Set-2: Compartment Modelling of Linear Systems

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CS302, Modeling and Simulation

In this lab, we modeled compartment systems to analyze the behavior of linear systems in various scenarios. Our study focused on the concentration of pollutants in a lake, the amount of a drug in a single dose of medicine, and its accumulation over a full course of medication. These models help understand how substances distribute and evolve within a system over time.

I. FORMULATION OF LINEAR SYSTEMS

Pollutant Concentration in a Lake

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 concentration of pollutant inflow into the lake, F is the fixed volumetric flow rate and V is the fixed volume of the lake (since the lake also drains out).

The C(t) concentration of the pollutant is given by

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

Single Dose Drug Model

A single dose of a drug is administered to a patient. The dynamics of the drug follows the equation $\dot{x} = -k_1x$, x(0) = x_0 in the GI tract, and $\dot{y} = k_1x - k_2y$, y(0) = 0 in the blood.

The amount of drug in the GI tract is given by

$$x = x_0e^{-k_1t} \tag{3}$$

and the amount of drug in blood is given by

$$y = \frac{k_1x_0}{k_2 - k_1}(e^{-k_1t} - e^{-k_2t}) \tag{4}$$

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

$$x = x_0e^{-kt} \tag{5}$$

$$y = kx_0te^{-kt} \tag{6}$$

Course of Medication Model

A course of medication is administered to the patient. The dynamics of the drug follows the equation $\dot{x} = I - k_1x$, x(0) = 0 in the GI tract, and $\dot{y} = k_1x - k_2y$, y(0) = 0 in the bloodstream.

The amount of drug in the GI tract is given by

$$x = \frac{I}{k_1}(1 - e^{-k_1t}) \tag{7}$$

The amount of drug in blood is given by

$$y = \frac{I}{k_2}(1 - e^{-k_2t}) - \frac{I}{k_2 - k_1}(e^{-k_1t} - e^{-k_2t}) \tag{8}$$

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

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

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

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II. GRAPHS

A. Plot the concentration of pollutants in the lake

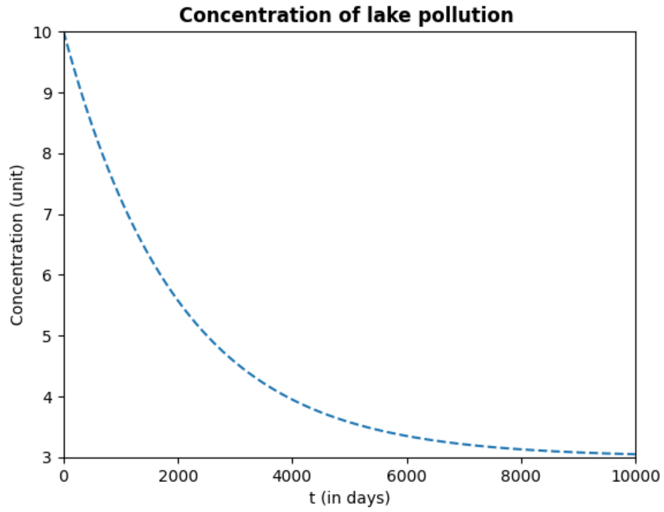

FIG. 1: The dotted graph shows the concentration of pollutants in the lake over time when C_{in} is not zero.

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.

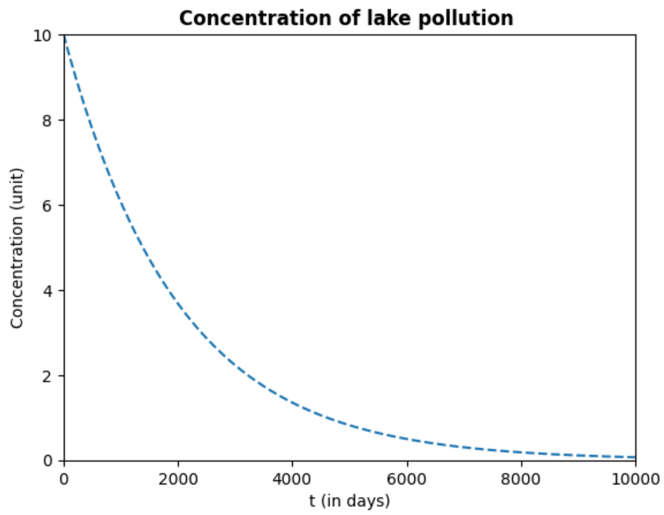

FIG. 2: The dotted graph shows the concentration of pollutants in the lake over time when C_{in} is zero.

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.

The time taken for C $= 0.5C_0$ is **2506 days** when C_{in} is not zero. The time taken for C $= 0.5C_0$ is **1387 days** when C_{in} is zero.

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

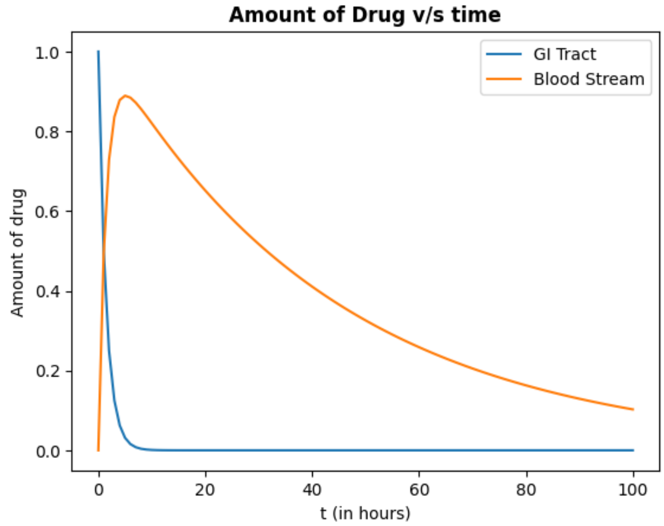

FIG. 3: The graph shows the amount of drug in GI tract and blood stream with respect to time when k_1 and k_2 are different.

Here,

$$k_1 = 0.6931\ hr^{-1}, \quad k_2 = 0.0231\ hr^{-1},$$

$$x_0 = 1 \text{ unit}, \quad y_0 = 0 \text{ unit}.$$

The maximum value of y (t) is **0.8893** units at **5 hours**.

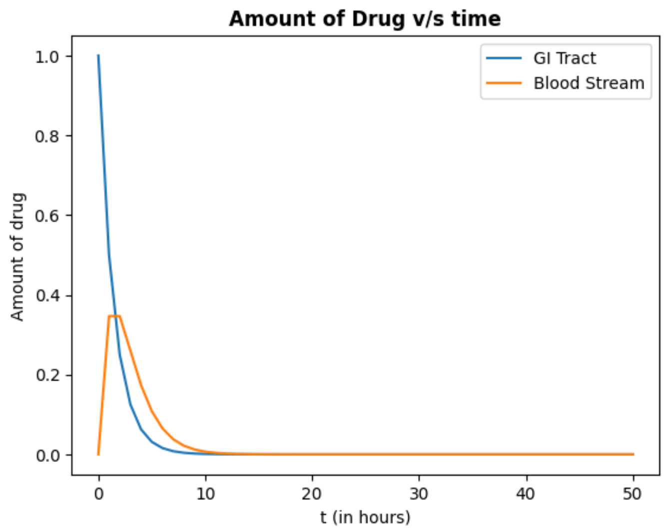

FIG. 4: The graph shows the amount of drug in GI tract and blood stream with respect to time when k_1 and k_2 are same as k_1.

Here,

$$k_1 = k_2 = 0.6931\ hr^{-1},$$

$$x_0 = 1 \text{ unit}, \quad y_0 = 0 \text{ unit}.$$

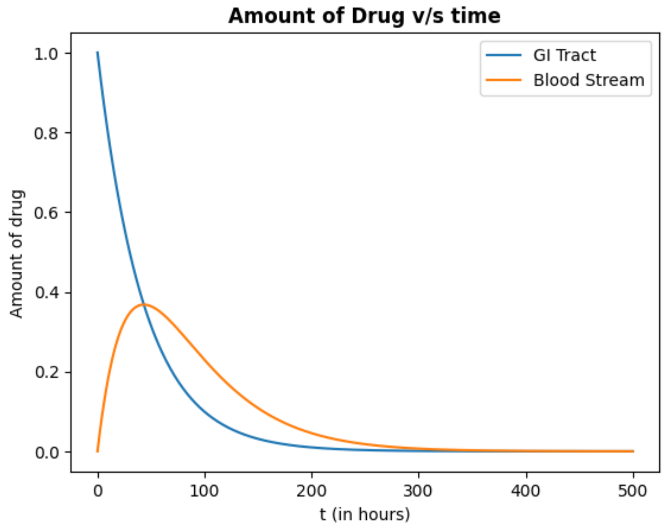

FIG. 5: The graph shows the amount of drug in GI tract and blood stream with respect to time when k_1 and k_2 are same as k_2.

Here,

$$k_1 = k_2 = 0.0231\ hr^{-1},$$

$$x_0 = 1 \text{ unit}, \quad y_0 = 0 \text{ unit}.$$

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

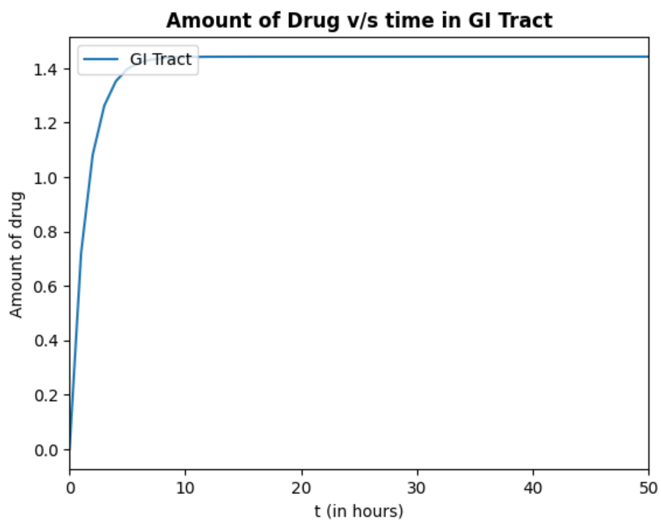

FIG. 6: The graph shows the amount of drug in GI tract with respect to time when k_1 and k_2 are different.

Here,

$$k_1 = 0.6931\ hr^{-1}, \quad k_2 = 0.0231\ hr^{-1}, \quad I = 1 \text{ unit}$$

$$x_0 = 0 \text{ unit}, \quad y_0 = 0 \text{ unit}.$$

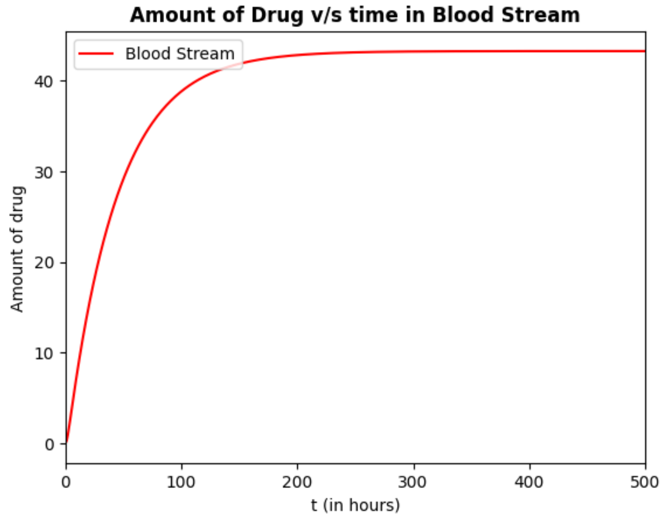

FIG. 7: The graph shows the amount of drug in blood stream with respect to time when k_1 and k_2 are different.

Here,

$$k_1 = 0.6931\ hr^{-1}, \quad k_2 = 0.0231\ hr^{-1}, \quad I = 1 \text{ unit}$$

$$x_0 = 0 \text{ unit}, \quad y_0 = 0 \text{ unit}.$$

The limiting value of x(t) is **1.4428** units and that of y(t) is **42.858** units.

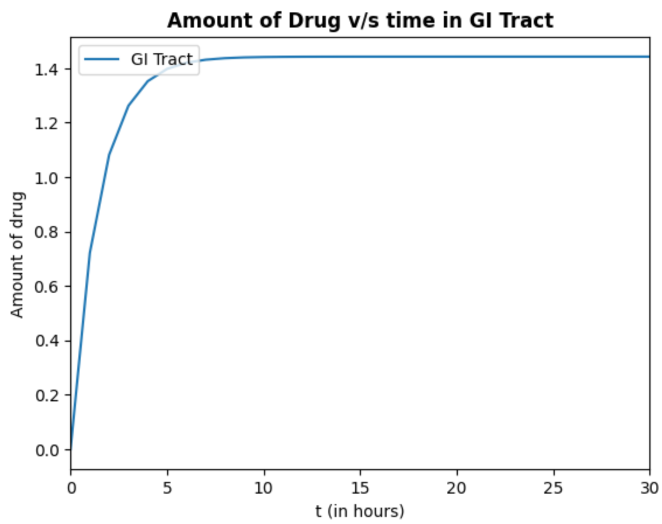

FIG. 8: The graph shows the amount of drug in GI tract with respect to time when k_1 and k_2 are same as k_1.

Here,

$$k_1 = k_2 = 0.6931\ hr^{-1}, \quad I = 1 \text{ unit}$$

$$x_0 = 1 \text{ unit}, \quad y_0 = 0 \text{ unit}.$$

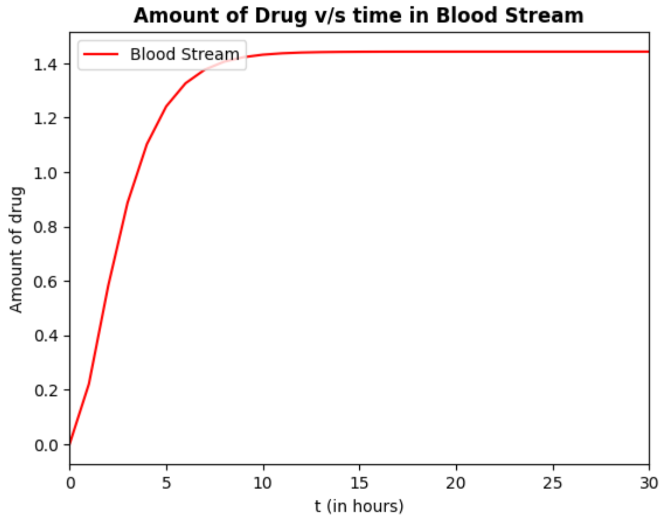

FIG. 9: The graph shows the amount of drug in Blood Stream with respect to time when k_1 and k_2 are same as k_1.

Here,

$$k_1 = k_2 = 0.6931\ hr^{-1}, \quad I = 1 \text{ unit}$$

$$x_0 = 1 \text{ unit}, \quad y_0 = 0 \text{ unit}.$$

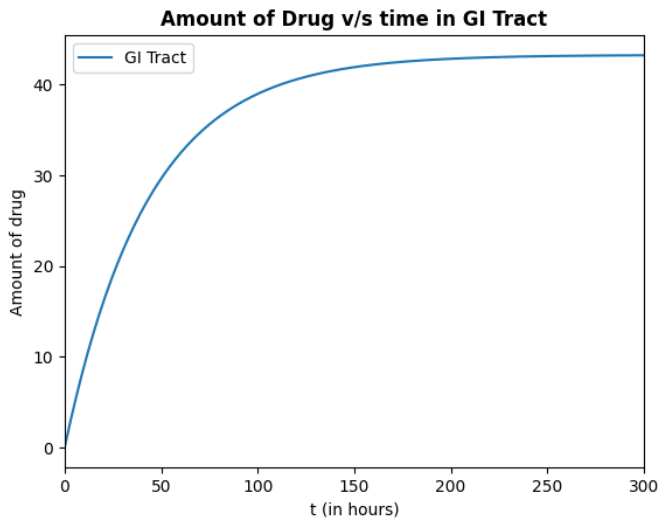

FIG. 10: The graph shows the amount of drug in GI tract with respect to time when k_1 and k_2 are same as k_2.

Here,

$$k_1 = k_2 = 0.6931\ hr^{-1}, \quad I = 1 \text{ unit}$$

$$x_0 = 1 \text{ unit}, \quad y_0 = 0 \text{ unit}.$$

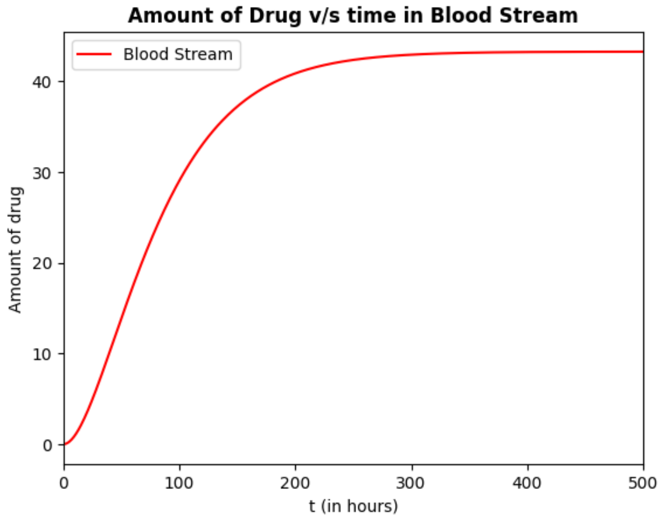

FIG. 11: The graph shows the amount of drug in Blood Stream with respect to time when k_1 and k_2 are same as k_2.

Here,

$$k_1 = k_2 = 0.6931\ hr^{-1}, \quad I = 1 \text{ unit}$$

$$x_0 = 1 \text{ unit}, \quad y_0 = 0 \text{ unit}.$$

III. SALIENT FEATURES:

1. Based on the results obtained, it is clear that whether or not the inflow of pollutants is zero, the concentration of pollutants in the lake saturates to the value of C_{in}.

2. In the case of a single dose of medicine, the concentration of medication in the gastrointestinal (GI) tract after a single dosage falls exponentially and converges to zero as t approaches infinity. In the meantime, the blood's medication concentration rises to its peak, falls exponentially, and eventually converges to zero. The values of k_1 and k_2 determine the convergence time.

3. When a course of medication is taken, $k_1 = k_2 =$ k indicates that the drug concentrations in the GI tract and blood both converge to the same value. In this case, the value of k determines the convergence time.