CS302-Modulation and Simulation

Lab 1

Undertaken By

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Contents

1 Newton's Cooling Law

Newton's law of cooling states 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 ambient temperature (T_m).

1.1 Assumptions

1. The heat transfer that occurs isn't by radiation.
2. The heat capacity of the substance should remain constant.
3. There is linear heat transfer involved. Here, we don't take into consideration convection or radiation.

1.2 Differential Equation Modelling Newton's Law

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

1.3 Analytical Solution

$$\int \frac{dT}{T-T_m} = \int -kdt$$

$$ln[T - T_m]_{T_0}^{T} = -kt$$

$$ln\frac{T-T_m}{T-T_0} = -kt$$

$$\frac{T-T_m}{T-T_0} = e^{-kt}$$

$$T(t) = T_m + (T_0 - T_m)e^{-kt} \tag{2}$$

1.4 Parameters

$T(t)$ = Temperature of the object under observation at time t
T_0 = Initial temperature of the object at time $t = 0$
T_m = Ambient Temperature
k = Positive Constant
t = Time

1.5 Examples

1.5.1 Example 1(c)

$T(t) = 20°\text{C}$
$T_0 = 6°\text{C}$
$T_m = 25°\text{C}$
$k = ?$
$t = 1$ hour

Putting the above values in the analytical solution:
$20 = 25 + (6 - 25)e^{-k}$
$19e^{-k} = 5$
$k = 1.335\ hr^{-1}$

1.5.2 Example 1(d)

$T(t) = 12°\text{C}$
$T_0 = 6°\text{C}$
$T_m = 25°\text{C}$
$k = 1.335\ hr^{-1}$
$t = ?$

Putting the above values in the analytical solution:
$12 = 25 + (6 - 25)e^{-1.335}$
$e^{-1.335} = 13/19$
$t = 17.0557\ mins$

1.6 Computational Model

1.6.1 Analysis of the Computational Model

Figure 1 shows the function for various values of h. Here, we aren't able to see the exact difference for the different values.

Figure 2 is a zoomed figure, here we see that as the value of h gets smaller we are able to get more precise values of the temperature.

A good value of h for this question would be $0.0001t$ i.e. 0.002. Here we will get the best results for the model.

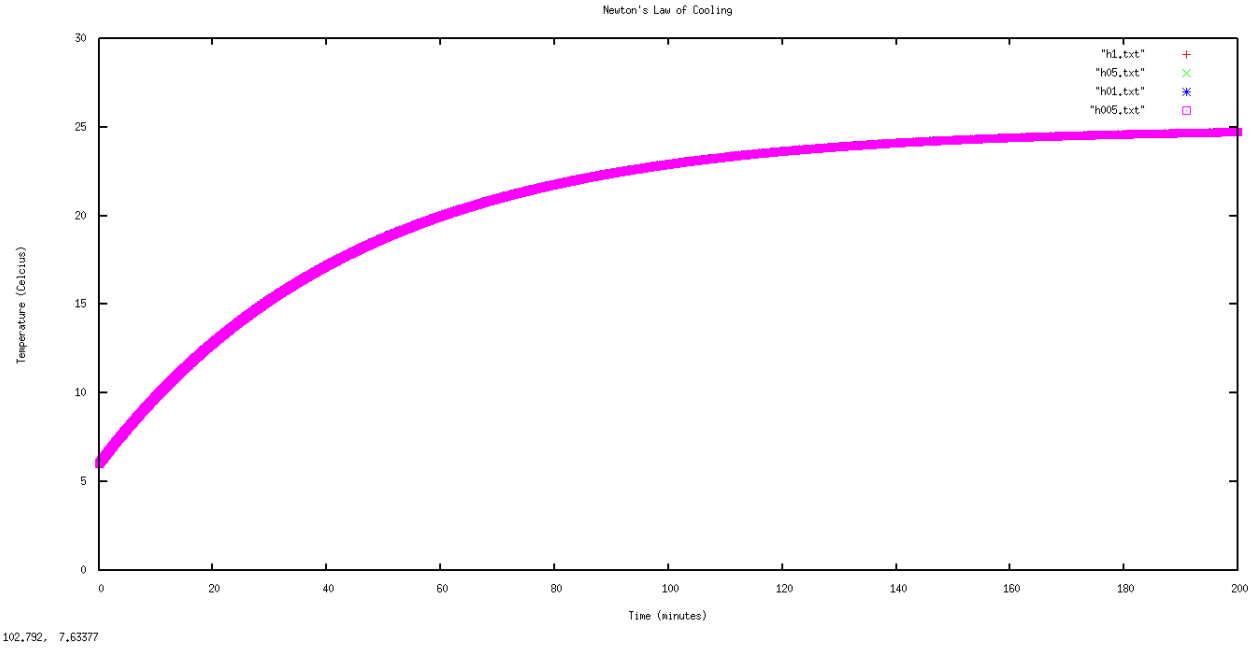


Figure 1: From Eq. (1) we can see that temperature starting from initial value $6°C$ reaches a saturation of $25°C$. The value of constant is k=0.02225 $min^{-}1$.

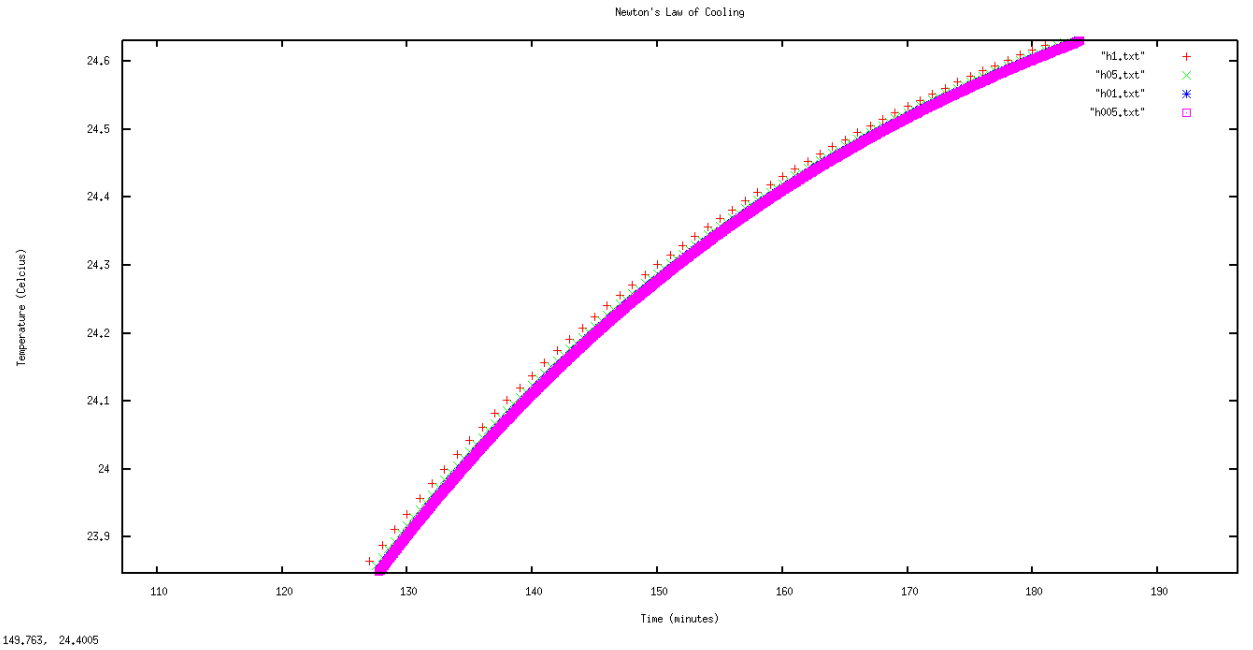


Figure 2: Zoomed image showing the difference in convergence for different values of 'h'.

2 Drug Dosage Model (Analytical)

$$\text{Drug} \longrightarrow \text{GI-tract} \longrightarrow (k_1)\text{Blood} \longrightarrow (k_2)\text{Elimination}$$

2.1 Model 1: Instantaneous Transfer from GI-Tract to Blood Stream

In this case the drug immediately dissolves in the blood stream from the GI-Tract. The drug then is eliminated from the blood stream through excretion. There is an initial amount of dosage, the compartment, i.e. the blood stream, and the movement out is the rate at which the drug leaves the body. This rate is decreasing and hence we can use the exponential decay function to determine the amount of drug in the body at any given time.

2.1.1 Assumptions

1. The whole body is one homogeneous compartment.
2. The drug immediately dissolves in the blood stream from the GI-Tract.
3. This model is similar to a one compartment model. Hence, it can be modelled using a single differential equation.
4. Rate of elimination depends on the metabolism of the individual's body.

2.1.2 Differential Model of the Instantaneous Transfer from GI-Tract to Blood Stream

$$\frac{dB(t)}{dt} = -k_2 B(t) \tag{3}$$

2.1.3 Analytical Solution

$$\int \frac{dB(t)}{B(t)} = \int -k_2 dt$$

$$ln[B(t)] = -k_2 t + ln(c_0)$$

$$Att = 0, B(t) = c_0$$

$$B(t) = c_0 e^{-k_2 t} \tag{4}$$

2.1.4 Parameters

$B(t)$ = Amount of drug in blood stream at time t
c_0 = Initial concentration of drug in bloodstream at time $t = 0$
k_2 = Excretion Constant (the rate at which the drug is removed from the body)
t = Time

2.2 Model 2: Instantaneous transfer into GI-Tract and then slow diffusion from GI-Tract to Blood Stream

In this case the drug immediately dissolves in the the GI-Tract. The drug then diffuses into the blood stream at a constant rate. Here, the drug is metabolized at two separate locations in the body. This results in two differential equations, one each for the GI tract and other for the blood stream. The rate of metabolism is directly proportional to the amount of drug present at that time in that compartment.

2.2.1 Assumptions

1. The drug immediately dissolves in the GI-Tract when it is ingested.

2.2.2 Differential Model of the Instantaneous transfer into GI-Tract and then slow diffusion from GI-Tract to Blood Stream

Amount of drug in GI Tract = Rate at which drug enters GI-Tract - Rate at which the drug diffuses into the blood stream

$$\frac{dG(t)}{dt} = -k_1 G(t) \tag{5}$$

Amount of drug in Blood Stream = Rate at which drug enters Blood Stream - Rate at which the drug is excreted out from the blood stream

$$\frac{dB(t)}{dt} = k_1 G(t) - k_2 B(t) \tag{6}$$

2.2.3 Analytical Solution

Applying Laplace Transformation,

For GI-Tract:

$$sG(t)' - G(0) = -k_1 G(t)'$$

$$\therefore G(t)' = \frac{G(0)}{s+k_1}$$

For Blood Stream:

$$sB(t)' - B(0) = k_1 G(t)' - k_2 B(t)' \; ; B(0) = 0$$

$$\therefore sB(t)' = k_1 B(t)' - k_2 G(t)'$$

$$\therefore B(t)' = \frac{k_1 G(t)}{s+k_2}$$

$$\therefore B(t)' = \frac{k_1}{s+k_2}\frac{G(0)}{s+k_1}$$

$$\therefore B(t)' = \frac{G(0).k_1}{(s+k_2)(s+k_1)}$$

$$\therefore B(t)' = \frac{G(0).k_1}{k_1-k_2}[\frac{1}{s+k_2} - \frac{1}{s+k_1}]$$

Inverse Laplace

$$\therefore B(t) = \frac{G(0).k_1}{k_1 - k_2}[e^{-k_2 t} - e^{-k_1 t}] \tag{7}$$

$$\therefore G(t) = G(0)e^{-k_1 t} \tag{8}$$

2.2.4 Parameters

$G(t)$ = Amount of drug in GI-Tract at time t
$B(t)$ = Amount of drug in blood stream at time t
$G(0)$ = Initial concentration of drug in GI-Tract at time $t = 0$
$B(0)$ = Initial concentration of drug in Blood Stream at time $t = 0$; $B(0) = 0$
k_1 = Diffusion Constant (the rate at which the drug is diffused from the GI-Tract to the Blood Stream)
k_2 = Excretion Constant (the rate at which the drug is removed from the body)
t = Time

2.3 Model 3: Drug is taken at regular intervals

This is the case of IV drips where the drug is given at specific intervals to the patient.

2.3.1 Differential Model of the regular interval drug dosage (for discrete case)

$$Q = Q_0$$

$$Q(T) = Q_0 e^{-kt} + Q_0 = Q_0(1 + r) \ ; \ r = e^{-kt}$$

$$Q(2T) = Q_0(1 + r)r + Q_0 = Q_0(1 + r + r^2)$$

$$\text{Similarly, } Q(nT) = Q_0(1 + r + r^2 + r^3 + ... + r^n) = Q_0\frac{1-r^{n+1}}{1-r}$$

2.3.2 Differential Model of the regular interval drug dosage (for continuous case)

For the continuous case, we are supposed to give a continuous dosage of the drug at discrete times. As a result the dosage will be a function of time as shown in the following model.

For GI-Tract:

$$\frac{dG(t)}{dt} = I(t) - k_1 G(t) \tag{9}$$

For Blood-Stream:

$$\frac{dB(t)}{dt} = k_1 G(t) - k_2 B(t) \tag{10}$$

2.3.3 Analytical Solution

$$\text{If n} \to \infty \ , \ Q \to \frac{Q_0}{1-r}$$

$$\text{Else, } Q(nT) = Q_0\frac{1-r^{n+1}}{1-r}$$

The continuous case is not integrable and hence analytical solution isn't possible.

2.3.4 Parameters

For Discrete Model:

$Q(t)$ = Amount of drug in the body at time t
$Q(0)$ = Initial concentration of drug in body at time $t = 0$
k= Rate of diffusion of the drug in the body t = Time

For Continuous Model:

$G(t)$ = Amount of drug in GI-Tract at time t
$B(t)$ = Amount of drug in blood stream at time t
$G(0)$ = Initial concentration of drug in GI-Tract at time $t = 0$
$B(0)$ = Initial concentration of drug in Blood Stream at time $t = 0$; $B(0) = 0$
k_1 = Diffusion Constant (the rate at which the drug is diffused from the GI-Tract to the Blood Stream)
k_2 = Excretion Constant (the rate at which the drug is removed from the body)
$I(t)$ = The continuous dosage that i given t = Time

3 Drug Dosage Model (Computational)

3.1 Graphical Analysis of GI-Tract and Blood Stream

3.1.1 Drug Dispersion in GI-Tract and Blood Stream

As seen in Figure 3, the amount of drug decreases from the GI-Tract continuously because from the GI-Tract all the drug is supposed to be diffused into the blood stream. The amount of drug increases in the blood stream initially and then decreases as it is removed by excretion. The rate of drug diffusion and excretion depends on the constants k_1 and k_2.

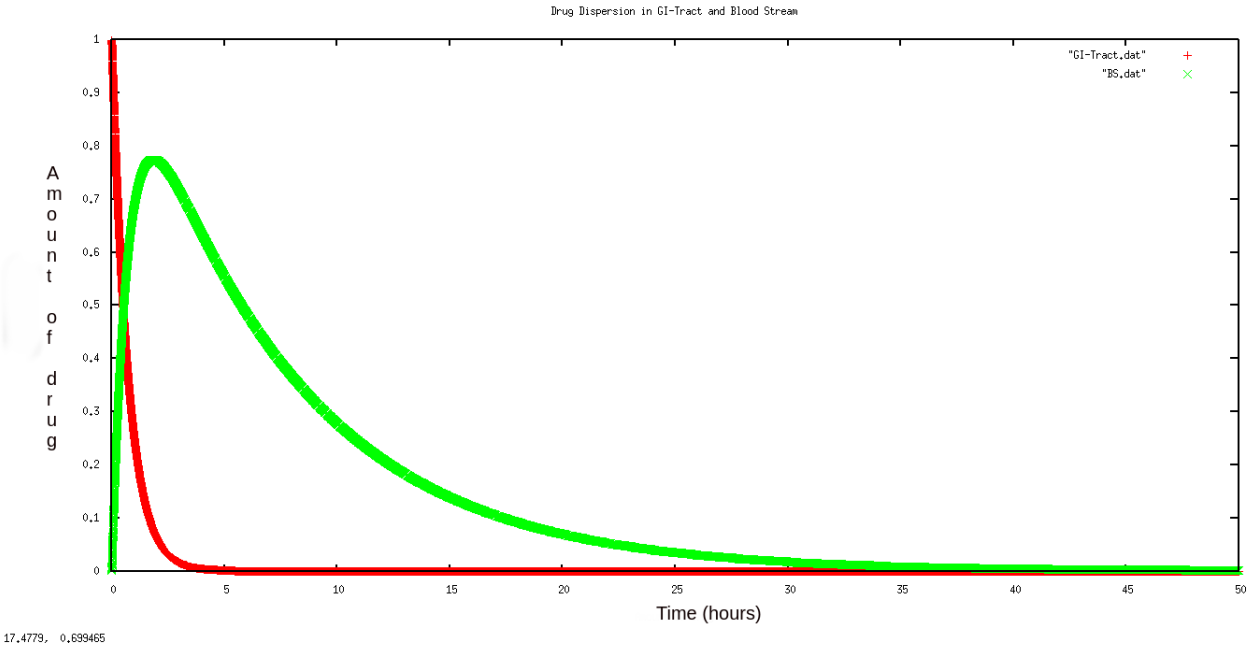


Figure 3: From Eq. (5) and Eq. (6) we can see the drug level in the GI-Tract and the Blood Stream

The highest concentration of the drug in the body is 0.77. This can be verified with a graph as well as analytical analysis.

3.1.2 Drug Dispersion in GI-Tract and Blood Stream for different excretion rates

Here. we have kept k_1 fixed and varied k_2 i.e. the excretion constant. We see that the amount of drug in the GI-Tract decreases as expected. For the blood stream the initial increase and decreases will depend on the excretion constant.

Now, if the excretion constant is high the amount of drug removed from the blood stream will increase at a faster rate. And so we will have low amount of drug in the body within a shorter time. Hence, there is a direct proportionality between the amount of drug and the excretion constant.

Also, we see that the highest concentration of the drug is dependent on the excretion rate. Lower the excretion rate, higher is the retention and the amount of drug present in the body.

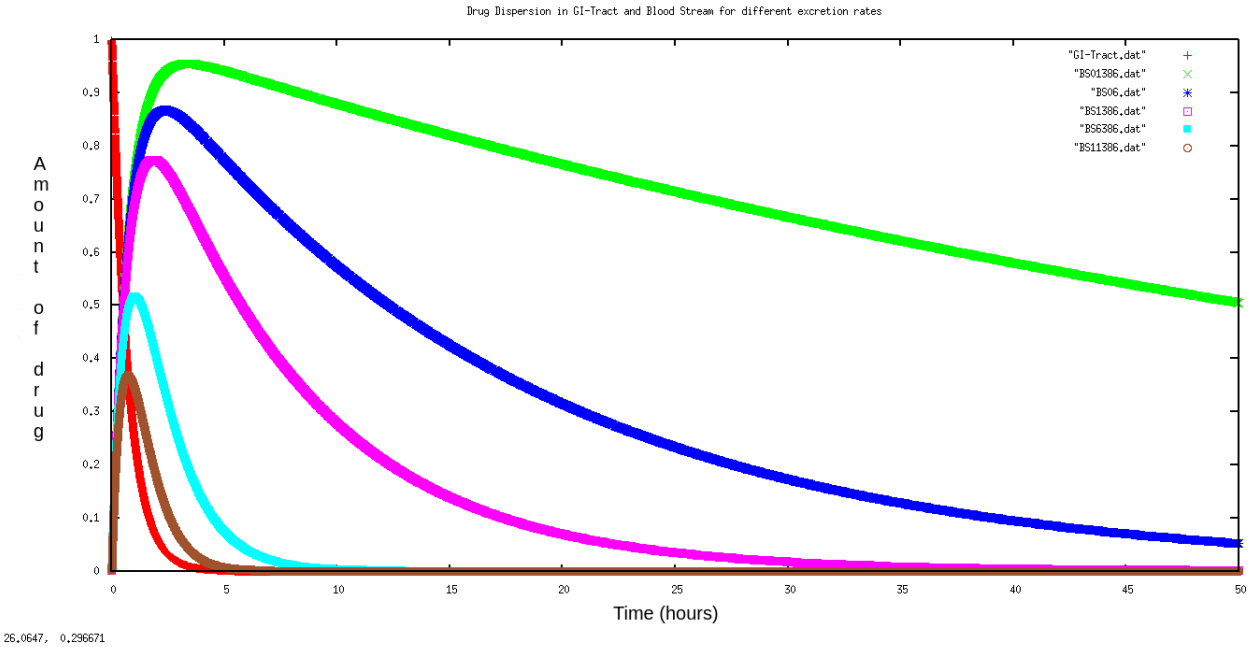


Figure 4: Drug dispersion for different k_2 values i.e. different excretion rates

3.1.3 Drug Dispersion in GI-Tract and Blood Stream for different diffusion rates

The diffusion constant won't affect the amount of drug excreted from the body. But it will affect the rate at which the drug is diffused from the GI-Tract of the blood stream.

Here, we see that for a constant excretion rate and for varying diffusion rates, the amount of drug in the GI-Tract is inversely proportional to the diffusion constant. As the diffusion constant increases the amount of drug in GI-Tract starts decreasing at a faster rate.

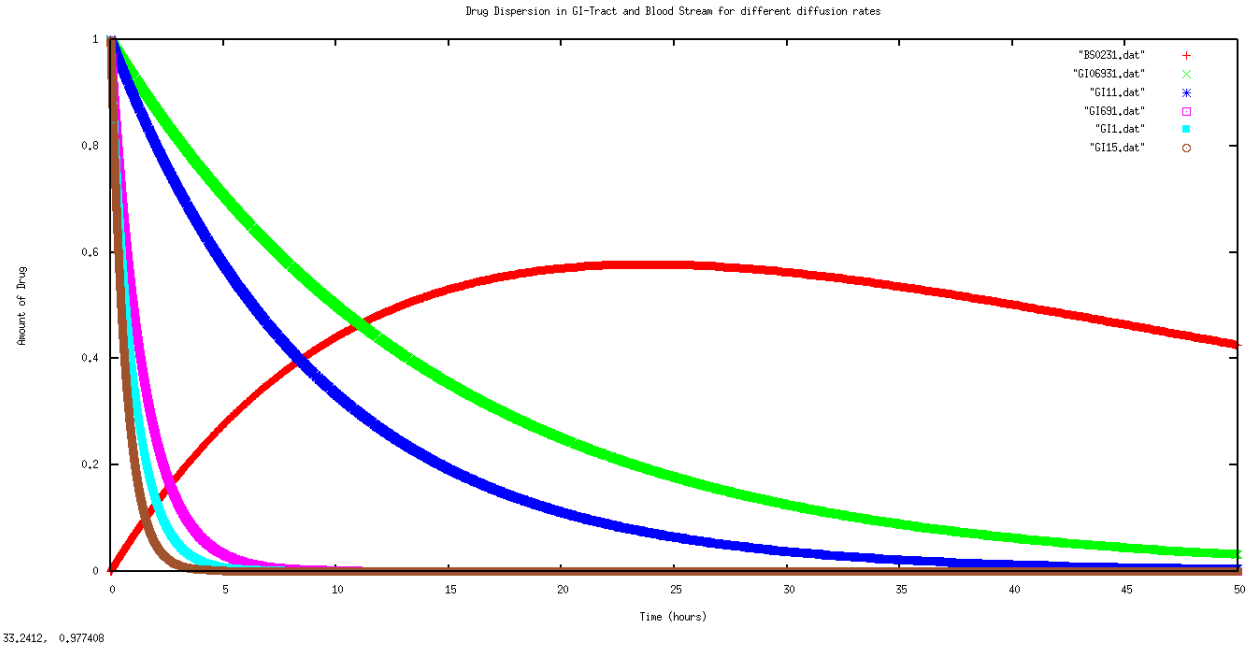


Figure 5: Drug dispersion for different k_1 values i.e. different diffusion rates

3.1.4 Drug Dispersion in GI-Tract and Blood Stream for Regular Dosage

As we have given a continuous flow of the drug in the GI-Tract, as we can see in the Fig. 3.1.4 the amount of drug in the GI-Tract will initially reduce and then remain constant, because it will diffuse at a rate lesser than the incoming rate. This rate would be proportional to the amount of drug in GI-Tract at that particular time and hence it too will get constant after a while.

The amount of drug in the blood stream is continuously increasing in the beginning. The excretion rate is very small as compared to the incoming drug rate, so it is an exponential rise. After a while, this too attains a constant rate.

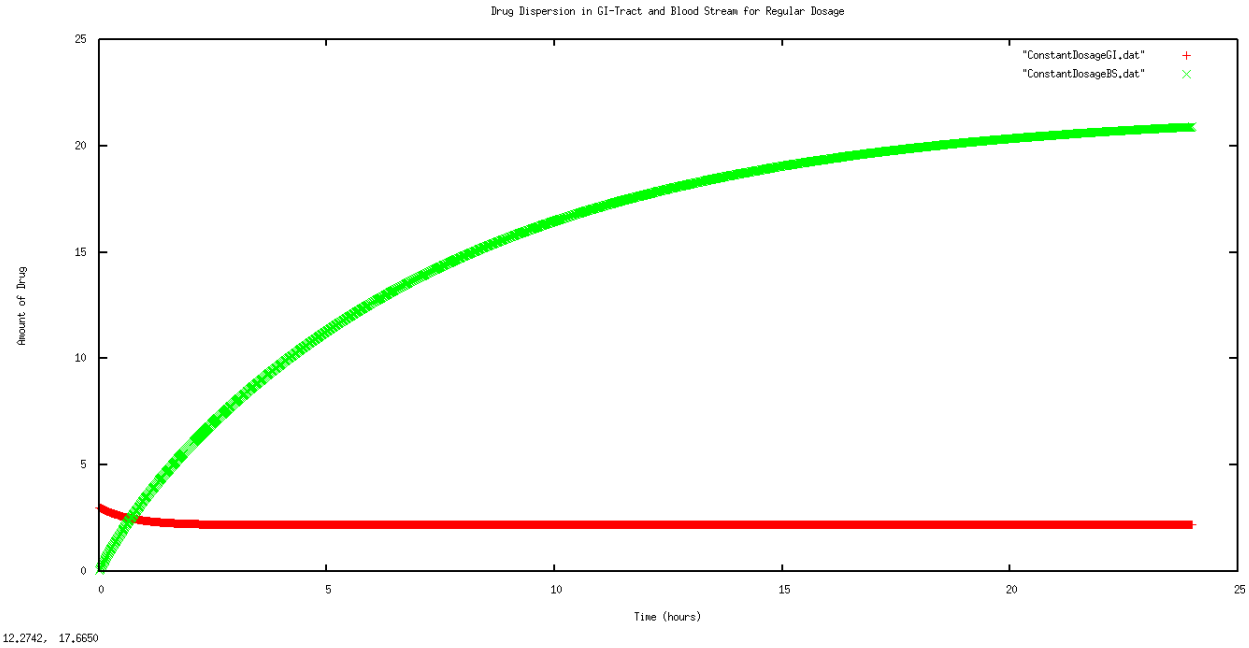


Figure 6: Drug dispersion for regular dosage at all times. Here, the fixed dosage is of 3 units. The model is plotted using Eq. (9) and Eq. (10)

3.1.5 Drug Dispersion in GI-Tract and Blood Stream for Continuous Dosage at regular intervals of 6 hours

When the drug is administered at regular intervals of 6 hours each, we see that the amount of drug in the blood keeps on increasing at a steady rate. This can have an adverse effect on the body.

Suppose, the maximum limit of the drug is 20 units in the blood, then after around 65 hours. Hence, after this time there would be an adverse effect on the patient.

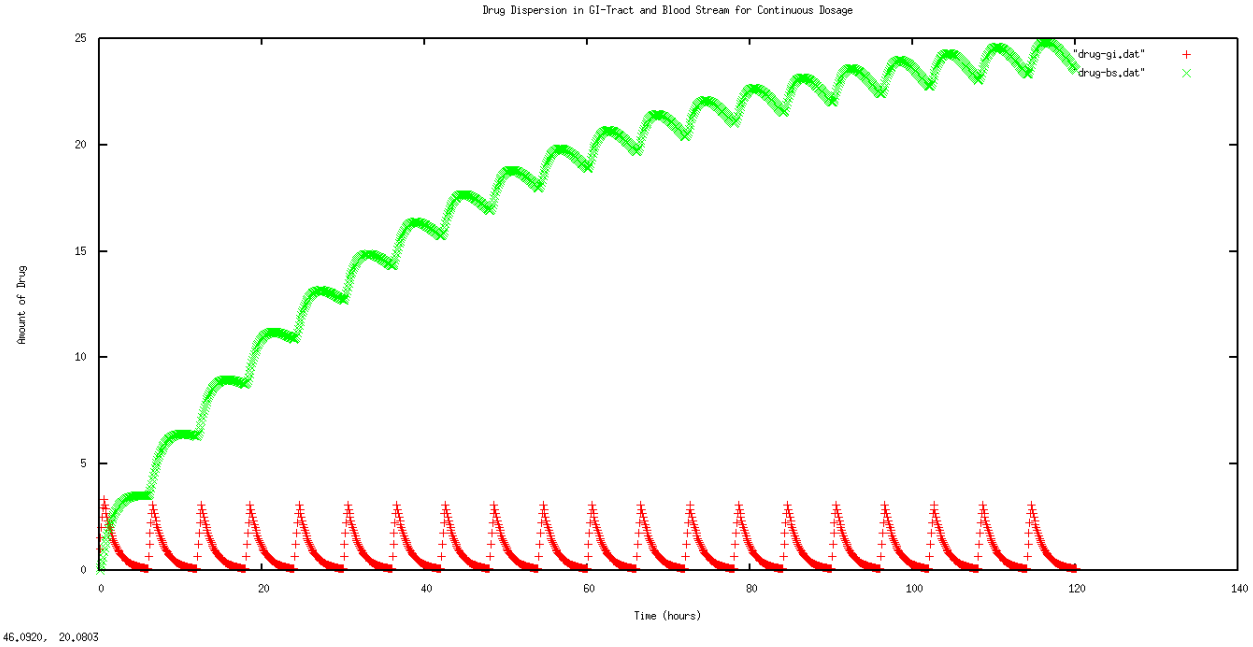


Figure 7: Drug dispersion in GI-Tract and Blood Stream for Continuous Dosage at regular intervals of 6 hours

3.1.6 Drug Dispersion in GI-Tract and Blood Stream for Continuous Dosage at regular intervals of 8 hours

If the drug is administered at regular intervals of 8 hours, we see that the drug level in the body doesn't go beyond 20 at any point of time and achieves a saturation around that level.

Hence, we can say that this is a safe time gap to administer the drug in the body.

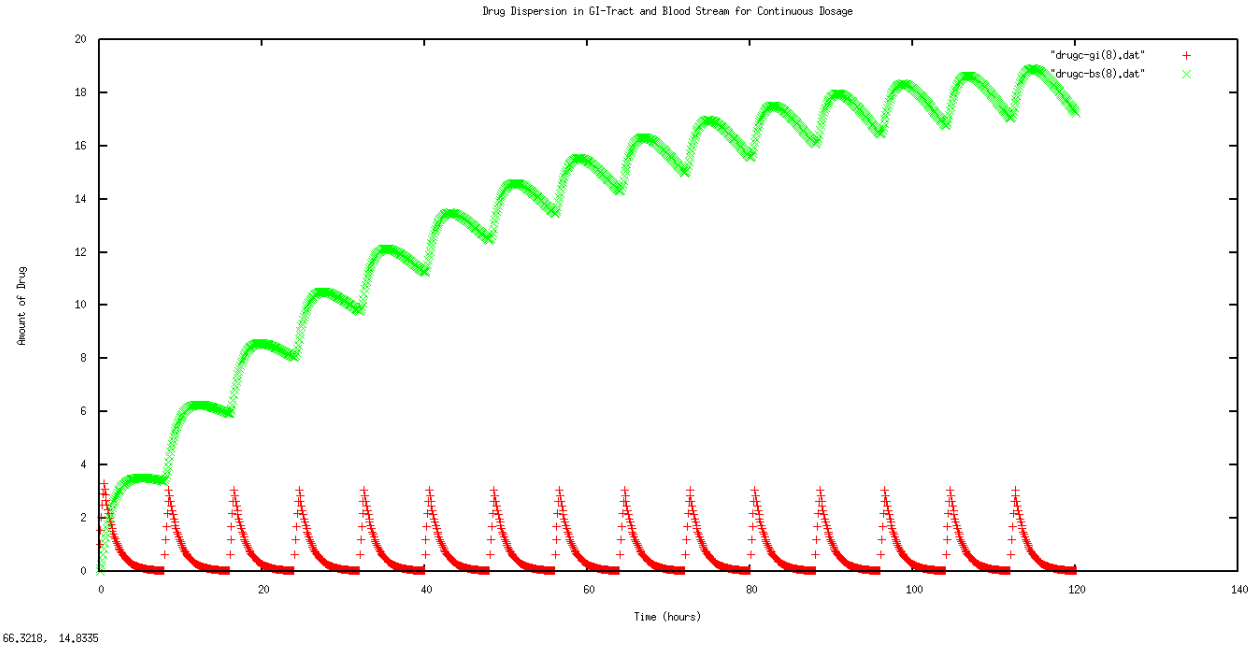


Figure 8: Drug dispersion in GI-Tract and Blood Stream for Continuous Dosage at regular intervals of 8 hours

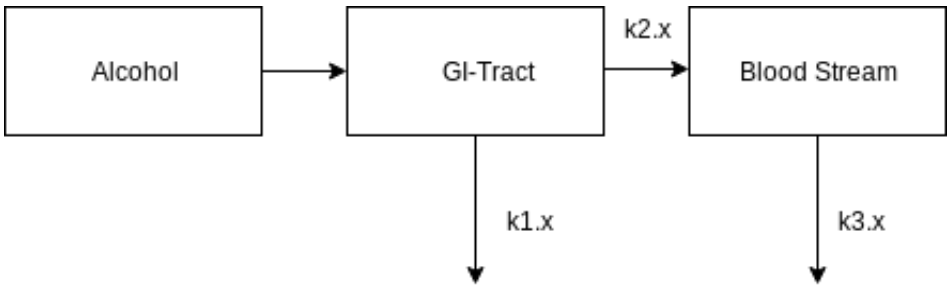
4 Blood Alcohol Level Analysis

We look at the blood alcohol level in this analysis. the various factors affecting the alcohol levels in a person's body are:

1. Person's Weight
2. Percentage of body fat
3. Age
4. Food in the GI-Tract

The blood alcohol level is directly proportional to the body weight of the person because it increases the absorption rate. It is inversely proportional to the age, because the metabolic rate of the body also affects the absorption rate.

4.1 Differential Equation Modelling Blood Alcohol Level in Human Body



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

$$\frac{dy}{dt} = k_2 x - \frac{k_3 y}{y + M} \tag{12}$$

4.2 Parameters

$x(t)$ = Amount of alcohol in the GI-Tract
y = Amount of alcohol in the Blood Stream
I = Alcohol Intake
k_1 = Positive dimensionless model showing the diffusion rate from the GI-Tract to the blood stream
k_2 = Positive dimensionless model showing the absorption rate at which the blood stream absorbs the alcohol
k_3 = Excretion constant for the removal of alcohol from the body
M = Constant in the Michaelis-Menton Function

4.3 Computational Analysis

The alcohol content in the body changes according to the Eq. (11) in the GI-Tract and the Eq. (12) in the blood stream. Now, when a person drinks on an empty stomach the initial concentration of the alcohol in his body is 0. Hence, $I = 0$.

Hence, $k_1 = k_2 = 6$

As the person is a 70kg male, we calculate k_3 as $8/10C$ where $C(bodyfluidsinL = 0.82w$ for males.

We see that, the amount of alcohol in the GI-Tract decreases at an exponential rate and the amount of alcohol in the body increases initially and then decreases. The increase and decrease are a exponential function of the amount of alcohol present in the body. When the BAL goes beyond 0.05 the person feels dizzy. Initially when the person drinks he may feel this sensation for around 1.5 hours and later this feeling would go and he would start feeling happy again.

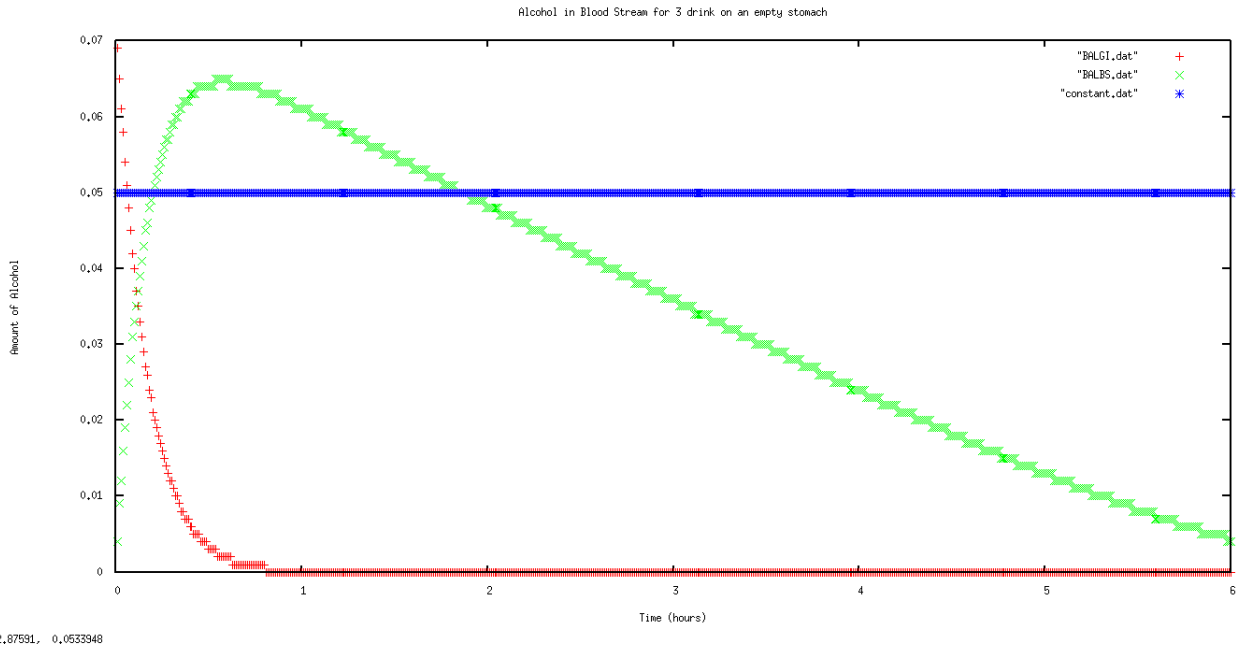


Figure 9: According to Eq. (11) and Eq. (12) Blood Alcohol Level in the body at an empty stomach at a constant 3 drinks; initial amount taken is 0 and the subject under observation is a 70kg male

As shown in Figure 10, when the person drinks continuously without stopping then the amount of alcohol in the change GI-Tract becomes stable after a while but the amount of alcohol in the blood stream keeps on increasing. Hence, the person would feel dizzy and at a later stage this can also result in several serious repercussions.

Here, the initial amount of alcohol in the body is taken as $I = 14n/10C$.

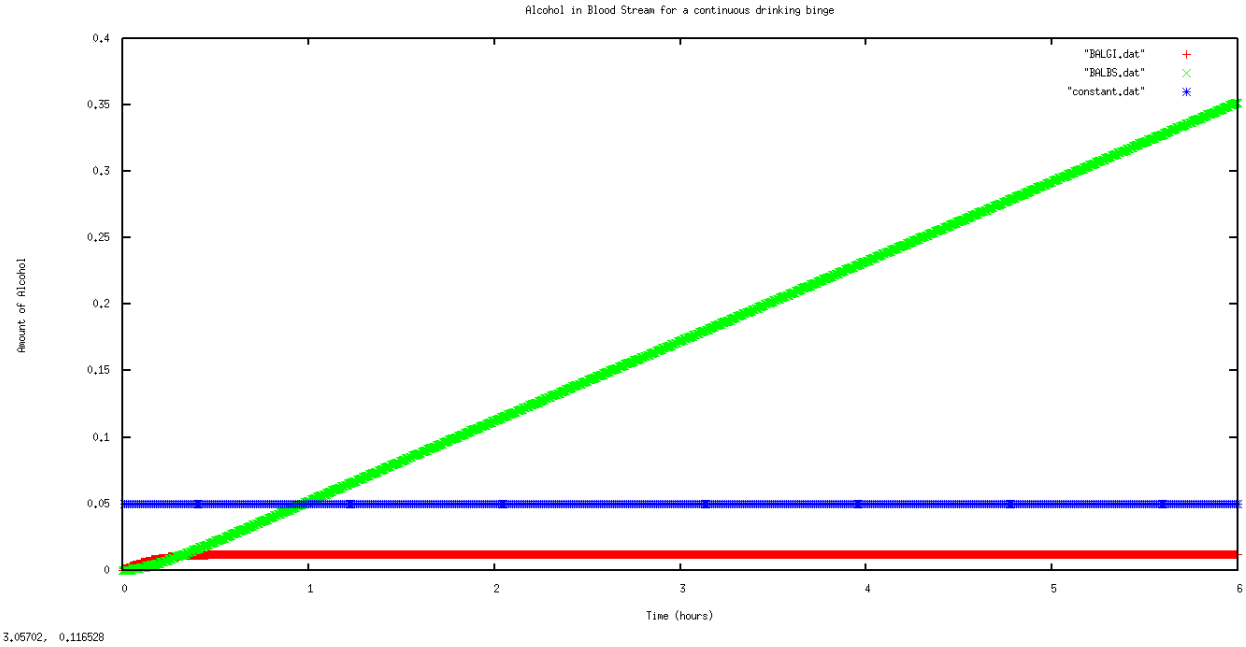


Figure 10: According to Eq. (11) and Eq. (12) Blood Alcohol Level in the body at an empty stomach when a person is binge drinking; initial amount taken is I and the subject under observation is a 70kg male

5 References

1. https://books.google.co.in/books?id=EUQrBgAAQBAJ