Modeling and Simulation, CS302

Lab-1

Due Date: Tuesday 21 Jan 2020

1. Consider the following different scenarios for drug delivery. In each of them construct appropriate abstract models, mathematical model and implement it on the computer to obtain the result.

   (a) Imagine a situation in which the drug immediately reaches the body, distributes almost instantaneously to all parts of the body and is eliminated out. It can be assumed that the rate at which the drug is excreted out depends on the instantaneous concentration. The rate at which the drug leaves the body is $k = 0.1386/hr$. Suppose that 6 units of the drug are taken initially. Based on your mathematical model show how the drug concentration changes in the bloodstream with time over a period of 1 day. Comment on how the behavior changes as the rate k is changed. Instead if the dosage was 6 units for the first 5 hours how would the behavior change in time.

   (b) Let us assume that the drug is taken at regular intervals of time (T). The other assumptions are the same as in part (a) above. The therapeutic level of the concentration of the drug is in between 10 and 25 units. The drug will be administered for upto 10 days. Estimate the range of intervals at which it should be administered so that it remains within the therapeutic levels. Does the time required to achieve constant levels depend on these intervals?

   (c) Let us assume that the therapeutic limit is between 250 and 600 units. Other conditions are similar to part (b) above, but to achieve this the drug is administered continuously for a certain duration (τ). During this duration ($T + \tau$) 6 units are administered at each instant (per minute). Numerically, obtain an estimate for both T and τ so that the drug is within the therapeutic limit.

   (d) Now consider the situation in which the drug enters the GI-tract instantaneously and then slowly diffuses into the blood stream. Let the proportionality constant for this process be k_1. Modify your model appropriately. Assume that $k_1 = 1.386/hr$ and $k = 0.1386/hr$. Let the initial intake be 6 units. What is the highest level of the drug in the blood. Understand the behavior observed. Now, administer a continuous supply of 6 units of drug at all times. Analyze the behavior for 24 hours.

(e) Assuming regular dosage at time T and with therapeutic level set to the one in part (b). Obtain a numerical estimate to the bounds for the intervals.

(f) Assume regular dosage for a duration τ. The therapeutic levels are assumed to be the same as in part (c). Numerically obtain an estimate for T and τ so that the concentration is within the therapeutic limits.

- **Report:** The above set of exercises are merely a way to develop an understanding via a model and numerical simulation. Write a report using the understanding developed above. The report should have the following abstract, introduction, model, result and conclusion. The abstract should tell the reader what to expect in the report. The introduction should introduce the topic with the relevant assumtptions and different scenarios. The model should introduce the mathematical model. All the constants and variables should be defined here. The result should be used to present the analysis. Since we are using two different frameworks (a)-(c) and (d) -(f) it would be important to do a comparative analysis of the behaviors observed.
- The report should not be more than 4 pages 2 columns. The latex template will be provided if required.