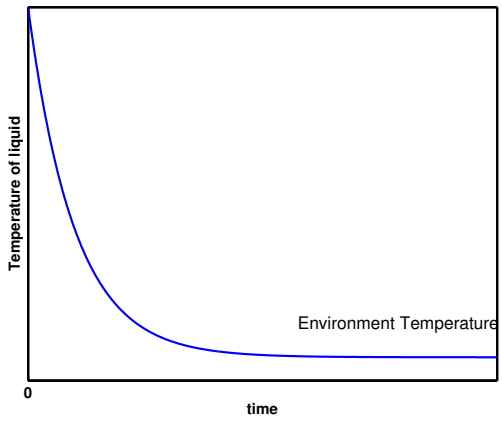
Modeling and Simulation, CS302

Lab-1

Due Date: Sunday 22nd Jan,2016

1. Newton's Law of Cooling: When a hot liquid is placed in a cooler environment, its temperature decreases to its surrounding. The figure below shows a typical decrease in the temperature of the liquid. Initially, there is a rapid decrease in the temperature, and finally it decreases to the value of the environment temperature. Newton's law of cooling assumes that the rate of change of temperature (T) with respect to time (t) of an object is proportional to the difference between the temperature of the object and its surroundings (T_m).



   (a) Write down the differential equation that models Newton's law.

   (b) Solve this equation for T as a function of t.

   (c) Assuming $T_m = 25^o$C, suppose cold water at 6^oC is placed in a room. After $1h$, the temperature of the water is 20^oC. Determine all the constants in the equation for T.

   (d) How long will it take for the water to warm to 12^oC in part (c) ?

   (e) Implement your model of Newton's law of cooling on the computer using Euler's method. Solve for time step $\Delta t = 1,\ 0.5,\ 0.1,\ 0.05$. What would be a reasonable time step for this model? (Use the values of the parameters from part (c) above). For comparison, plot on the same figure.

2. Consider a two compartment model of drug dosage. The two compartments here can be thought of to represent the gastrointestinal tract (GI-tract) and blood stream. The pill or

drug that is taken first goes to the GI-tract from where it dissolves in the blood stream and then is finally eliminated. Assuming that the rate of change of the drug in either of the compartments is proportional to the amount present model the following three scenarios.

(a) If the drug in the GI-tract immediately dissolves to the blood stream, what would be a reasonable model. Assume that the proportionality constant for drug elimination from the blood stream is k_2 ($k_2 > 0$). Solve analytically.

(b) 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. How will the instantaneous intake be incorporated in your equations. Solve analytically.

(c) If we now break the assumption of instantaneous intake of pills but rather assume that it is taken at regular intervals, how would you modify your model.

3. Implementation on a computer (I suggest that you use Matlab but not the inbuilt ODE solver)

(a) For part(1b) above write a code and obtain the evolution in time of the amount of drug in GI-tract and blood stream. Assume that $k_1 = 1.386/hr$ and $k_2 = 0.1386/hr$. Let the initial intake be 1 units. What is the highest level of the drug in the blood.

(b) Take different values of k_2 ($k_2 = 0.01386,\ 0.06,\ 0.1386,\ 0.6386,\ 1.386$ per hour) and study the effect. Comment on the different behaviors observed. k_1 and initial conditions are the same as in part(2a).

(c) Take $k_2 = 0.0231$ and study the effect of having different values of k_1. ($k_1 = 0.06931, 0.11, 0.691, 1.0, 1.5$).

(d) Part (1c) is for regular dosage. First have a constant supply of 3 units of the drug at all times. Analyze the behavior for 24 hours. Assume that at $t = 0$ there is no drug in the GI-tract or blood stream. Initial conditions are the same as in part(2a).

(e) Now modify your code for repeated dosage. Assume that the drug is administered for 1/2 hour every 6 hours. Assume that during the administration phase this intake is a constant at 6 units. Take $k_1 = 0.6931$ and $k_2 = 0.0231$ per hour. How does the amounts in GI-tract and blood stream change over a period of 24 hours.

(f) Assuming that the maximum therapeutic limit is at 20 units in the blood stream what is the time duration after which the drug will have adverse effect.

(g) Now assume that the drug is taken every 8 hours. Assume all other conditions to be the same as in part (f) determine if the drug will have an adverse effect or not.

4. In this problem we attempt to look at a simple blood alcohol levels in humans. There are many factors that influence the body's ability to absorb alcohol. These include person's weight, percentage of body fat and age. An important quantity is the blood alcohol level (BAL), more body weight implies that a person has more water in his body and hence alcohol can be absorbed quickly. Older people absorb alcohol at a slower rate due to their decreased metabolic activity. The presence of food in the GI-tract can also effect the BAL. Soon after the alcohol enters the blood it enters the liver for elimination, which eliminates most of the alcohol. The equation for such a simple model is usually written as:

$$\begin{aligned} \dot{x} &= I - k_1 x \\ \dot{y} &= k_1 x - \frac{k_3 y}{y + M} \end{aligned}$$

$x(t)$ is the alcohol level in the GI tract and $y(t)$ represents the alcohol level in the bloodstream. The typical units are $g/100mL$. The first equation has two terms, I represents the alcohol intake and the second term represents the diffusion from GI tract into the bloodstream. The y equation has the inflow and outflow to the liver term. The outflow is most aptly represented by what is called a Michaelis-Menton function. For $y >> M$ it equals a constant k_3. M is a constant with value 0.005.

Some other information that is relevant is the total volume of body fluid in liters (C) is $0.67w$ for males and $0.82w$ for females, w being the body weight in kilograms. $I = 14n/10C$ where n is the number of drinks (we assume the glass size to be the same in all cases), and $k_3 = 8/10C$. Both I and K_3 have units g/100mL while k_1 and k_2 are dimensionless. Also, for empty stomach drinking we assume $k_1 = k_2$ and for drinking after a substantial meal we assume $k_2 = k_1/2$.

(a) Assuming $k_1 = 6$ and the person takes 3 drinks initially explore the alcohol concentrations in bloodstream and GI tract with time. If BAL above 0.05 leads to dizziness and below it leads to happy feeling, which scenario above would lead to dizziness.

(b) Assuming continuous drinking explore what happens in (a).