PHARMACOKINETICS IS A DESCRIPTION OF DRUGS AND THEIR BEHAVIOR IN THE HUMAN BODY BY BUILDING A MATHEMATICAL MODEL

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ABSTRACT

This article builds a mathematical model of the movement of drugs in the human body, thereby helping to determine the time of action of drugs on the body and to study their effects on damaged areas.

In [1], the mathematical model of the distribution of drugs in the compartments of the blood and tissue environment was studied for three cases: through the mouth, through the vein and through the tissue. Exactly what kind of medicine is not reflected in what kind of situation. In [3], the characteristics of antibiotic drugs were considered.

We focus on medicinal substances. Here is the movement of drugs in the human body and the connection of this movement with mathematics. This is to determine how much and how much time to give the medicine to a person depending on his age, weight and other symptoms.

The pharmacokinetics process consists of 5 stages:

• Liberation - the drug is released from the formulation.

• Absorption - the drug enters the body.

• Distribution - the drug spreads throughout the body

• Metabolism - the drug is broken down by the body.

• Excretion – the drug is removed from the body.

Each drug has some effect on the body. Some drugs must be absorbed quickly (for example, nitroglycerin in the case of a heart attack) and eliminated quickly (otherwise toxins will accumulate in the blood). For other drugs, we want slow absorption, so we get the maximum benefit and don't lose much from the release.

So, when a doctor prescribes (say), "take 2 tablets 3 times a day after meals", it is based on the desired levels of drug concentration and certain levels of distribution, metabolism and excretion in the body.

What is mathematics?

Mathematical analysis always leads to the optimal solution of various complex problems. Thus, it is mandatory to establish a mathematical model to estimate the drug concentration in different places and in the blood. When the drug is administered orally, the gastrointestinal tract dissolves the drug. From there, the

drugs diffuse into the blood and circulate throughout the body with the bloodstream. Medicines are gradually cleared from the blood by the liver and kidneys. The flow of drugs in the body is modeled by treating different parts of the body as compartments and then observing when the drug enters and leaves each compartment. In the following cases, it is intended to consider the use of drugs to restore the damaged part.

When the drug is administered to the body for the first time, the concentration of the drug in the bloodstream is zero. As the drug moves through the body and is metabolized, the concentration of the drug increases and reaches a peak level where it begins to decline. This is the period when the drug is fully distributed and metabolized. Over time, the concentration of the drug decreases and falls below a certain effective amount. To repeat these actions, it is necessary to take several more pills.

We can mathematically model such a situation using a differential equation. It consists of two parts - absorption part and elimination part. Initially, absorption (increase in drug concentration) dominates, and over time, elimination (decrease in concentration) is the most important element.

We have the following variables:

D = dose of drug administered

V = volume distributed in the body

C = rate of change of drug concentration at time t

F = fraction of absorbed dose (also called bioavailability)

A = absorption rate constant

E = elimination rate constant

t = time

Fraction of Absorption: It depends on the amount of drug administered, the fraction absorbed and the rate constant of absorption. It will decrease over time. The expression of suction is expressed as follows:

$$A \cdot F \cdot D \cdot e^{-At}$$

Elimination (disappearance) part: The dynamics of elimination is influenced by the elimination constant, the volume distributed in the body and the remaining concentration of the drug. The expression of this part is:

$$E \cdot V \cdot C$$

For our model, we need to subtract the elimination part from the absorption part (because the absorption part increases the concentration of the drug and the elimination part decreases it). Our differential equation is:

$$\frac{dC}{dt} = \frac{1}{V}\left(A \cdot F \cdot D \cdot e^{-At} - E \cdot V \cdot C\right), \quad C(0) = 0$$

We solve the differential equation for the one-dimensional part

$$\frac{dC(t)}{dt} = \frac{A \cdot F \cdot D}{V} \cdot e^{-At} - E \cdot C(t) \tag{1}$$

$$\frac{dC(t)}{dt} = -E \cdot C(t) \Rightarrow \frac{dC(t)}{C(t)} = -E \cdot dt \Rightarrow \ln C(t) = -E \cdot t + \ln C_1$$

$$\frac{dC(t)}{dt} = -EC(t) \rightarrow \frac{dC(t)}{C(t)} = -Edt \rightarrow lnC(1) = -Et + C1$$

$$C(t) = e^{-E \cdot t} \cdot C_1(t) \tag{2}$$

$$C'(t) = -E \cdot e^{-E \cdot t} \cdot C_1(t) + C_1'(t) \cdot e^{-E \cdot t}$$

(1) into Eq

$$-E \cdot e^{-E \cdot t} \cdot C_1(t) + C_1'(t) \cdot e^{-E \cdot t} = \frac{A \cdot F \cdot D}{V} \cdot e^{-A \cdot t} - E \cdot e^{-E \cdot t} \cdot C_1(t)$$

$$e^{-E \cdot t} \cdot C_1'(t) = \frac{A \cdot F \cdot D}{V} \cdot e^{-A \cdot t}$$

$$C_1'(t) = \frac{A \cdot F \cdot D}{V} \cdot e^{(E-A) \cdot t}$$

$$C_1(t) = \frac{A \cdot F \cdot D}{V(E-A)} \cdot e^{(E-A) \cdot t} + C_2$$

$C_1(t)$ put to (2) $$C(t) = e^{-E \cdot t} \cdot \left(\frac{A \cdot F \cdot D}{V(E-A)} \cdot e^{(E-A) \cdot t} + C_2 \right)$$ and use $C(0) = 0$

$$C_2 = -\frac{A \cdot F \cdot D}{V(E-A)}$$

$$C(t) = e^{-E \cdot t} \cdot \left(\frac{A \cdot F \cdot D}{V(E-A)} \cdot e^{(E-A) \cdot t} - \frac{A \cdot F \cdot D}{V(E-A)} \right)$$

$$C(t) = \frac{A \cdot F \cdot D}{V(E-A)} \cdot \left(e^{-A \cdot t} - e^{-E \cdot t} \right)$$
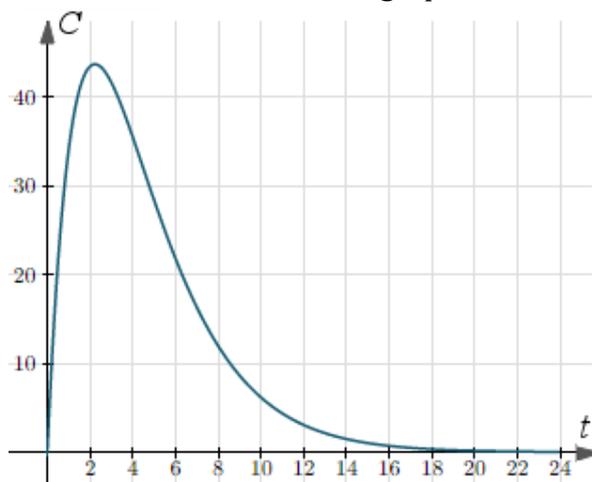
We will have the following function.

If we take the constants without units for simplicity,

$$V = 15; \; A = 0,5; \; E = 0,4; \; F = 2; \; D = 800$$

(These values are available from the pharmaceutical staff.)

$$C(t) = 533,3 \cdot \left(e^{-0,5 \cdot t} - e^{-0,4 \cdot t} \right)$$

And we draw its graph

On the graph, we can see the concentration rise (up to about t = 2) and the levels. Then the concentration drops to almost zero at t = 24.

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