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On prognosis of dissolution of a medicinal product in an organism

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Abstract
We consider a model of dissolution of a medicinal drug in an animal with account of it's dissolution and changing of conditions of the process. In the framework of the model one shall to calculate distribution of concentration of the above substance in space and time during it's dissolution in an animal. To analyze the introduced model we consider an approach to solve the equations, which were used in the framework of the model. The approach gives a possibility to solve the above equations analytically.

Keywords: Dissolution of a medicinal product, spatio-temporal distribution of concentration of a medicinal product, changing of speed of dissolution of a medicinal product, analytical approach for analysis

Introduction

In the present time one can find fast increasing of quantity of new medicinal products as well as intensive development of old medicinal products with questionable efficacy and safety [1-5]. Usually influence of a medicinal products on organism could be done experimentally. Some time required dose of the considered products with influence on organism could be estimated. Also one can find another actual problem is speed of dissolution of a medicinal products in organism. In this paper we consider a model for estimation of distribution of concentration of a medicinal product in space and time. Based on the model we analyzed the above concentration with account possible changing of properties of organism.

Method of solution

In this section we consider a model for estimation and analysis of dissolution of a medicinal product in an organism. To estimate of distribution of concentration of a medicinal product in space and time we solve the second Fick's law in the following form [4, 5].

$$\frac{\partial C(x,t)}{\partial t} = \frac{\partial}{\partial x}\left[D(x,t)\frac{\partial C(x,t)}{\partial x}\right] + \frac{S}{V\,h}D(x,t)\,C(x,t)N(x,t), \qquad (1)$$

where $C(x,t)$ is the spatio-temporal distribution of concentration of the considered medicinal product; $D(x,t)$ is the diffusion coefficient of the product, which depends on tissue conditions in organism; S is the square of available for dissolution of solid surface; V is the volume of dissolution media; h is the width of the diffusion layer; $K(x,t)$ is the parameter of interaction of the considered product with another substances in organism; $N(x,t)$ is the concentration of other substances in organism, which interacting with infused product. Initial and boundary conditions for concentration of the considered medicinal product could be written in the following form

$$C(x,0) = f_C(x),\quad \left.\frac{\partial C(x,t)}{\partial x}\right|_{x=0} = 0,\quad C(L,t) = 0. \qquad (2)$$

Next let us to solve the Eq. (1) with conditions (2) by method of averaging of function corrections [6-8]. First of all we transform Eq. (1) to the following integral form

$$C(x,t)=C(x,t)+\frac{1}{L^2}\left\{\int_0^t\int_0^x D(v,\tau)\,C(v,\tau)\,d\,v\,d\,\tau-\int_0^t\int_0^x (x-v)C(v,\tau)\frac{\partial D(v,\tau)}{\partial v}d\,v\,d\,\tau+\right.$$

$$+\frac{S}{V\,h}\int_0^t\int_0^x (x-v)D(v,\tau)C(v,\tau)N(v,\tau)\,d\,v\,d\,\tau-\int_0^t\int_0^L D(v,\tau)C(v,\tau)\,d\,v\,d\,\tau+\int_0^L (L-v)\ \times$$

$$\left.\times\,C(v,t)\,d\,v+\int_0^x (x-v)\,f(v)\,d\,v+\int_0^t\int_0^L (L-v)C(v,\tau)\frac{\partial D(v,\tau)}{\partial v}d\,v\,d\,\tau-\int_0^x (x-v)\,C(v,t)\,d\,v\right\}. \quad (3)$$

In the framework of the considered method we substitute not yet known average value of the required concentration α_1 instead of the above concentration in the right sides of Eqs. (3). The substitution gives a possibility to obtain equations to calculate the first-order approximations of concentration of the considered product in the following form

$$C_1(x,t)=\alpha_1+\frac{1}{L^2}\left[\int_0^x (x-v)\,f(v)\,d\,v+\frac{\alpha_1 S}{V\,h}\int_0^t\int_0^x (x-v)D(v,\tau)N(v,\tau)\,d\,v\,d\,\tau+\alpha_1\frac{L^2-x^2}{2}\right] \quad (4)$$

Average value of concentration of medical product α_1 could be obtain by the following standard relation [6-8].

$$\alpha_1=\frac{1}{L\Theta}\int_0^\Theta\int_0^L C_1(x,t)\,d\,x\,d\,t \quad (5)$$

Substitution of relation (4) into relation (5) gives a possibility to obtain relation to determine average value α_1 in the final form

$$\alpha_1=V\,h\,\Theta\int_0^L (L^2-x^2)\,f(x)\,d\,x\Big/\left\{S\left[\int_0^\Theta(\Theta-t)\int_0^L (L^2-x^2)D(x,t)N(x,t)\,d\,x\,d\,t-\right.\right.$$

$$\left.\left.-2\int_0^\Theta(\Theta-t)\int_0^L x(L-x)D(x,t)N(x,t)\,d\,x\,d\,t\right]-\frac{2}{3}V\,h\,\Theta\,L^3\right\} \quad (6)$$

The second-order approximation of the considered concentration in the framework of the method of averaging of function corrections could be determined by using the following standard procedure: replacement of the considered concentration in the right sides of Eq. (3) on the sum $C(x,t)\to\alpha_2+C_1(x,t)$ [6-8]. The replacement gives a possibility to obtain the following equations to determine the concentration of the considered medicinal product

$$C_2(x,t)=\alpha_2+C_1(x,t)+\frac{1}{L^2}\left\{\int_0^t\int_0^x D(v,\tau)\,[\alpha_2+C_1(v,\tau)]\,d\,v\,d\,\tau-\int_0^t\int_0^x (x-v)[\alpha_2+C_1(v,\tau)]\times\right.$$

$$\times\frac{\partial D(v,\tau)}{\partial v}d\,v\,d\,\tau+\int_0^x (x-v)\,f(v)\,d\,v+\frac{S}{Vh}\int_0^t\int_0^x (x-v)D(v,\tau)[\alpha_2+C_1(v,\tau)]N(v,\tau)\,d\,v\,d\,\tau+$$

$$+\int_0^L (L-v)\,[\alpha_2+C_1(v,t)]\,d\,v+\int_0^t\int_0^L (L-v)[\alpha_2+C_1(v,\tau)]\frac{\partial D(v,\tau)}{\partial v}d\,v\,d\,\tau-\int_0^x[\alpha_2+C_1(v,t)]\times$$

$$\left.\times\,(x-v)\,d\,v-\int_0^t\int_0^L D(v,\tau)[\alpha_2+C_1(v,\tau)]\,d\,v\,d\,\tau\right\} \quad (7)$$

Average value of the second-order approximation of the above concentration α_2 could be calculated by using the following standard relation [6-8].

$$\alpha_2=\frac{1}{L\Theta}\int_0^\Theta\int_0^L [C_2(x,t)-C_1(x,t)]\,d\,x\,d\,t \quad (8)$$

Substitution of relations (7) into relation (8) gives a possibility to obtain the following relations for the required average value α_2

$$\alpha_2 = \left[\frac{1}{2}\int_0^\Theta (\Theta - t)\int_0^L (L + x)^2 C_1(x,t)\frac{\partial D(x,t)}{\partial x} d\,x\,d\,t - \int_0^\Theta (\Theta - t)\int_0^L (x - v) D(x,t) C_1(x,t)\, d\,x\,d\,t + \right.$$

$$+ 2\int_0^\Theta (\Theta - t)\int_0^L x^2 C_1(x,t)\frac{\partial D(x,t)}{\partial x} d\,x\,d\,t + \frac{S}{2V h}\int_0^\Theta (\Theta - t)\int_0^L (L + x)^2 D(x,t) C_1(x,t) N(x,t) d\,x\,d\,t +$$

$$+ \frac{2S}{Vh}\int_0^\Theta (\Theta - t)\int_0^L x^2 D(x,t) C_1(x,t) N(x,t) d\,x\,d\,t - \frac{1}{2}\int_0^\Theta (\Theta - t)\int_0^L \left(L^2 - x^2\right) C_1(x,t)\frac{\partial D(x,t)}{\partial x} d\,x\,d\,t -$$

$$- \int_0^\Theta \int_0^L x(L - x)\, f(x) d\,x\,d\,t - L\int_0^\Theta \int_0^L (L - x) C_1(x,t) d\,x\,d\,t + L\int_0^\Theta \int_0^L (L - x) D(x,t) C_1(x,t)\, d\,x \times$$

$$\times (\Theta - t)\, d\,t + \frac{1}{2}\int_0^\Theta (\Theta - t)\int_0^L \left(L^2 + x^2\right) D(x,t) C_1(x,t) d\,x\,d\,t + 2\int_0^\Theta \int_0^L x^2 C_1(x,t) D(x,t)\, d\,x \times$$

$$\times (\Theta - t)\, d\,t \Big] \left[\int_0^\Theta (\Theta - t)\int_0^L (x - v) D(x,t)\, d\,x\,d\,t - \frac{1}{2}\int_0^\Theta (\Theta - t)\int_0^L (L + x)^2 \frac{\partial D(x,t)}{\partial x} d\,x\,d\,t - \right.$$

$$- \frac{S}{2V h}\int_0^\Theta (\Theta - t)\int_0^L (L + x)^2 D(x,t) N(x,t)\, d\,x\,d\,t - \frac{2S}{Vh}\int_0^\Theta (\Theta - t)\int_0^L x^2 D(x,t) N(x,t)\, d\,x\,d\,t +$$

$$\left. + \Theta^2 \frac{L^3}{4} + 2\int_0^\Theta (\Theta - t)\int_0^L x^2 \frac{\partial D(x,t)}{\partial x} d\,x\,d\,t \right]^{-1} \tag{9}$$

Spatio-temporal distribution of concentration of medicinal product was analyzed analytically by using the second-order approximation in the framework of method of averaging of function corrections. The approximation is usually enough good approximation for to make qualitative analysis and to obtain some quantitative results. All obtained results have been checked by comparison with results of numerical simulations.

Discussion

In this section we present an analysis of spatio-temporal distribution of concentration of medicinal product in organism. Figs. 1 and 2 shows typical dependences of the considered concentration on time and coordinate, respectively. The obtained dependences qualitatively coincides with analogous experimental distributions. Increasing of temperature of organism leads to acceleration of interaction of the considered medicinal product with other substances of the organism.

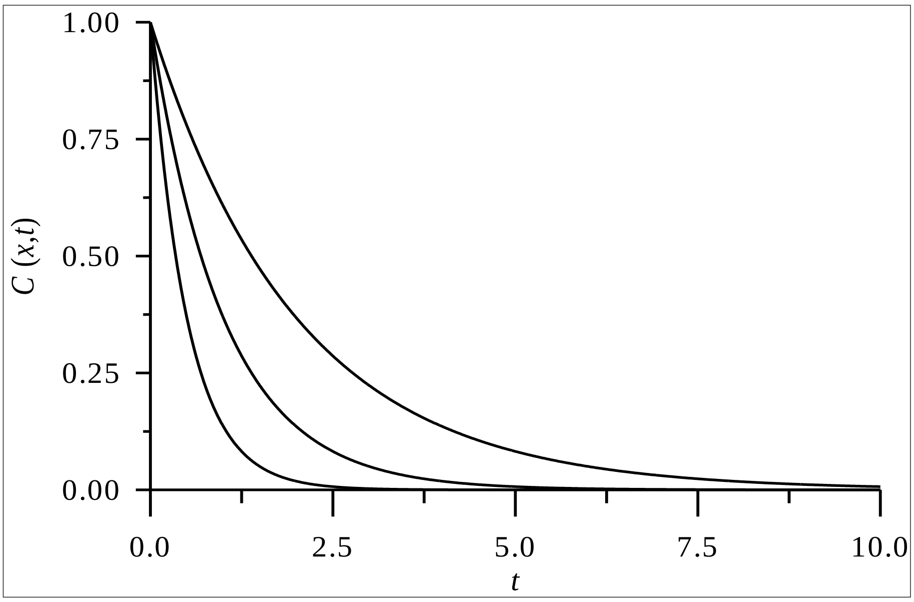

Fig 1: Typical dependences of concentration of considered product on time

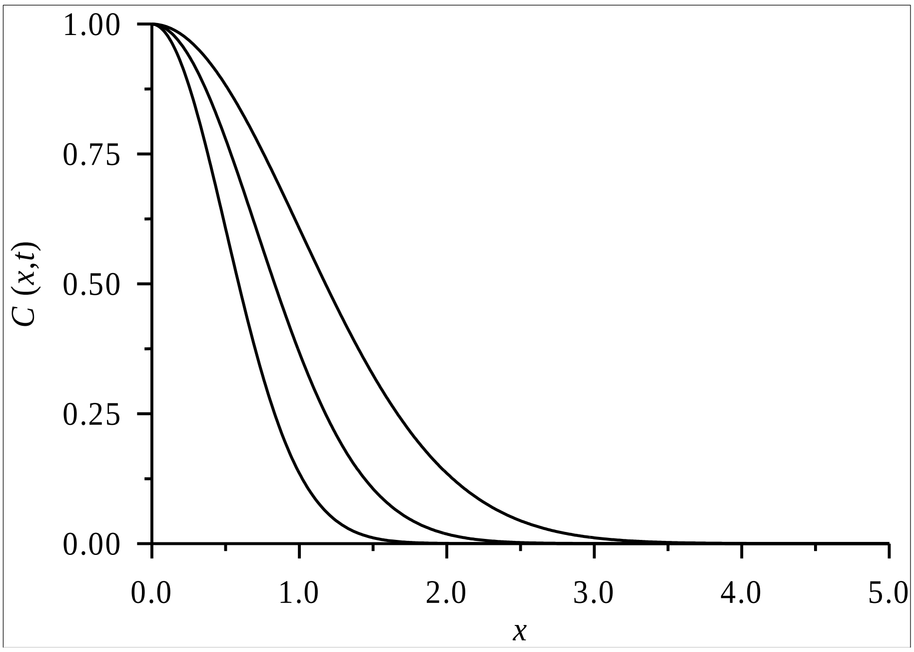

Fig 2: Typical dependences of concentration of considered product on coordinate

Conclusion

In this paper we consider analysis of dissolution of a medicinal product in an organisms. The analysis based on estimation of spatio-temporal distribution of concentration of the above product during the dissolution. We introduce an analytical approach for analysis of the above dissolution with account changing of it's conditions. We consider possibility to accelerate and decelerate of dissolution of medicinal products in organisms.

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