Set - 2 : Compartment modelling of linear systems

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CS302, Modelling and Simulation

I. 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

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

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

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

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

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

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

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

II. RESULTS

A. Plot the concentration of pollutants in the lake

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

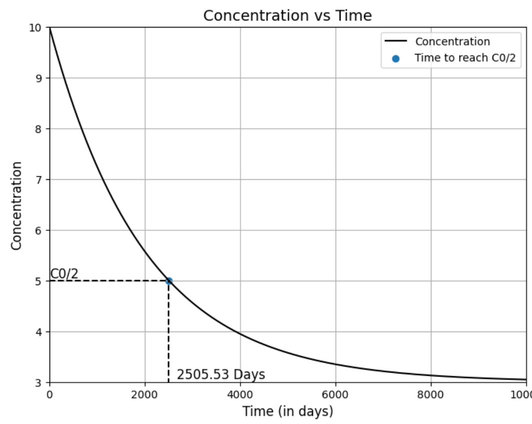

FIG. 1: Here F = $5\times10^8 m^3/day, V = 10^{12} m^3, C_{in} = 3$ unit and C(0) = C_0 = 10 unit

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Fig. 2 shows the concentration of pollutants in the lake over time.

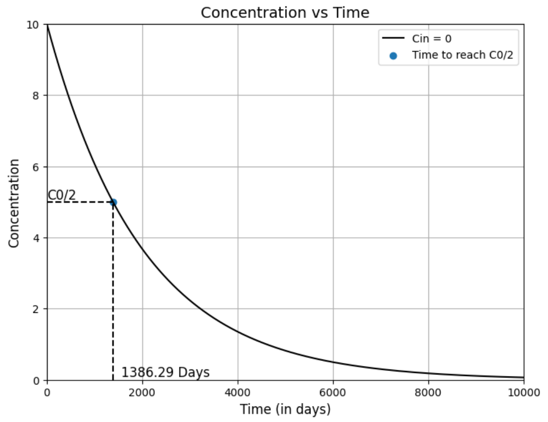

FIG. 2: Here F $= 5\times10^8 m^3/day, V = 10^{12} m^3, C_{in} = 0$ unit and C(0) $= C_0 = 10$ unit

The time taken for C $= 0.5C_0$ is **2505.53 days** when C_{in} is not zero. The time taken for C $= 0.5C_0$ is **1386.29 days** when C_{in} is zero.

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.

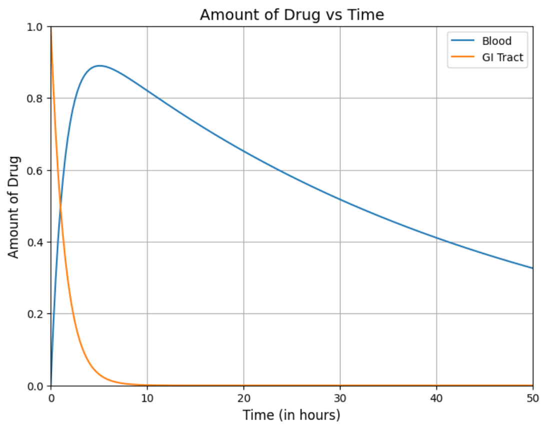

FIG. 3: Here $k_1 = 0.6931$ hr$^{-1}, k_2 = 0.0231$ hr^{-1}*and* $I = 1$ unit.

The peak value of y(t) is **0.889** units at **4.88 hours**.

Fig. 4 shows the amount of drug in GI tract and blood stream with respect to time when k$_1 = k_2 = 0.6931$.

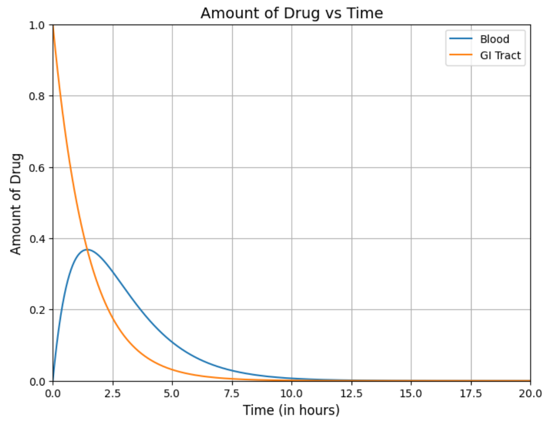

FIG. 4: Here $k_1 = k_2 = 0.6931$ hr^{-1}*and* $I = 1$ unit.

Fig. 5 shows the amount of drug in GI tract and blood stream with respect to time when k$_1 = k_2 = 0.0231$.

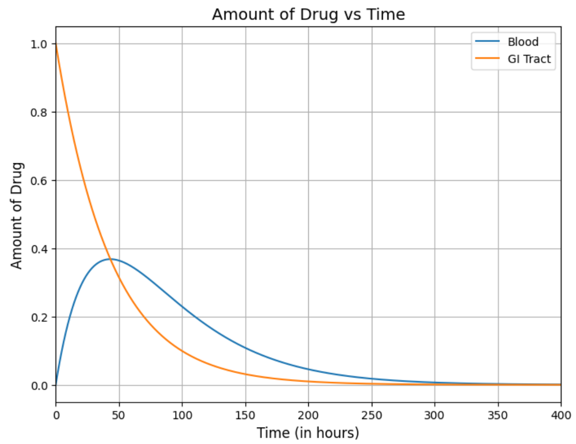

FIG. 5: Here $k_1 = k_2 = 0.0231$ hr^{-1}*and* $I = 1$ unit.

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

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

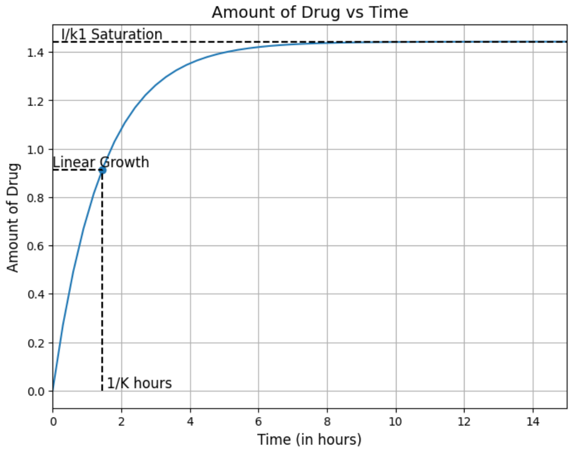

FIG. 6: $k_1 = 0.6931 hr^{-1}$, $k_2 = 0.0231 hr^{-1}, x_0 = 1\,unit, y_0 = 0\,unit$

The limiting value of x(t) is **1.44** units and that of y(t) is **43.29** units.

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

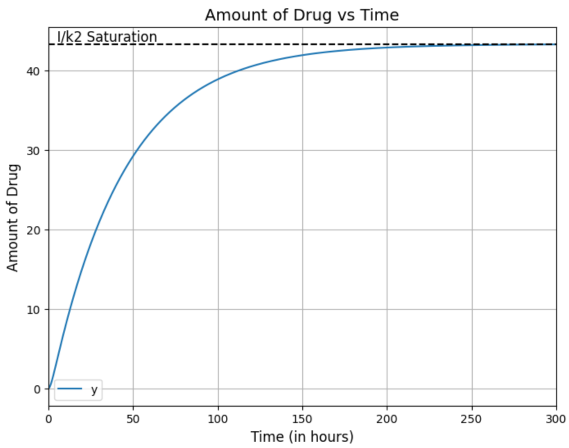

FIG. 7: $k_1 = 0.6931 hr^{-1}$, $k_2 = 0.0231 hr^{-1}, x_0 = 1\,unit, y_0 = 0\,unit$

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

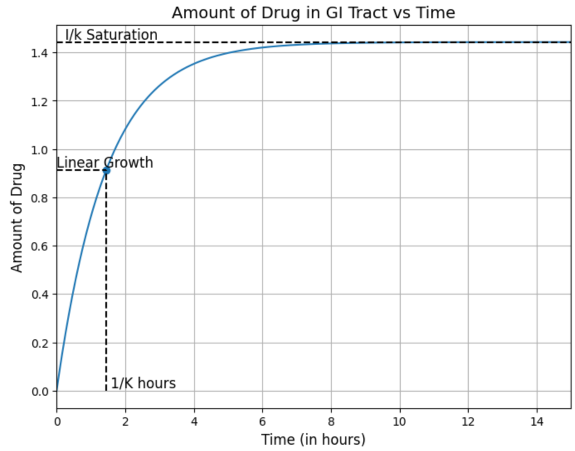

FIG. 8: $k_1 = k_2 = 0.6931 hr^{-1}$, $x_0 = 1\,unit, y_0 = 0\,unit$

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

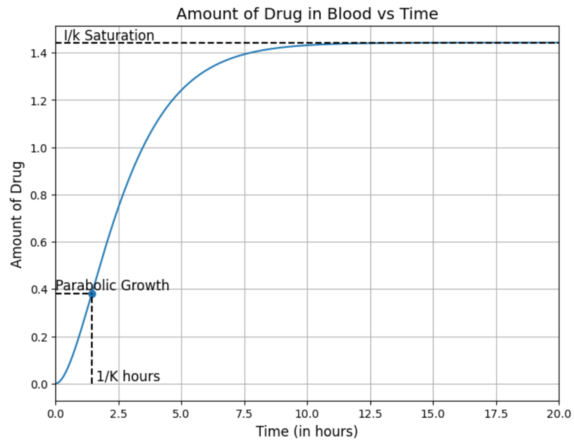

FIG. 9: $k_1 = k_2 = 0.6931 hr^{-1}$, $x_0 = 1\,unit, y_0 = 0\,unit$

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

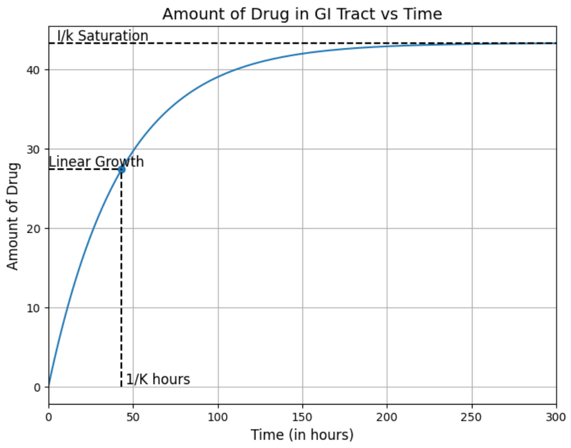

FIG. 10: $\mathrm{k}_1 = k_2 = 0.0231 hr^{-1}$, $\mathrm{x}_0 = 1\, unit, y_0 = 0\, unit$

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

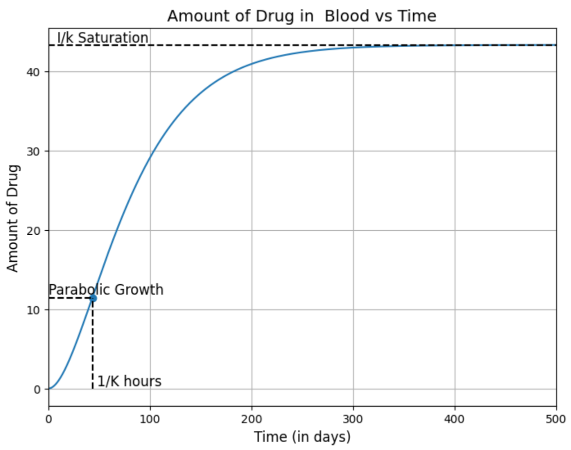

FIG. 11: $\mathrm{Pk}_1 = k_2 = 0.0231 hr^{-1}$, $\mathrm{x}_0 = 1\, unit, y_0 = 0\, unit$

III. CONCLUSIONS

- Based on the obtained results, 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 Cin.

- 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 K1 and K2 determine the convergence time.

- When a course of medication is taken, K1 = K2 = 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.