The study of drug diffusion through a mathematical model

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Abstract

This independent study is aimed to study the model of the diffusion of paracetamol in the body through the stomach, small intestine, blood vessels, tissues, liver and kidneys at a certain time period and study the change in drug concentration by finding the exact solution and using numerical methods. It was found that the drug concentration in each organ changed as follows: The stomach is the first part that receives the drug with the initial concentration. The drug concentration in the stomach gradually decreases until the concentration is close to zero. When the drug concentration in the stomach starts to decrease for a while, the concentration in the small intestine increases continuously until reach a highest threshold then the drug concentration slightly decreases. After that, the drug concentration in blood vessels, tissues, liver and kidney slightly increases until meet a maximum threshold. Then the blood concentration in those organs slowly decreases.

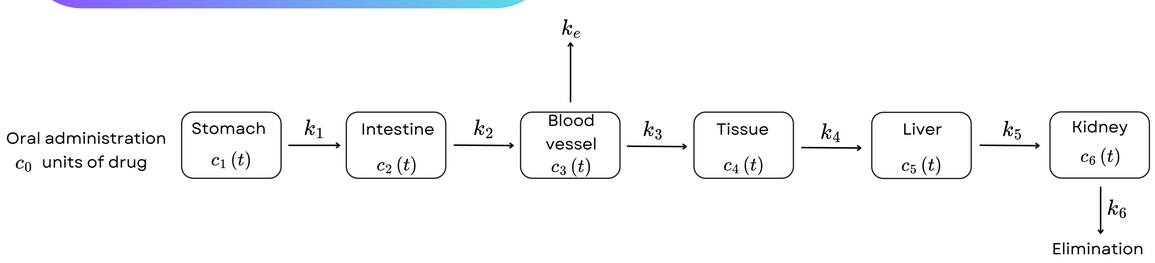
Introduction

The distribution of drugs is a crucial process in the human body. Studying the mechanisms of changes in drug concentration within the body is essential for observing how drugs spread to various organs. A widely method for analyzing this process is the mathematical modeling, which systematically predicts and explains drug behavior in the body. This study focuses on paracetamol, a common and easily accessible medication. We aim to examine the changes in drug concentration over time as it passes through different organs, including the stomach, small intestine, blood vessels, tissues, liver, and kidneys. Drug diffusion rates and elimination rates, are considered to gain a understanding of the behavior of paracetamol and its concentration levels at different time intervals.

Methodology

We use a numerical approach with the ode45 algorithm to study the behavior of paracetamol concentration changes over time. Additionally, we analyze the effects of varying diffusion rates in different organs. The parameter values are as follows: $k_1 = 0.91$, $k_2 = 0.63$, $k_3 = 0.52$, $k_e = 0.43$, $k_4 = 0.41$, $k_5 = 0.36$ and $k_6 = 0.31$ while initial variable is $c_0 = 500$

Mathematical Model



Definitetion of variables and parameters in mathematical model

c_0	is the initial concentration of drug dosage.	k_1	is the rate constants from stomach to intestine.
$c_1(t)$	is the concentration of drug in stomach.	k_2	is the rate constants from intestine to blood vessel.
$c_2(t)$	is the concentration of drug in intestine.	k_3	is the rate constants from blood vessel to tissue.
$c_3(t)$	is the concentration of drug in blood vessel.	k_e	is the elimination rate from the blood vessel.
$c_4(t)$	is the concentration of drug in tissue.	k_4	is the rate constants from tissue to liver.
$c_5(t)$	is the concentration of drug in liver.	k_5	is the rate constants from liver to kidney.
$c_6(t)$	is the concentration of drug in kidney.	k_6	is the elimination rate from the kidney.

This model is described with the following system of ordinary differential equations

$$\frac{dc_1(t)}{dt} = -k_1 c_1(t) \qquad c_1(0) = c_0$$

$$\frac{dc_2(t)}{dt} = k_1 c_1(t) - k_2 c_2(t) \qquad c_2(0) = 0$$

$$\frac{dc_3(t)}{dt} = k_2 c_2(t) - (k_3 + k_e) c_3(t) \qquad c_3(0) = 0$$

$$\frac{dc_4(t)}{dt} = k_3 c_3(t) - k_4 c_4(t) \qquad c_4(0) = 0$$

$$\frac{dc_5(t)}{dt} = k_4 c_4(t) - k_5 c_5(t) \qquad c_5(0) = 0$$

$$\frac{dc_6(t)}{dt} = k_5 c_5(t) - k_6 c_6(t) \qquad c_6(0) = 0$$

Results and discussion

Numerical solutions

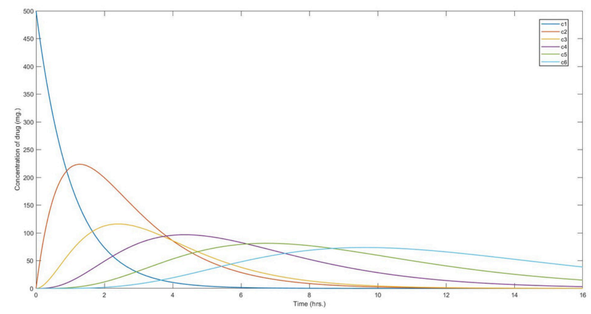


Figure 1

By using the initial concentration of paracetamol and the given parameters, it is observed that form Figure 1 the drug concentration in the stomach continuously decreases until it approaches zero. As the drug concentration in the stomach declines ($c_1(t)$), the concentration in the small intestine ($c_2(t)$) begins to increase. Subsequently, the drug concentration in the blood vessel ($c_3(t)$), tissues ($c_4(t)$), kidneys ($c_5(t)$) and liver ($c_6(t)$) increase. Once the concentration reaches its peak, it gradually decreases over time.

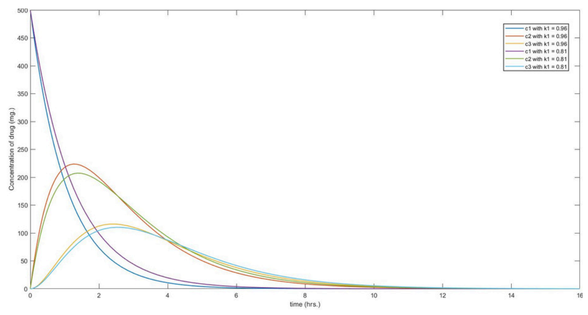


Figure 2

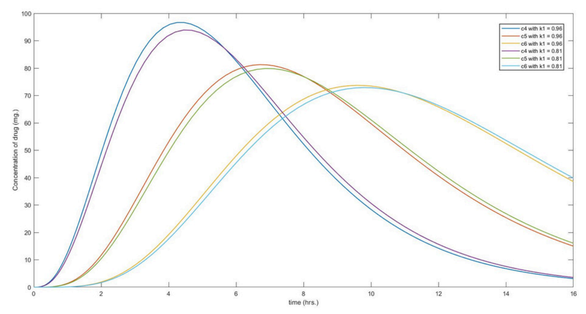


Figure 3

Figure 2 and 3 show that the study examines the impact of the diffusion rate from the stomach to the small intestine on drug concentration in various organs. By changing the value of k_1 from 0.96 to 0.81, it is observed that the drug concentration in the stomach ($c_1(t)$) increases, while the concentration in other organs($c_2(t)$ to $c_6(t)$) decreases.

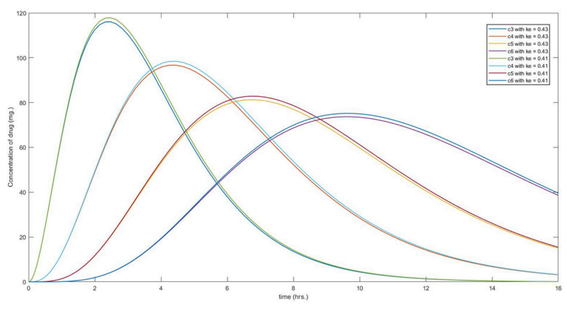


Figure 4

Figure 4 indicates that the study examines the impact of the diffusion rate from the bloodstream to the tissues on drug concentration in various organs. By changing the value of k_e from 0.43 to 0.41, it is observed that the drug concentration in the blood vessel ($c_3(t)$) increases, which also leads to an increase in drug concentration in other organs ($c_4(t)$ to $c_6(t)$).

Conclusion

The diffusion of paracetamal through stomach, intestine, blood vessel, tissue, liver and kidney is studied by using a mathematical model. The concentration of paracetamal in stomach gradually decreases while the concentration of paracetamal in other organ slowly increase. We also study the affect of diffusion rate $k_1, k_2, k_3, k_4, k_5, k_6$ and k_e. The concentration of drug in intestine ,blood vessel ,tissue ,liver and kidney decrease when the parameters (k_1 - k_6) decrease. On the other hand, the concentration of paracetamal in those organs (blood vessel ,tissue ,liver and kidney) increase when the elimination rate (k_e) decreases.

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