Lab Report for Lab -1

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CS-302 Modeling and Simulation course, DA-IICT

NEWTON'S LAW OF COOLING

Problem and Assumptions

Newton's Law of Cooling states that when a hot liquid is placed in a cooler environment, its temperature decreases to its surrounding.

- Hot liquid and the cooler environment consists an isolated system and both have uniform temperature among each of them.
- No energy exchange occurs outside of this isolated system.
- Energy released or gained from cooling or heating of liquid does not affect environment in any ways (i.e. Temperature of environment does not change)

Model and Solution

Newton's law of cooling assumes that the rate of change of temperature of an object (T) with respect to time (t) is proportional to the difference between the temperature of the object and temperature of environment (T_m).

$$\frac{dT}{dt} \propto (T_m - T)$$

$$\frac{dT}{dt} = k(T_m - T) \tag{1}$$

Solving equation(1) using Laplace transform we get,

$$T(t) = (T(0) - T_m)\mathrm{e}^{-kt} + T_m \tag{2}$$

Given initial conditions, $T_m = 25°C$, $T(0) = 6°C$

At time t=1hr, T(t) = 20°C

Solving the equation (2) for k, the value of k is found to be 1.335 hr^{-1}.

To find how long will it take for the water to warm to 12°C, subtitute the value of T(t) = 12 °C in equation (2), the time taken, $t = 0.2842\ hr \approx 17\ minutes$

Results

As we can see from figure 1, for Δt less than or 0.1, no oscillations are observed and the values are closer to an exponential curve i.e. approximation is better. Hence $\Delta t = 0.1\ or\ 0.05$ would be a reasonable time-step for this model.

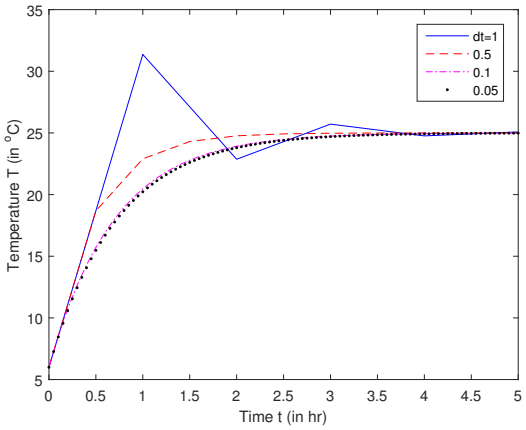


FIG. 1: Numerical simulation of Eq. (1) using Euler's method for different step sizes. The initial conditions are $T_0 = 6^oC,\ T_m = 25^oC,$ and $k = 1.335\ hr^{-1}$.

Conclusion

DRUG DOSAGE MODEL

Problem and Assumptions

Drug dosage model consists of two compartment, 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. The rate of change of the drug in either of the compartments is proportional to the amount present model the following three scenarios.
Some of assumptions taken to model system effectively are as below.

- Drug enters the GI-tract instantaneously.
- Blood and GI tract are homogeneous system. i.e Concentration of drug is same in entire system.
- Initially drug present in system is zero.

One compartment model

the drug in the GI-tract immediately dissolves to the blood stream, and drug elimination occurs from the blood stream.

Let Q(t) be the concentration of drug present in blood at any time t(in hours). Now as drug elimination is proportional to amount present in blood.

$$\frac{dQ}{dt} \propto -Q$$

$$\frac{dQ}{dt} = -k_2 Q \tag{3}$$

Solving eq. 3, we get

(4)

Two compartment model
In this model drug enters the GI-tract instantaneously and then slowly diffuses into the blood stream then in blood

inflow from GI-tract and outflow due to drug elimination occurs.

Let $X(t)$ be the concentration of drug present in GI tract at any time t(in hours) and $Y(t)$ be the concentration of drug present in blood at time t. Now as drug elimination is proportional to amount present in GI tract.

$$\frac{dX}{dt} \propto -X$$

$$\frac{dY}{dt} \propto X - Y$$

$$\frac{dX}{dt} = -k_1 X \tag{5}$$

$$\frac{dY}{dt} = k_1 X - k_2 Y \tag{6}$$

Solving equations (5) and (6) we get,

$$X(t) = X(0)\mathrm{e}^{-k_1 t} \tag{7}$$

$$Y(t) = \frac{k_1 X(0)}{k_1 - k_2}[\mathrm{e}^{-k_2 t} - \mathrm{e}^{-k_1 t}] \tag{8}$$

Two compartment model with regular intervals intake

In this model we add some amount of drug into GI-tract at discrete time which dissolves immediately and slowly diffuses into blood stream.

Here if drug is taken at T intervals then using $X(t) = X_0 - e^{k_1 t}$ and $X(t)$ with $X(t+T)$ we get,

$$X(t+nT) = nX_0 - [e^{-k_1 T}\frac{e^{nk_1 T} - 1}{e^{-k_1 T} - 1}] - e^{-k_1 t}$$

here n = 0,1,2...

Results

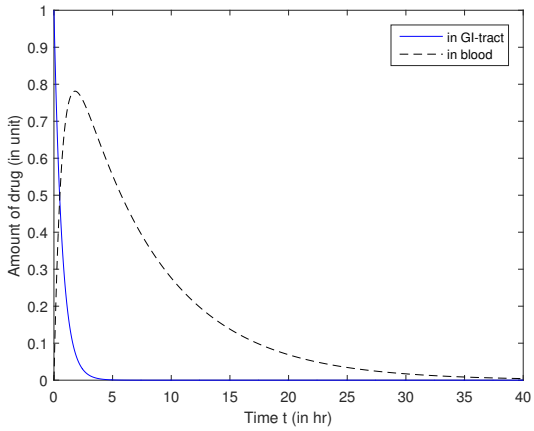


FIG. 2: Numerical simulation of Eq. (5) and Eq. (6) using Euler's method with conditions $k1 = 1.386\ hr^{-1}$, $k2 = 0.1386\ hr^{-1}$ and initial intake $X_0 = 1\ unit$..

In the case shown in fig. 2, the highest level of the drug in the blood is 0.7813 unit. This attains when the drug in GI-tract fully dissolves to the blood stream. Then slowly the amount in blood decreases, and the effect of drug wears off after nearly 40 hours.

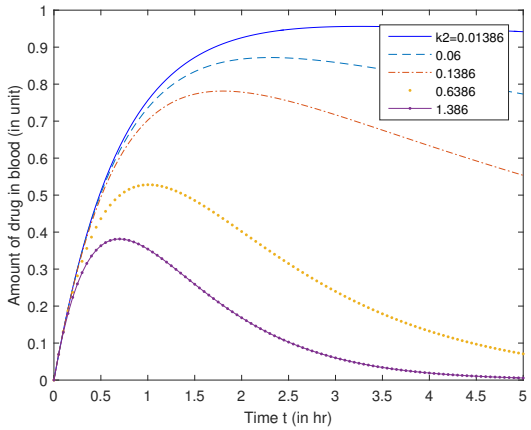
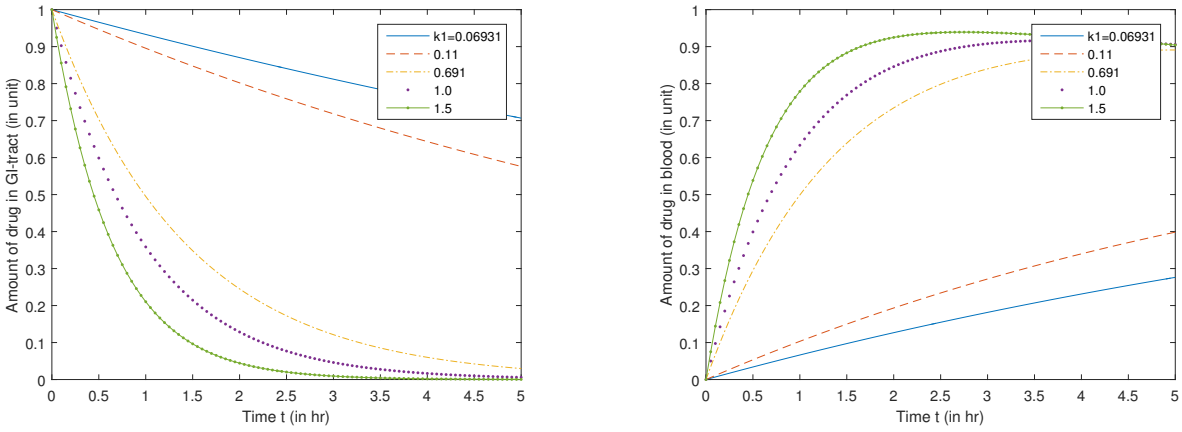


FIG. 3: Numerical simulation of Eq. (6) using Euler's method for different values of k_2 with conditions $k_1 = 1.386\ hr^{-1}$ and initial intake $X_0 = 1\ unit$.

In the case shown in fig. 3, as the value of k_2 increases the highest level of the drug in the blood is attained faster, and then the effect of drug (i.e. amount of drug in blood) wears off quickly. While, the maximum level of drug in the blood attained decreases, as the value of k_2 increases which can be seen in table I.



((a)) ((b))

FIG. 4: Numerical simulation of Eq. (5) and Eq. (6) using Euler's method for different values of k_1 with conditions $k_2 = 0.0231\ hr^{-1}$ and initial intake $X_0 = 1\ unit$.

In the case shown in fig. 4(a), as the value of k_1 increases, the drug in GI-tract dissolves faster into the blood, and drug is removed totally from GI-tract quickly.

In the case shown in fig. 4(b), as the value of k_1 increases the highest level of the drug in the blood is attained slower, and the effect of drug (i.e. amount of drug in blood) doesn't wears off quickly but remains for a longer time. While, the maximum level of drug in the blood attained increases, as the value of k_1 increases which can be seen in table II.

k_2	Highest level of drug in blood
0.01386	0.9561
0.06	0.8719
0.1386	0.7813
0.6386	0.5281
1.386	0.3814

TABLE I: Highest level of drug in the blood for different values of k_2

k_1	Highest level of drug in blood
0.06931	0.2762
0.11	0.3985
0.691	0.8909
1.0	0.9168
1.5	0.9391

TABLE II: Highest level of drug in the blood for different values of k_1

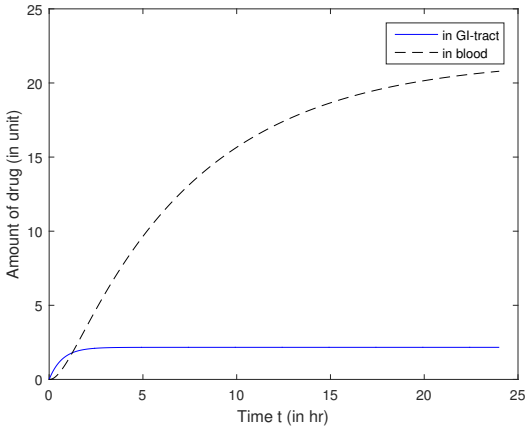


FIG. 5: Two compartment model with regular dosage

Taking regular dosage of 3 units all time for 24 hours with no initial drug present in GI-tract at t=0. We get amount of drug present in system as a function of time as mentioned in Fig. 5.

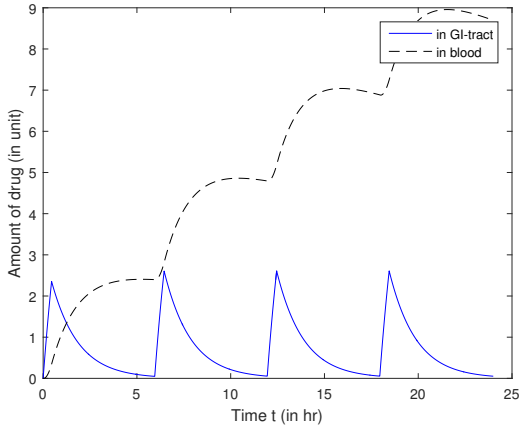


FIG. 6: Two compartment model with regular dosage

Now taking regular dosage of 6 units for 1/2 hour at every 6 hour in 24 hour. We get amount of drug in a system as a function of time as given in fig. 6.

After *103.5 hours* we get to the maximum therapeutic limit which is 20 units in the blood stream. Hence after 103.5 hours drug have adverse effects. After sufficiently long time drug concentration in blood becomes constant for here it is 22.02 units.

Now doing regular dosage for 1/2 hour at every 8 hours, we see that maximum amount of drug present in blood is 16.746 units which is less than maximum therapeutic limit. Hence we can avoid any adverse effect of drugs by taking it at every 8 hours instead of 6 hours.

Conclusion

BLOOD ALCOHOL LEVEL

Problem and Assumptions

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.
- The volume of body fluid is different in males and females.
- The presence of food in the GI-tract can also effect the BAL.
- Both GI-tract and blood stream are homogeneous system i.e. alcohol mixes instantaneously as it enters into the system.

Model

Suppose x(t) is the alcohol level in the GI tract and y(t) represents the alcohol level in the bloodstream. The equation for this simple model is:

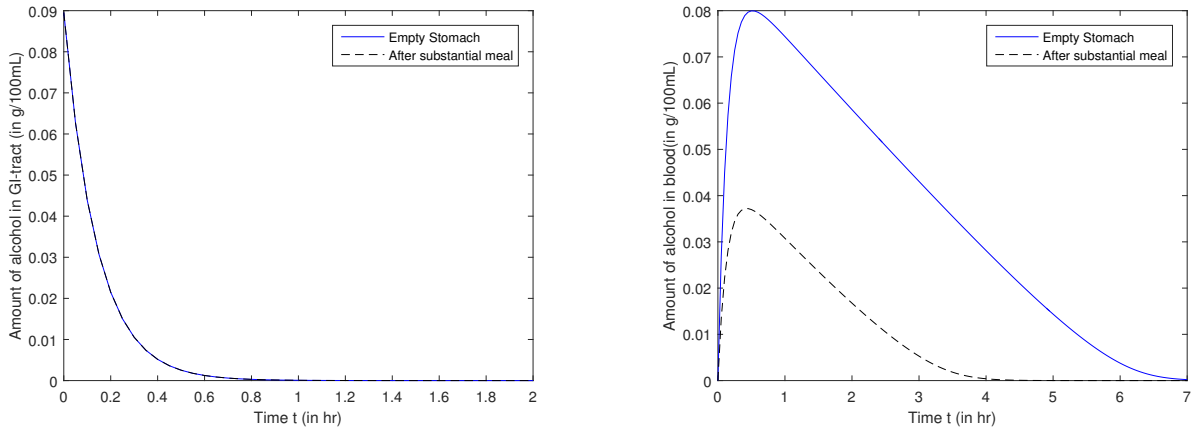
$$\frac{dx}{dt} = I - k_1 x \tag{9}$$

$$\frac{dy}{dt} = k_2 x - \frac{k_3 y}{y + M} \tag{10}$$

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. M is a constant with value 0.005. Total volume of body fluid in liters (C) is 0.67w for males and 0.82w for females, where w is the body weight in kilograms. $I = \frac{14n}{10C}$ where n is the number of drinks, and $k_3 = \frac{8}{10C}$. Also, for empty stomach drinking we assume $k_1 = k_2$ and for drinking after a substantial meal we assume $k_2 = \frac{k_1}{2}$.

Results

Case 1: Person only intakes alcohol initially



((a)) Alcohol level in GI-tract ((b)) Alcohol level in blood

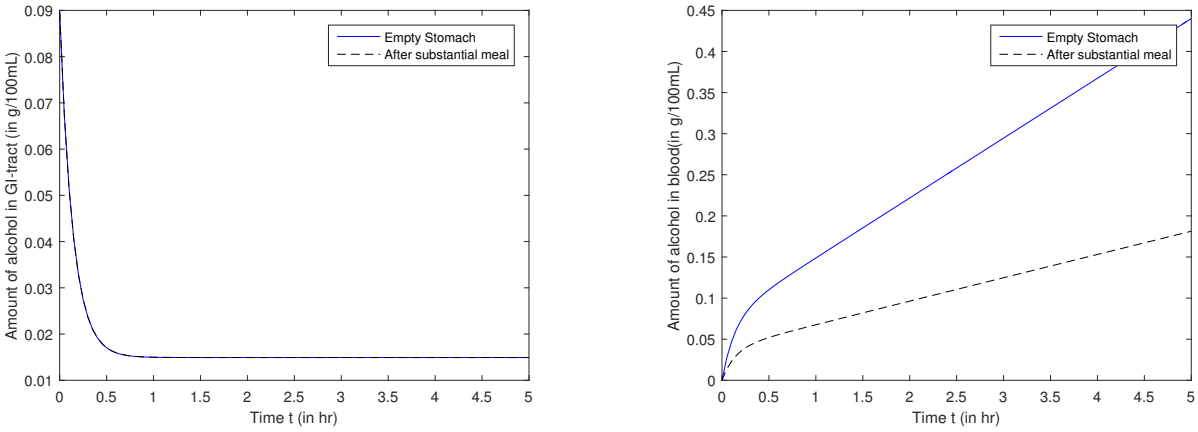
FIG. 7: Numerical simulation of Eq. (11) and Eq. (10) using Euler's method. The value of $k_1 = 6$ and $n = 3$ and person considered is a male with weight $w = 70\ kg$

In the first case shown in figure 7, since the alcohol intake takes place only initially, the term I is not considered in Eq. 9,

$$\frac{dx}{dt} = -k_1 x \tag{11}$$

Since, BAL above 0.05 leads to dizziness and below it leads to happy feeling, we can see from figure 7, for empty stomach drinking, the maximum BAL value attained is near to 0.08, which leads to dizziness. While, for drinking after a substantial meal, the maximum BAL value attains less than 0.04, which leads the person to happy feeling. A possible explanation is that some amount of alcohol gets used up in the GI-tract for digestion of food, and hence the amount of alcohol flowing from GI-tract to blood is smaller compared to the case of empty stomach drinking.

Case 2: Continuous drinking (i.e. the person intakes alcohol continuously)



((a)) Alcohol level in GI-tract ((b)) Alcohol level in blood

FIG. 8: Numerical simulation of Eq. (9) and Eq. (10) using Euler's method. The value of $k_1 = 6$ and $n = 3$ and person considered is a male with weight $w = 70\ kg$

In the case of continous drinking, the change in alcohol level in GI-tract becomes zero, when the amount of alcohol, $x = \frac{I}{k_1}$. In this case, $I = 0.0896$. As the amount of alcohol is blood i.e. y increases, the out flow term (a Michaelis-Menton function) in Eq. 10, for $y >> M$, equals a constant k_3 whose value in this case is 0.01705.

1. Empty Stomach: Since $k_1 = k_2$, the change in amount of alcohol in blood is equal to $k_2x - k_3 = I - k_3$, and hence the amount will always increase.

2. After substantial meal: If the person drinks after a substantial meal, $k_2 = \frac{k_1}{2}$. Therefore, the change in amount of alcohol in blood is equal to $k_2x - k_3 = \frac{I}{2} - k_3$ which is a constant greater than zero and hence the amount will always increase.

If the person instead of drinking 3 glasses as mentioned in the initial conditions, drinks only 1 glass(i.e. n = 1), then after some time the amount of alcohol in blood becomes constant in a case, when he/she has taken a substantial meal(≈ 0.04 *unit*), dizziness doesn't occur.

Conclusion

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