ON NUMERICAL SOLUTION OF AXISYMMETRIC REACTION-DIFFUSION EQUATION AND SOME OF ITS APPLICATIONS TO BIOPHYSICS

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Abstract

The numerical solution of the axi-symmetric reaction-diffusion equation is obtained by means of the second order accurate implicit finite difference schemes. The result is applied to the model of oxygen diffusion at the brain capillary.

Key words and phrases: Boundary value problems, Reaction-diffusion equation, Finite difference schemes, Blood Flaw.

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1 Introduction

Let us consider a diffusion process accompanied by a chemical reaction at the cylindrical area with the radius R_0 and length l. We suppose that this process is axi-symmetrical and the substance moves along the inner boundary of the cylinder at a constant speed. In this case the process is described by the axi-symmetric reaction-diffusion equation with the appropriate initial-boundary conditions [1]

$$\frac{\partial U}{\partial t} = D\left(\Delta U + \frac{1}{r}\frac{\partial U}{\partial r}\right) - \beta(U,t), \quad (\beta > 0),$$

where U is an unknown function and β is a velocity of the chemical reaction, which is generally non-linear function of U and t. We consider this equation in case of $\beta = \beta t$, where β is a constant.

Our purpose is to solve the corresponding initial boundary value problems for the reaction-diffusion equation by means of finite-difference schemes.

2 Setting of the problem

Let G be the rectangle $\{0 < x < l, r_0 < r < R_0\}$, in the coordinate system Oxr. This rectangle is a lateral cross-section of the cylindrical area.

Consider the following

Problem 1. In the area $Q_T = G \times \{0 < t < T\}$, find a function U continuous on $\bar{Q_T}$, having second order derivatives in Q_T, and satisfying the following equation

$$\frac{\partial U}{\partial t} = D\left(\Delta U + \frac{1}{r}\frac{\partial U}{\partial r}\right) - \beta t, \quad (\beta > 0), \tag{1}$$

with the initial and boundary conditions

$$U(x, r, 0) = f(x, r, 0), \tag{2}$$

$$U|_S = f(x, r, t),\ t > 0,$$

where β is the velocity of the chemical reaction, U is the substance concentration, D is a diffusion coefficient, S is the boundary of G,

$$f = \frac{R_0^2 - r^2}{R_0^2 - r_0^2}\left\{C_0 e^{-\frac{V_0}{D}x} e^{\frac{V_0^2}{D}t} - C_0 V_0^2 \frac{\beta}{D} t\right\}. \tag{3}$$

The function (3) for $r = r_0$ is the solution of the following equation

$$\frac{\partial f}{\partial t} = D\frac{\partial^2 f}{\partial x^2} - \beta \tag{4}$$

with the boundary condition

$$f|_{x=V_0 t, r=r_0} = C_0 - C_0 V_0^2 \frac{\beta}{D} t.$$

The second condition of (2), (3) and (4) means that the substance is moving along the boundary $r = r_0$ at the constant velocity V_0.

3 The algorithm

Let us consider more general equation

$$\frac{\partial U^*}{\partial t} = D\left(\Delta U^* + \frac{1}{r}\frac{\partial U^*}{\partial r}\right) + f_0(x, r, t), \tag{5}$$

with the following boundary conditions

$$U^*(x, r, 0) = f_1(x, r),$$

$$\begin{aligned} &U^*(0, r, t) = f_2(r, t),\ U^*(l, r, t) = f_3(r, t), \\ &U^*(x, r_0, t) = f_4(x, t),\ U^*(x, R_0, t) = f_5(x, t) = 0, \end{aligned} \tag{6}$$

where $f_0,\ f_1,\ f_2,\ f_3,\ f_4$ are the given continuous functions.

The equation (5) is a parabolic type linear equation. A numerical treatment of the parabolic type equations by means of different types of finite difference schemes was considered by numerous authors [1–8]. We will construct the new type of economical finite difference schemes for the equation (5)with the boundary conditions (6) and consequently for the equation (1) with the boundary conditions (2).

We divide the area of integration $\bar{Q}_T = \overline{G} \times [0,T]$ by the planes $x_i = ih_1,\ r_j = jh_2,\ t_n = n\tau,(i = 0,1,2,\dots,M,\quad j = 0,1,2,\dots,N,\quad n = 0,1,2,\dots L,)$ into cells, where $h_1 = \frac{l}{M},\quad h_2 = \frac{R_0 - r_0}{N},\quad \tau = \frac{T}{L}$.

Consequently, for the areas $\bar{G}$ and $[0,T]$ we introduce the following grids

$$\overline{\omega}_h = \{x_i = ih_1, r_j = jh_2, i = 0,1,\dots,M, j = 0,1,\dots,N\},$$

$$\overline{\omega}_\tau = \{t_j = \tau,\ j = 0,1,\dots,\ L\}.$$

For net functions and their difference derivatives we introduce the following notation

$$y_{x_1} = \frac{1}{h_1}(y(x+h_1,r) - y(x,r),$$
$$y_{r_2} = \frac{1}{h_2}(y(x,r+h_2) - y(x,r),$$
$$y_{\bar{x}_1} = \frac{1}{h_1}(y(x,r) - y(x-h_1,r)),$$
$$y_{\bar{r}_2} = \frac{1}{h_2}(y(x,r) - y(x,r-h_2)),$$
$$\Delta_2 y = y_{\overset{\circ}{r}_2} = \frac{1}{2}(y_{r_2} + y_{\bar{r}_2}),$$
$$\Delta_{11} y = y_{x\bar{x}},\ \Delta_{22} y = y_{r\bar{r}},$$

$$y((n+\frac{1}{2})\tau) = y^{n+\frac{1}{2}}.$$

We introduce the following symmetric finite difference schemes

$$\frac{y^{n+\frac{1}{2}} - y^n}{\frac{1}{2}\tau} = \sigma D\left[\Delta_{11}(y^{n+\frac{1}{2}} - y^n)\right] + D(\Delta_{11} + \Delta_{22})y^n + \frac{D}{jh_2}\Delta_2 y^n + f_0^{(n+\frac{1}{4})\tau}, \tag{7}$$

$$\frac{y^{n+1} - y^{n+\frac{1}{2}}}{\frac{1}{2}\tau} = \sigma D\left[\Delta_{22} y^{n+1} - y^{n+\frac{1}{2}})\right] + D(\Delta_{11} + \Delta_{22})y^{n+\frac{1}{2}} + \frac{D}{jh_2}\Delta_2 y^{n+\frac{1}{2}} + f_0^{(n+\frac{3}{4})\tau}, \tag{8}$$

$$
\begin{aligned}
&-\frac{\sigma\tau D}{2h_1^2} y_{i-1,j}^{n+\frac{1}{2}} + \left(1+\frac{\sigma\tau D}{h_1^2}\right) y_{ij}^{n+\frac{1}{2}} - \frac{\sigma\tau D}{h_1^2} y_{i+1,j}^{n+\frac{1}{2}} = \Phi_1, \\
&-\frac{\sigma\tau D}{2h_2^2} y_{i,j-1}^{n+1} + \left(1+\frac{\sigma\tau D}{h_2^2}\right) y_{ij}^{n+1} - \frac{\sigma\tau D}{2h_2^2} y_{i,j+1}^{n+1} = \Phi_2,
\end{aligned} \tag{9}
$$

$$
\begin{aligned}
&y(x_i, r_j, 0) = U_h^*(x, r, 0) = f_{1n}(x_i, r_j), \\
&y(0, r_j, t_n) = f_{2n}(r_j, t_n), \\
&y(l, r_j, t_n) = f_{3n}(r_j, t_n), \\
&y(x_i, r_0, t_n) = f_{4n}(x_i, t_n), \\
&y(x_i, R_0, t_n) = f_{5n}(x_i, t_n) = 0,
\end{aligned} \tag{10}
$$

where y_{ij}^n, $f_{1n}, \ldots, f_{5n}$ are the net functions of U^*, $f_1, \ldots, f_5$ and Φ_1 and Φ_2 are given by

$$
\begin{aligned}
\Phi_1 = &-\frac{\sigma\tau D}{2h_1^2} y_{i-1,j}^n + \left(1+\frac{\sigma\tau D}{2h_1^2}\right) y_{ij}^n - \frac{\sigma\tau D}{2h_1^2} y_{i+1,j}^n \\
&+\frac{1}{2}\tau D \left(\frac{y_{i-1,j}^n - 2y_{ij}^n + y_{i+1,j}^n}{h_1^2} + \frac{y_{i,j-1}^n - 2y_{ij}^n + y_{i,j+1}^n}{h_2^2}\right) \\
&+\frac{1}{2}\frac{\tau D}{jh_2}\frac{y_{i,j-1}^n - y_{i,j+1}^n}{2h_2} + \frac{1}{2}\tau f_0^{(n+\frac{1}{4})\tau},
\end{aligned}
$$

$$
\begin{aligned}
\Phi_2 = &-\frac{\sigma\tau D}{2h_2^2} y_{i,j-1}^{n+\frac{1}{2}} + \left(1+\frac{\sigma\tau D}{h_2^2}\right) y_{ij}^{n+\frac{1}{2}} - \frac{\sigma\tau D}{2h_2^2} y_{i,j+1}^{n+\frac{1}{2}} \\
&+\frac{1}{2}\tau D \left(\frac{y_{i-1,j}^{n+\frac{1}{2}} - 2y_{ij}^{n+\frac{1}{2}} + y_{i+1,j}^{n+\frac{1}{2}}}{h_1^2} + \frac{y_{i,j-1}^{n+\frac{1}{2}} - 2y_{ij}^{n+\frac{1}{2}} + y_{i,j+1}^{n+\frac{1}{2}}}{h_2^2}\right) \\
&+\frac{1}{2}\frac{\tau D}{jh_2}\frac{y_{i,j+1}^{n+\frac{1}{2}} - y_{i,j-1}^{n+\frac{1}{2}}}{2h_2} + \frac{1}{2}\tau f_0^{(n+\frac{3}{4})\tau}.
\end{aligned}
$$

The parameter σ is chosen from the condition $\sigma \geq \frac{c_2 n^2}{\nu(n-1)}$.

The stability and complete approximation of these schemes were proved in [8]. The accuracy is $O(\tau + h^2)$, where τ and h are steps along time and axis $h = (h_1, h_2)$.

Putting $f_0 = f_1 = f_2 = f_3 = f_4 = f$ in (7), (8), (9), (10), we obtain the schemes for the equation (1).

Below the example is given for the oxygen diffusion process in the human brain.The numerical results are obtained using the programming language C^{++} and the graph of this process is plotted.

4 Numerical examples

Here we consider the oxygen diffusion process in the human brain capillary across the radial direction. We admit that the capillary radius is about $r_0 = 3\mu m$ [9,10, 11] and choose the Krogh model [11,12]. We consider the capillary as a cylinder. Oxygen carried by RBC (red blood cell) is diffused along the capillary endothelium to the cylindrical area with the average radius $R_0 = 7\mu m$ of the brain tissue (the thickness of the capillary endothelium is about$1\mu m$) [9,10, 11]. Simultaneously oxygen is solved in the blood plasma, and consumed by the capillary endothelium and tissues. The initial saturation of oxygen at the tissue is denoted by C_*. Our purpose is estimation of the dynamics of saturation i.e. $C - C_*$.

We use the following data: the volume of the brain is $60sm^3$ and weight $14kg$ [9, 10], cerebral blood flow is about$100mL$ per $100g$ of brain per minute, arterial blood in the brain contains $19.6mL$ oxygen per $100mL$, the cerebral oxygen consumption is approximately $30mL$ per min [9, 10,11]. According to this $C_0 = 1.17pkL$; $\beta = 0.43pkL/sec$. We also take into the account capillary length $1\,mm$; and velocity of the blood $V_0 = 0.5(0.2)\,mm/sec$.

$$l = 0.5\,mm;\ C_0 = 1.17pkL;\ \beta = 0.43pkL/sec;$$

$$D = 0.13;\ V_0 = 0.5(or0.2)\,mm/sec;$$

The dynamics of saturation is given in Fig. 1 and Fig. 2

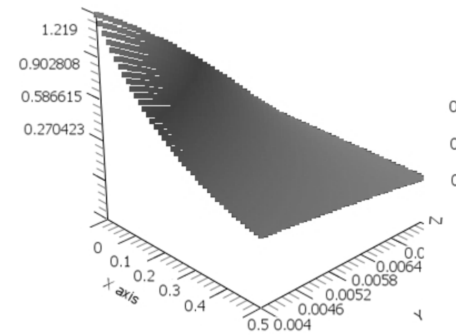

Fig 1. T=0,3; V_0=0,5;

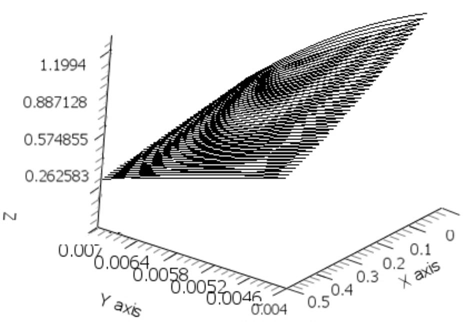

Fig 2. T=0,3; V_0=0,2;

Note 1. The schemes (7), (8), (9), (10), could be applied also to the case when to the write hand side of (1) the term αU, where α is a given constant, is added.

Note 2. The schemes (7), (8), (9), (10), also could be applied to the equation (1) with the discontinuous boundary conditions, when discontinuities are of the first order. I.E. Let us consider the following problem

Problem 2. In the area $Q_T = G \times \{0 < t < T\}$, to find a function U continuous on $\bar{Q_T}$, having second order derivatives in Q_T, and satisfies the following equation

$$\frac{\partial U}{\partial t} = D\left(\Delta U + \frac{1}{r}\frac{\partial U}{\partial r}\right) - \beta t, \quad (\beta > 0),$$

with the initial and boundary conditions

$$U(x,r,0) = C_0(x,r),\ U|_{r=r_0} = f(x,t),$$

$$U|_S = 0,\ t > 0,\ (r \neq r_0),$$

where

$$f = \frac{R_0^2 - r^2}{R_0^2 - r_0^2}\left\{C_0 e^{-\frac{V_0}{D}x} e^{\frac{V_0^2}{D}t} - C_0 V_0^2 \frac{\beta}{D} t\right\}.$$

Putting the data from the Example 1. we have obtained the following graphs

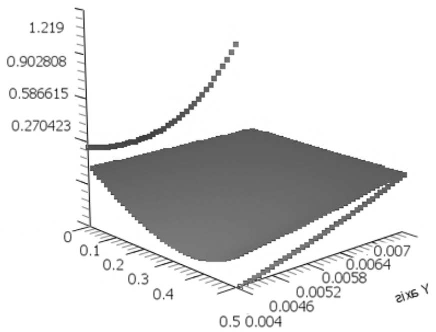

Fig 3. T=0,3; V_0=0,5;

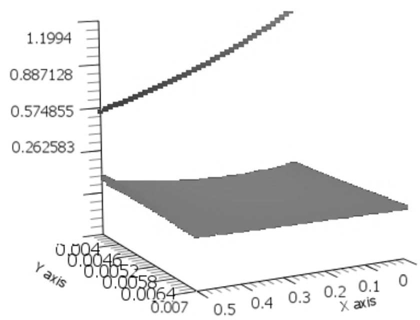

Fig 4. T=0,3; V_0=0,2;

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