mathrm{X} + \mathrm{Y}$$
$$\mathrm{X} + \mathrm{Y} \xrightarrow{k_y} \mathrm{X} + 2\,\mathrm{Y}$$
$$\mathrm{X} \xrightarrow{d_x}$$
$$\mathrm{Y} \xrightarrow{d_y}$$

The first two "reactions" are reproduction, producing female (X) and male (Y) offspring, respectively. The last two "reactions" represent death. One can imagine *many* improvements to such a model.

(a) Write down the mass-action differential equations for this model. [4 marks]

(b) Determine the equilibrium points of this model. [6 marks]

(c) Carry out **one** of the following analyses:

- A phase-plane analysis of the model
- A linear stability analysis of the two equilibria

Based on your analysis, what does this model predict about the population? [10 marks]

Note: if you try both, **clearly indicate which one I am to grade**. I will **only** grade **one** solution. Absent clear directions from you, I will grade the first solution I find.

5. The peroxidase-oxidase reaction is an enzyme-catalyzed redox reaction that displays bistability in an CSTR. An early model for this reaction involved uncompetitive substrate inhibition, i.e. an unproductive ES_2 complex.[1] The overall rate equation is **16 marks**

$$\frac{dS}{dt} = Q(S_0 - S) - \frac{VS}{1 + \frac{S}{K_M} + \frac{S^2}{K_M K_I}}.$$

(a) Transform this differential equation to dimensionless form. Because we want to vary Q, *do not* use Q in the definitions of your dimensionless *variables*. [5 marks]

(b) What is the equilibrium point when $Q = 0$? [1 mark]

(c) Experimentally, it is easy to vary Q, which represents a pumping rate. Your dimensionless equations should contain a parameter proportional to Q. Generate a bifurcation diagram varying this parameter using AUTO, and demonstrate that there is a range of bistability. Your answer should include a sketch of the bifurcation diagram along with the values of the parameter at the two bifurcation points. Also make sure to name the type of bifurcation observed. [10 marks]

Here are some parameters you can use: $S_0 = 10\,\mu\text{M}$, $V = 1\,\text{s}^{-1}$, $K_M = 1\,\mu\text{M}$, $K_I = 0.5\,\mu\text{M}$. You will of course have to calculate the parameters of your dimensionless representation using these.

[1] Degn, *Nature* **217**, 1047.