Introduction to Reactor Design, 3K4

Tutorial 7/Assignment 4

Kevin Dunn, kevin.dunn@mcmaster.ca **Due as part of assignment 4, 15 March**

Objectives of this short assignment:

- To set up reactor models for the human body.
- To carefully plan a reactor design strategy.

Question 1

A drug is taken orally to treat infections in the body. It is effective when a concentration above 0.4 mg/L of body fluid is maintained in the bloodstream (based on volume of body fluid). Ideally, a concentration of around 1.0 mg/L should be maintained in the blood. Side effects can occur if the concentration in the blood exceeds 1.5 mg/L.

The drug is depleted by two pathways, both of which are first order: (1) It can be absorbed into the bloodstream through the stomach walls or (2) it can pass out through the gastrointestinal tract and not be absorbed into the blood. Both of these processes are first order in terms of the drug's concentration in the stomach. Once in the bloodstream, the drug attacks the target cells and is degraded by a zero-order process. The drug can also be removed from the blood and excreted in urine through a first-order process within the kidneys.

One dose of the drug is 300 mg in liquid form; and the volume of fluid in a typical adult body is approximately 45 L.

In the stomach there is absorption into the blood with $k_1 = 0.15\,\text{hour}^{-1}$ and elimination through the gastrointestinal tract at $k_2 = 0.6\,\text{hour}^{-1}$.

In the bloodstream the drug degrades with $k_3 = 0.1\,\text{mg.L}^{-1}\text{.hour}^{-1}$ [*note*: a zero-th order reaction can only proceed if the reactant is present]. Elimination through urine is according to $k_4 = 0.2\,\text{hour}^{-1}$.

1. Plot the concentration of the drug in the blood stream as a function of time when a single dose is taken. Clearly state all your assumptions. Clearly describe your plan to solve this problem at the start of your answer.
2. Simulate a 48 hour period in the body and find how often the patient should be told to take the drug.
3. Comment on any potential hazards; e.g. what should a patient do if they take two doses instead of one? What would happen if a patient takes half a dose, but twice as frequent?
4. How might the rate constants, k_1 and k_2 change if the drug is taken on a full stomach; or an empty stomach?

5. Simulate the case of an empty stomach and observe what happens to the drug concentration in the blood stream.

END