Set 2 -Utilizing Compartment Modeling to Analyze Drug Dosage and Lake Pollution

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CS302, Modelling and Simulation

In this lab, we tackle compartment modeling problems. We start by analyzing a lake pollution model that takes inflow and outflow into account. Subsequently, we examine medication dosage problems for both single dose administration and constant injection rates, taking into account rate equations for both the gastrointestinal system and blood.

I. INTRODUCTION

Within this study, we utilize mathematical equations to model and analyze lake pollution and drug dosage systems. This analysis will culminate in a concise examination of the amount of pollution in lake, and amount of drug in GI tract and in blood over time.

II. MODEL

A. Lake Pollution Model

The concentration of pollutant in the lake follows the equation

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

$$\textit{where} \quad a = \frac{F}{V} \cdot C_{\text{in}} \quad \textit{and} \quad b = \frac{F}{V}$$

Here, C is the concentration of pollutant in the lake, F is the inflow rate (as well as outflow rate), V is the volume of water in the lake, and C_{in} is the concentration of pollutant in the inflow water.

The solution to the differential equation, incorporating initial conditions, can be expressed as:

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

where, C_0) is initial amount of pollutant in the lake.

Now, time taken for concentration to go from C_0 to C while the inflow rate if C_in

$$t = \frac{V}{F} \ln\left(\frac{C_{\text{in}} - C_o}{C_{\text{in}} - C}\right) \tag{3}$$

B. Single dose of medicine

The amount of drug in GI tract and blood follows the given differential equations.

$$\dot{x} = -k_1 x \tag{4}$$

$$\dot{y} = k_1 x - k_2 y \tag{5}$$

with initial conditions $x(0) = x_0$ and $y(0) = 0$.

In this system, x represents the amount of drug in the gastrointestinal (GI) tract, y represents the amount of drug in the blood, k_1 is the decay constant for the GI tract, and k_2 is the decay constant for the blood.

The integral solutions to these equations, incorporating initial conditions, can be expressed as:

$$x = x_0 e^{-k_1 t} \tag{6}$$

$$y = \frac{k_1 x_0}{k_2 - k_1}\left(e^{-k_1 t} - e^{-k_2 t}\right) \tag{7}$$

The time when the value of y(amount of drug in blood) is maximum

$$t = \frac{\ln\left(\frac{k_1}{k_2}\right)}{k_1 - k_2} \tag{8}$$

Now, for the same decay constant case, the equations are:

$$x = x_0 e^{-kt} \tag{9}$$

$$y = k x_0 t e^{-kt} \tag{10}$$

The time when the value of y(amount of drug in blood) is maximum

$$t = \frac{1}{k} \tag{11}$$

and the maximum amount is

$$y_{max} = \frac{x_0}{e} \tag{12}$$

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C. Course of medicine

The amount of drug in GI tract and blood follows the given differential equations.

$$\dot{x} = I - k_1 x \tag{13}$$

$$\dot{y} = k_1 x - k_2 y \tag{14}$$

with initial conditions $x(0) = 0$ and $y(0) = 0$.

In this system, x represents the amount of drug in the gastrointestinal (GI) tract, y represents the amount of drug in the blood, I is the constant ingestion rate,k_1 is the decay constant for the GI tract, and k_2 is the decay constant for the blood.

The integral solutions to these equations, incorporating initial conditions, can be expressed as:

$$x = \frac{I}{k_1}(1 - e^{-k_1 t}) \tag{15}$$

$$y = \frac{I}{k2}(1 - e^{-k_2 t}) - \frac{I}{k_2 - k_1}(e^{-k_1 t} - e^{-k_2 t}) \tag{16}$$

Now, for the same decay constant case, the equations are:

$$x = \frac{I}{k_1}(1 - e^{-k_1 t}) \tag{17}$$

$$y = \frac{I}{k}(1 - (kt + 1)e^{-kt}) \tag{18}$$

The time when the value of y(amount of drug in blood) is maximum

$$t = \frac{1}{k} \tag{19}$$

and the maximum amount is

$$y_{max} = 0.26\frac{I}{k} \tag{20}$$

III. RESULTS

A. Lake Pollution

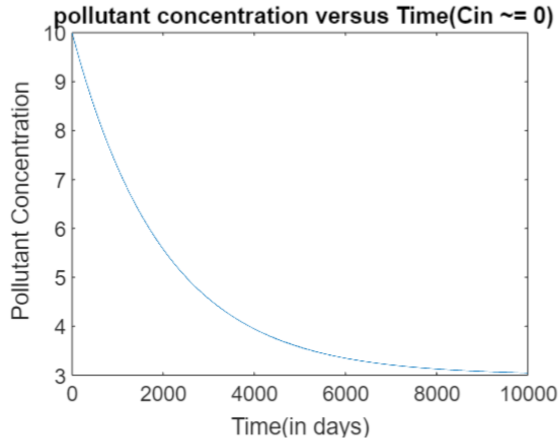

FIG. 1: Plot of $C(t)$: Concentration of pollutant in the lake as a function of time. Here, $F = 5 \times 10^8$ m^3/day, $V = 10^{12}$ m^3, $C_{\text{in}} = 3$ units, and $C(0) = C_0 = 10$ units.

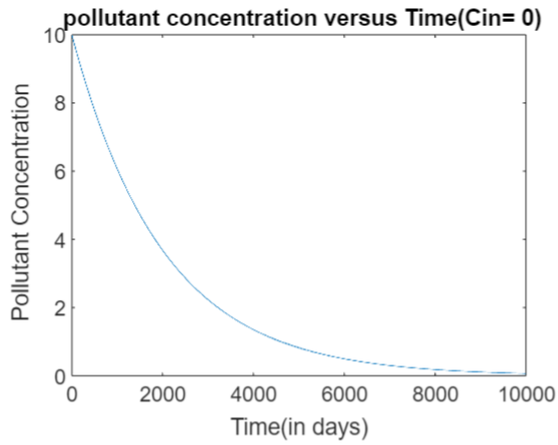

FIG. 2: Plot of $C(t)$: Concentration of pollutant in the lake as a function of time. Here, $F = 5 \times 10^8$ m^3/day, $V = 10^{12}$ m^3, $C_{\text{in}} = 0$ units, and $C(0) = C_0 = 10$ units.

The time taken for $C = 0.5C_0$ is 2505 days (6.86 years) when $C_{\text{in}} = 3$ and 1386 days (3.7981 years)

B. Single dose of medicine

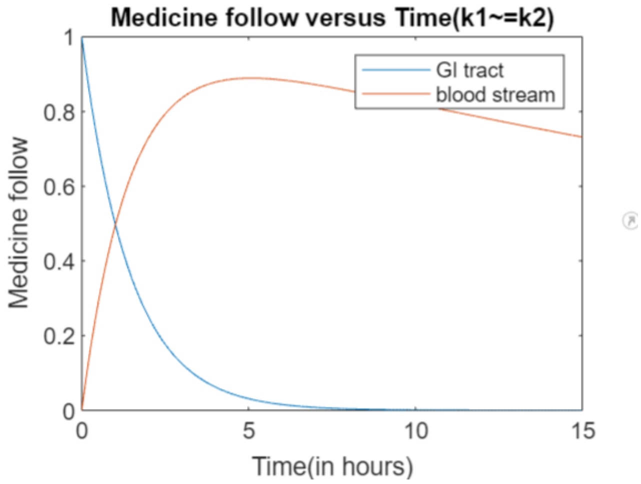

FIG. 3: Plot of $y(t)$ and $x(t)$: amount of drug in the GI trace and blood as a function of time. Here, $k1 = 0.6931hr^{-1}$, $k2 = 0.0231hr^{-1}$ and $x_0 = 1$ unit, The peak value of $y(t)$ is 0.8893 at time $t = 5.0766$ hours.

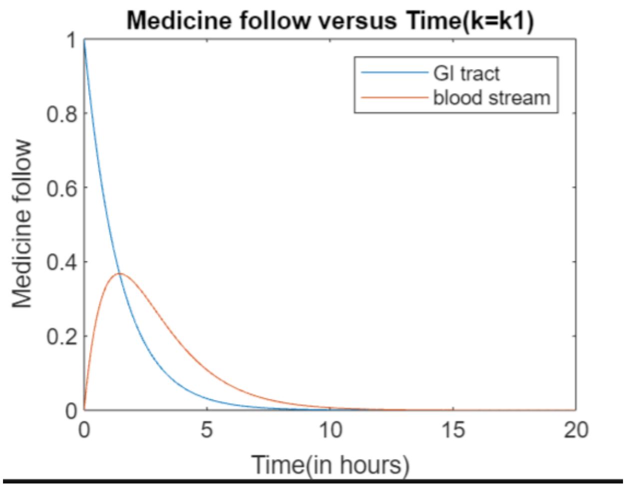

FIG. 4: Plot of $y(t)$ and $x(t)$: amount of drug in the GI trace and blood as a function of time. Here, $k1 = k2 = 0.6931hr^{-1}$ and $x_0 = 1$ unit, The peak value of $y(t)$ is 0.3679 at time $t = 1.4428$ hours.

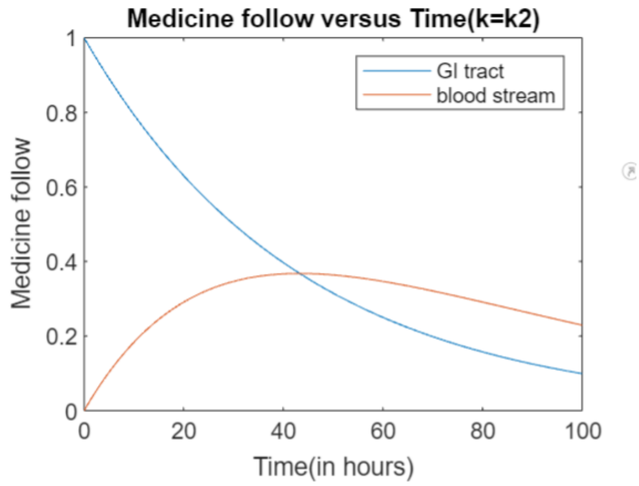

FIG. 5: Plot of $y(t)$ and $x(t)$: amount of drug in the GI trace and blood as a function of time. Here, $k1 = k2 = 0.0231hr^{-1}$ and $x_0 = 1$ unit, The peak value of $y(t)$ is 0.3679 at time $t = 43.2900$ hours.

C. Course of medicine

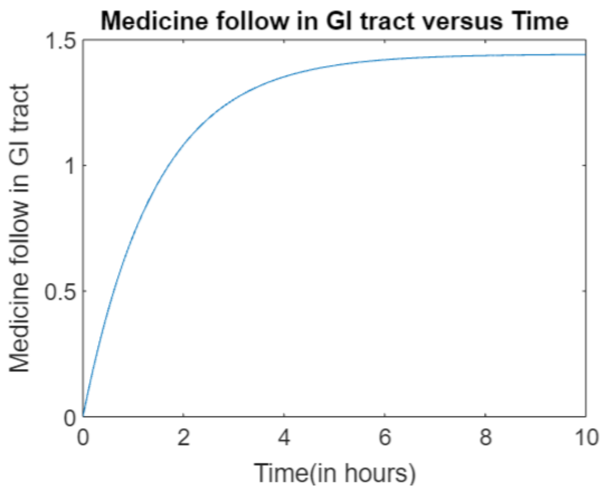

FIG. 6: Plot of $x(t)$: amount of drug in the GI trace as a function of time. Here, $k1 = 0.6931hr^{-1}$, $I = 1$, and $x_0 = 0$ unit, The peak value of $x(t)$ is 1.4428 which matches with I/k_1

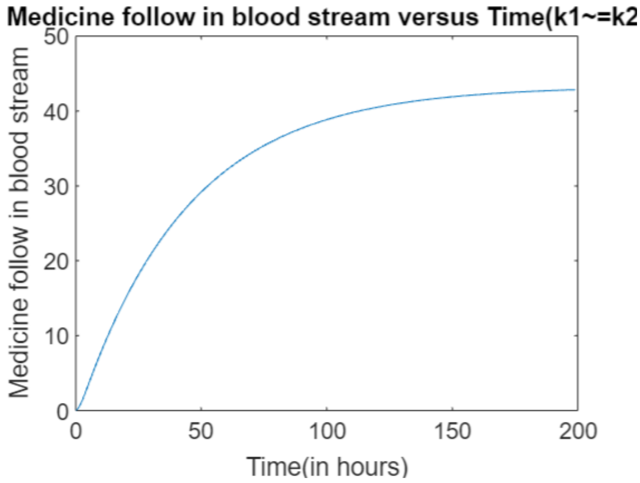

FIG. 7: Plot of $y(t)$: amount of drug in the blood as a function of time. Here, $k1 = 0.6931hr^{-1}$,$k2 = 0.0231hr^{-1}$, $I = 1$, and $x_0 = 0$ unit, The peak value of $y(t)$ is 43.2900 which matches with I/k_2

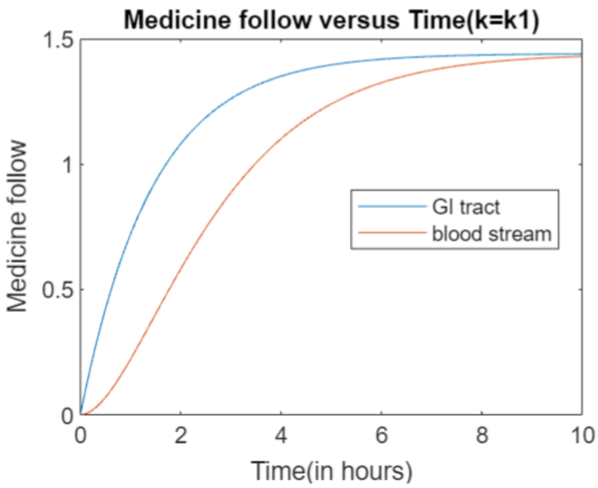

FIG. 8: Plot of $x(t)$ and $y(t)$: amount of drug in the GI trace and blood as a function of time. Here, $k1 = k2 = 0.6931hr^{-1}$, $I = 1$, and $x_0 = 0$ unit, The peak value of $x(t)$ and $y(t)$ is 1.4428 which matches with I/k

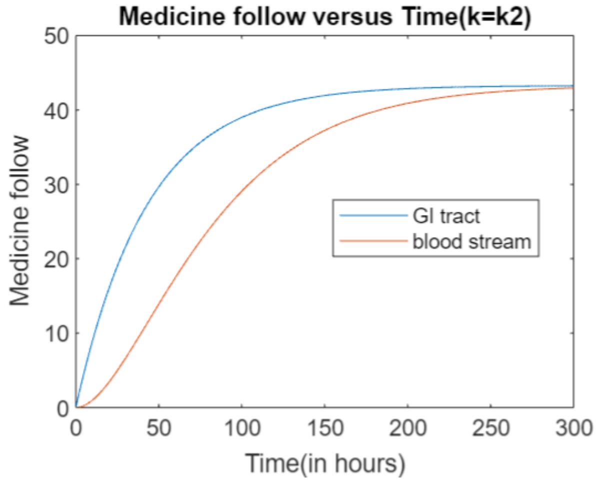

FIG. 9: Plot of $x(t)$ and $y(t)$: amount of drug in the GI trace and blood as a function of time. Here, $k1 = k2 = 0.0231hr^{-1}$, $I = 1$, and $x_0 = 0$ unit, The peak value of $x(t)$ and $y(t)$ is 43.2896 which matches with I/k

IV. CONCLUSIONS

- According to the lake pollution model, the pollutant concentration falls exponentially and saturates at a point where the input(inflow) rate equals the concentration.

- When there are identical rate constants in drug dosage-1, changes in the rate constants have no effect on the maximum value for the bloodstream. But the rate constant determines how long it takes to attain this value, thus lower values of k mean longer times to reach saturation.

- The The rate constants k_1 (GI Tract) and k_2 (Bloodstream) are inversely proportional to the peak saturation value at drug dosage -2.With large values of k we can get peak value (which is small/lower) in small duration of time.