

Compartments

Compartment is a homogeneous mathematical quantity. It represents a simplified model of reality, used to represent events. They can be small or large, but they are always abstract units. Typical compartments include plasma (possibly also blood), intracellular and extracellular fluid, fatty tissue etc. They are separated from each other by membranes. A set of compartments between which a substance is exchanged is described as a system.

Compartment Models

Compartment models are the basis of pharmacokinetic data analysis. They are dependent on substance concentration c and time t . For simplicity, one-, two- and three-compartment models are used.

Single compartment model

This type of model is the simplest. The whole body is considered here as a single compartment. It is assumed that after application, the substance is quickly and uniformly dispersed in the system. For this reason, it is impossible to accurately represent the distribution of the substance in the organism. This type of model is important when describing and predicting the movement of a drug, e.g. during repeated administration.

For data analysis purposes, it is most advantageous to work with concentration. The amount of substance D_0 (substance in the compartment) is divided by the volume unit (distribution volume).

$$C_0 = D_0/V_d$$

- C_0 = substance concentration at time $t = 0$;
- D_0 = amount of substance at $t = 0$;
- V_d = volume of distribution.

The modified equation for the one-compartment model can be expressed as:

$$C = C_0 \times e^{-kt} [1]$$

- C = concentration at time t ;
- C_0 = initial concentration;
- k = elimination constant;
- e = Euler's number.

The given equation describes the decreasing concentration of the administered substance in the compartment. The decrease is due only to the elimination of the substance.

Two-compartment model

Some substances cannot be immediately dispersed throughout the body volume. A two-compartment system is used to simulate this fact. The first is central and the second is peripheral. We assume an exchange of substance between compartments in order to maintain equilibrium.

Differential equation for the **central compartment**:

$$dC_1/dt = -C_1 \times (k_e + k_{1,2}) + C_2 \times k_{2,1}$$

Differential equation for the **peripheral compartment**:

$$dC_2/dt = C_1 \times k_{1,2} - C_2 \times k_{2,1}$$

- $k_{1,2}, k_{2,1}$ = rate constants that indicate the amount of substance exchanged per unit of time

The previous two equations can be combined into one:

$$C_t = Ae^{-\alpha t} + Be^{-\beta t} [1]$$

- $Ae^{-\alpha t}$ = distribution phase;
- $Be^{-\beta t}$ = elimination phase;
- α, β = slope of the curve during the distribution and elimination phase.

In this case, the loss of substance in the central compartment is dependent on the rate of elimination and the amount that is exchanged with the second compartment.

Three-compartment and multi-compartment model

As the number of compartments increases, the system becomes more complex.

The three-compartment system consists of a central compartment and two peripheral ones. The central one is better blooded than the other two.

$$dC_1/dt = -C_1 \times (k_e + k_{1,2} + k_{sub>1,3}) + C_2 \times k_{2,1} + C_3 \times k_{3,1}$$

Links

References

1. BURTIS, Carl A – ASHWOOD, Edward R – BRUNS, David E. *Tietz textbook of clinical chemistry and molecular diagnostics*. 4. edition. Wed. Louis, Mo : Elsevier Saunders, 2006. 2412 pp. ISBN 978-0-7216-0189-2.

External links

- Multi-compartment model - (English) (https://en.wikipedia.org/wiki/Multi-compartment_model%7C)

Resources

- BURTIS, Carl A – ASHWOOD, Edward R – BRUNS, David E. *Tietz textbook of clinical chemistry and molecular diagnostics*. 4. edition. Elsevier Saunders, 2006. 2412 pp. pp. 1237-1247. ISBN 978-0-7216-0189-2.
- DIPIRO, Joseph T. *Concepts in Clinical Pharmacokinetics*. 5th Edition edition. 2010. 250 pp. pp. 1-9. ISBN 978-1-58528-241-8.
- Pharmacokinetic analysis - Department of Pharmacology and Toxicology, UK (<https://www.faf.cuni.cz/~staud/lectures/obecna/06-PKanalyza.pdf>)