

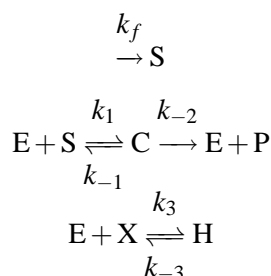
# Chemistry 5850 Fall 2005 Assignment 12

Due: Monday, Dec. 12.

Weight of this assignment: 32 marks

Everybody loves a question to which the professor doesn't know the answer, right?

Quite a few years ago, we studied the open competitive inhibition mechanism [1]:



We can prove that the steady state is locally stable for all values of the parameters. I have never however checked whether a Turing bifurcation was possible.

1. Write down rate equations for the concentrations of S, C and X. Use two mass conservation relations to eliminate other variables from the rate equations. [4 marks]

Note: In the original paper, I used S, E and X, for reasons which had to do with ease of computation of a slow manifold. Here however, it will turn out to be more convenient to use the above variables.

2. Find a scaling in which you can apply Tikhonov's theorem to the rate equation for C, i.e. determine the conditions under which [C] is a fast variable. Use this condition to eliminate [C] from the model, leaving you with a set of dimensionless equations in two variables. [8 marks]

Note: We're doing this because, under the conditions where I think there might be a possibility of a Turing bifurcation, [C] is in fact a fast variable. Moreover, it's much easier to analyze systems in two variables than in three.

3. Now carry out a Turing stability analysis of the two-variable system obtained. Note that, since the steady state of the system is always stable in the absence of diffusion, you don't need to do the stability analysis for that case. You may however have to resort to numerics to search for the Turing bifurcation (assuming there is one, which I'm not at all sure about). In case you do, here is an interesting set of parameters for you to work with:

$$\begin{array}{ll} k_f = 0.45 \text{ M/s} & k_3 = 1000 \text{ M}^{-1} \text{ s}^{-1} \\ k_1 = 10^6 \text{ M}^{-1} \text{ s}^{-1} & k_{-3} = 0.1 \text{ s}^{-1} \\ k_{-1} = 10 \text{ s}^{-1} & [E]_0 = 0.01 \text{ M} \\ k_{-2} = 90 \text{ s}^{-1} & [X]_0 = 0.02 \text{ M} \end{array}$$

[E]<sub>0</sub> and [X]<sub>0</sub> are the total amounts of enzyme and inhibitor. [20 marks]

Note: If there is a Turing bifurcation in this system, it would be very publishable. Whether you are doing the assignments for credit or not, you are therefore encouraged to try your hand at the analysis. If we find anything, everyone who contributed will be included as a coauthor.

## References

- [1] Ngo, L.G., Roussel, M.R.: A new class of biochemical oscillator models based on competitive binding. *Eur. J. Biochem.* **245**, 182–190 (1997)