Set - 2 : Dynamic Analysis of Compartmental Systems

Rakshit Pandhi (202201426)* and Kalp Shah (202201457)†

Dhirubhai Ambani Institute of Information & Communication Technology, Gandhinagar, Gujarat 382007, India

CS302, Modelling and Simulation

In this lab, we numerically and analytically analyze the lake pollution model, The dynamics of the medicine in blood and in GI tract with single dose of a medicine and by course of medicine with using mathematical tools and simulation software.

I. INTRODUCTION

This lab explores compartment modeling in linear systems, predicting pollution concentration in a lake over time. It also examines drug dynamics in the GI tract and bloodstream, plotting concentration changes for single and multiple doses.

II. MODEL

A. Lake Pollution Model

The concentration C(t) of pollutants in a lake follows the equation

$$\dot{C} = a - bC \tag{1}$$

where $a = FC_{in}/V$ and b = F/V . Here C_{in} in the constant pollutant concentration of inflow into the lake, F is the fixed volumetric flow rate and V is the fixed volume of the lake (as the lake also drains out).

The concentration C(t) of pollutant is given by

$$C = C_{in} + (C_0 - C_{in})e^{-Ft/V} \tag{2}$$

B. Single Medicine Dose

A single dose of a medicine is administered to a patient. The dynamics of the medicine follows the equation $\dot{x} = -k_1 x$, x(0) = x_0 in the GI tract, and $\dot{y} = k_1 x - k_2 y$, y(0) = 0 in the blood.

The amount of drug in GI tract is given by

$$x = x_0 e^{-k_1 t} \tag{3}$$

and the amount of drug in blood is given by

$$y = \frac{k_1 x_0}{k_2 - k_1}(e^{-k_1 t} - e^{-k_2 t}) \tag{4}$$

However for the same values of rate constants k_1 and k_2 the above equations differ as

$$x = x_0 e^{-kt} \tag{5}$$

$$y = k x_0 t e^{-kt} \tag{6}$$

C. Course of Medicine

A course of medicine is administered to a patient. The dynamics of the medicine follows the equation $\dot{x} = I - k_1 x$, x(0) = 0 in the GI tract, and $\dot{y} = k_1 x - k_2 y$, y(0) = 0 in the blood stream.

The amount of drug in GI tract is given by

$$x = \frac{I}{k_1}(1 - e^{-k_1 t}) \tag{7}$$

The amount of drug in blood is given by

$$y = \frac{I}{k_2}(1 - e^{-k_2 t}) - \frac{I}{k_2 - k_1}(e^{-k_1 t} - e^{-k_2 t}) \tag{8}$$

However for the same values of rate constants k_1 and k_2 the above equations differ as

$$x = \frac{I}{k}(1 - e^{-kt}) \tag{9}$$

$$y = \frac{I}{k}[1 - (kt + 1)e^{-kt}] \tag{10}$$

*Electronic address: 202201426@daiict.ac.in

†Electronic address: 202201457@daiict.ac.in

III. RESULTS

A. Plot the concentration of pollutants in the lake

Fig. 1 shows the concentration of pollutants in the lake over time.

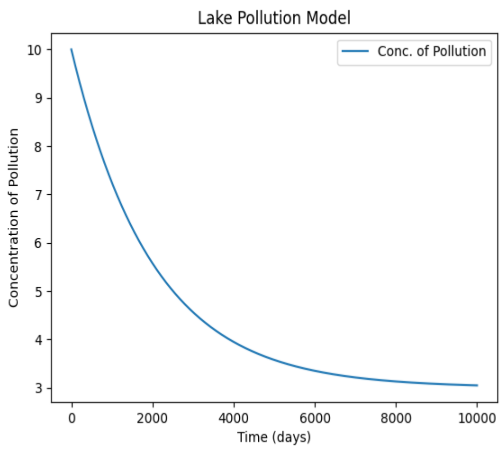

FIG. 1: Here F = $5{\times}10^8 m^3/day$, $V = 10^{12} m^3$, $C_{in} = 3$ unit and C(0) $= C_0 = 10$ unit.

The time taken for C $= 0.5C_0$ is **2505.525 days** when C_{in} is not zero. The time taken for C $= 0.5C_0$ is **1386.29 days** when C_{in} is zero.

Fig. 2 shows the concentration of pollutants in the lake over time when C_{in} is zero.

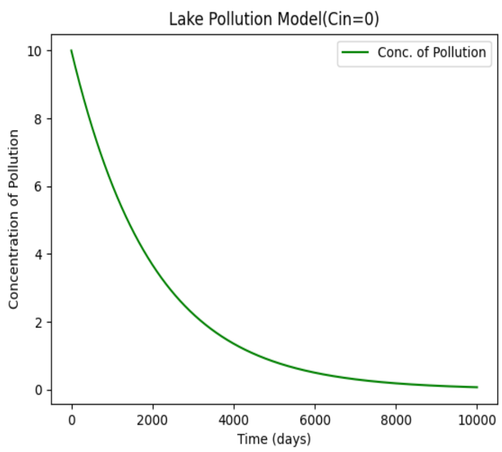

FIG. 2: Here F = $5{\times}10^8 m^3/day$, $V = 10^{12} m^3$, $C_{in} = 0$ unit and C(0) $= C_0 = 10$ unit.

B. Plot the amount of drug in a single dose of medicine

Fig. 3 shows the amount of drug in GI tract and blood stream with respect to time.

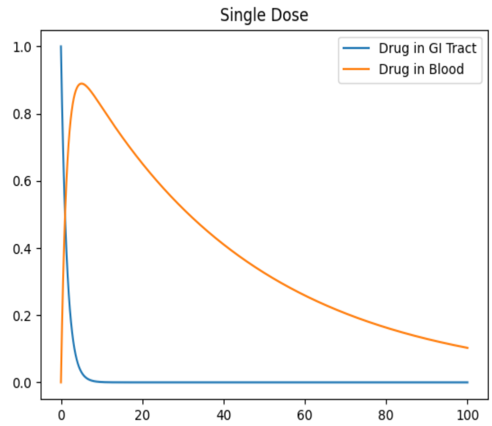

FIG. 3: k$_1 = 0.6931 hr^{-1}$, k$_2 = 0.0231 hr^{-1}, x_0 = 1\,unit$, $y_0 = 0\,unit$

The peak value of y(t) is **0.888** units at t = **5.1** years. Time t is found by using the equation :

$$t_p = \ln\left(\frac{k_1}{k_2}\right) \times \frac{1}{k_1 - k_2}$$

Fig. 4 shows the amount of drug in GI tract and blood stream with respect to time when k1=k2.

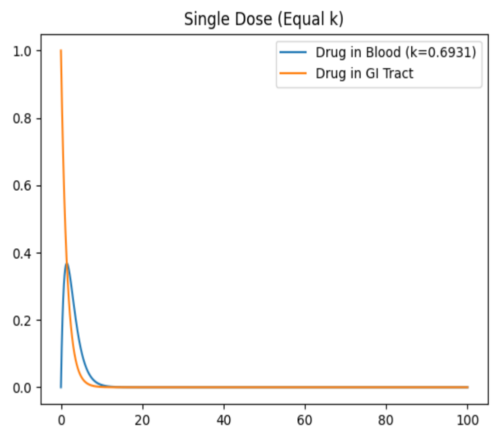

FIG. 4: k$_1 = k_2 = 0.6931 hr^{-1}$, , x$_0 = 1\,unit, y_0 = 0\,unit$

Fig. 5 shows the amount of drug in GI tract and blood stream with respect to time when k1=k2.

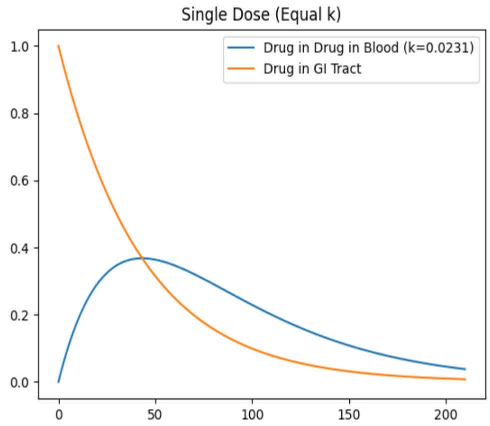

FIG. 5: $k_1 = k_2 = 0.0231 hr^{-1}$, $x_0 = 1\,unit$, $y_0 = 0\,unit$

C. Plot the amount of medicine in a course of medicine

Fig. 6 shows the amount of medicine in GI tract with respect to time.

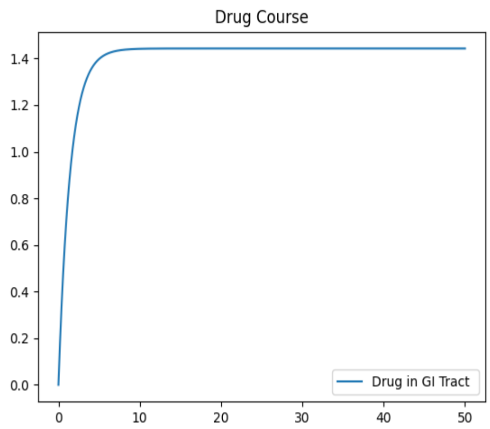

FIG. 6: $k_1 = 0.6931 hr^{-1}$, $k_2 = 0.0231 hr^{-1}, x_0 = 0\,unit$, $y_0 = 0\,unit$, , $I = 1\,unit$

The limiting value of x(t) is **1.4467** units .

Fig. 7 shows the amount of medicine in blood with respect to time.

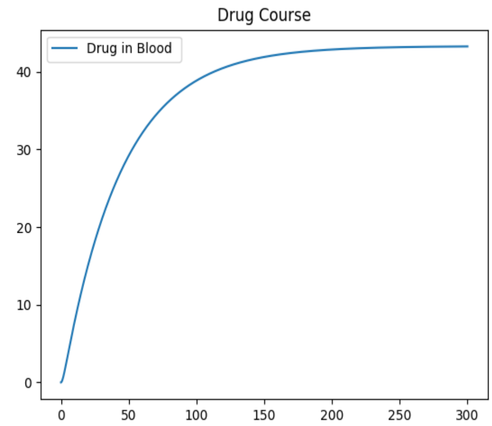

FIG. 7: $k_1 = 0.6931 hr^{-1}$, $k_2 = 0.0231 hr^{-1}$, $x_0 = 0\,unit$, $y_0 = 0\,unit$, , $I = 1\,unit$

The limiting value of y(t) is **43.4** units .

Fig. 8 shows the amount of medicine in GI tract with respect to time when k1=k2.

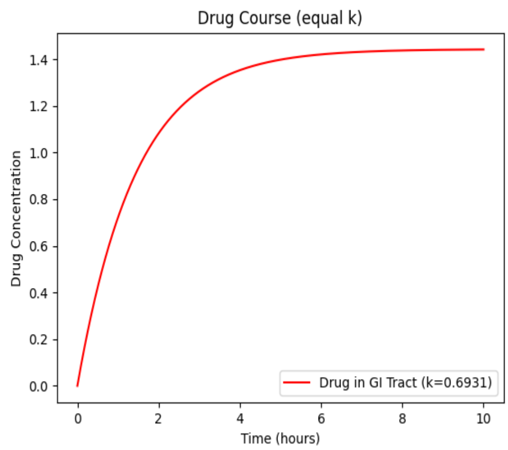

FIG. 8: $k_1 = k_2 = 0.6931 hr^{-1}$, $x_0 = 0\,unit$, $y_0 = 0\,unit$, $I = 1\,unit$

Fig. 9 shows the amount of medicine in blood with respect to time when k1=k2.

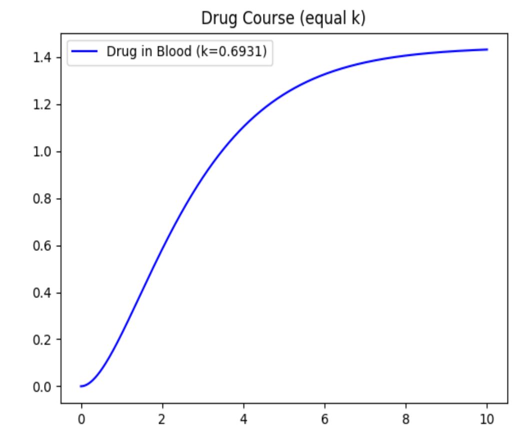

FIG. 9: $k_1 = k_2 = 0.6931 hr^{-1}$, $x_0 = 0\,unit$, $y_0 = 0\,unit$, $I = 1\,unit$

Fig. 10 shows the amount of medicine in GI tract with respect to time when k1=k2.

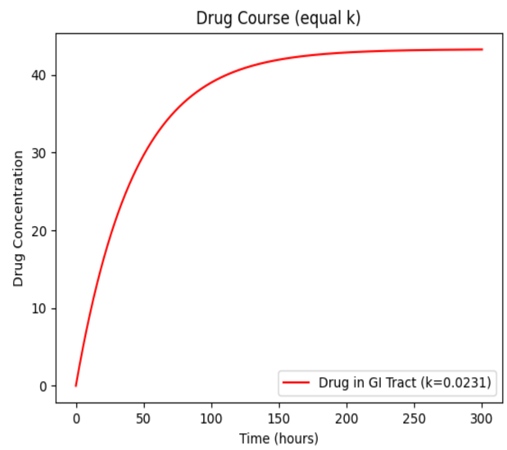

FIG. 10: $k_1 = k_2 = 0.0231 hr^{-1}$, $x_0 = 0\,unit$, $y_0 = 0\,unit$, $I = 1\,unit$

Fig. 11 shows the amount of medicine in blood with respect to time when k1=k2.

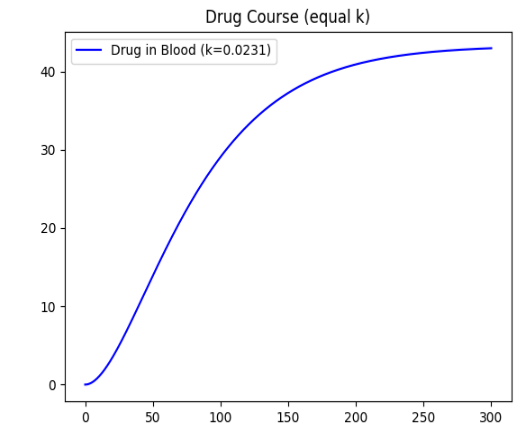

FIG. 11: $k_1 = k_2 = 0.0231 hr^{-1}$, $x_0 = 0\,unit$, $y_0 = 0\,unit$, $I = 1\,unit$

IV. CONCLUSIONS

- The results indicate that the pollutant concentration in the lake eventually stabilizes at the inflow concentration (C_{in}), whether it is zero or non-zero.
- For a single dose, the GI tract's concentration decays exponentially toward zero, while the bloodstream's concentration first peaks before gradually falling back to zero. The parameters K_1 and K_2 dictate the rate of these changes.
- When taking medicine as a course, the concentrations in both the bloodstream and the GI tract stabilize at the same value if $K_1 = K_2 = k$. The time required for convergence is determined by the value of K.
- Larger the k it takes lesser time to saturate and vice-versa, as k has the dimension of T^{-1}.