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EXPONENTIAL REPLACEMENT IN FINITE ELEMENT METHOD FOR THE PROBLEM OF ADVECTION-DIFFUSION

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The mathematical model of the distribution of drugs in the artery wall during the catheter treatment of atherosclerosis, which is the initial boundary value problem for a system of two differential equations, was considered. This process has such features as large Peclet number. During the first numerical experiment it was revealed that direct application of the finite element method with standard linear and quadratic basis functions leads to the loss of stability of the solution. This is due to the specifics of input parameters of the problem, in fact a significant advantage over advection coefficients of diffusion coefficients. The solution is to use special exponential replacement inside finite element method.

Key words: advection-diffusion, FEM, Peclet number, exponential replacement.

1. INTRODUCTION

Mathematical and computer modelling of physiological processes is relevant area of research. The research problem, describing the distribution of drugs in the artery wall during catheter treatment of atherosclerosis, will help optimize the procedure of the treatment [1].

Drugs are represented by set of nanoparticles, each containing encapsulated bioactive substances. After absorbing nanoparticles in blood vessels, a process of further transfer is mainly due to the advection-diffusion process during which the encapsulated drugs are released, providing a therapeutic effect on the target area of the artery.

The mathematical model of distribution of drugs in the artery wall during the catheter treatment of atherosclerosis was considered. During first numerical experiment it was found that in the case of actual biological and chemical numerical parameters the solution, obtained by finite element method with linear and quadratic basis functions is unstable, due to a significant advantage of advection coefficients over diffusion coefficients.

Problems with such feature as large Peclet number should be solved by using special numerical methods.

2. FORMULATION OF THE PROBLEM

The problem is to find such C_1, C_2 – unknown concentrations of nanoparticles and encapsulated drug, respectively, which meet a system of differential equations in Ω [3]

$$\begin{cases} \dfrac{\partial C_1}{\partial t} + \nabla \cdot (VC_1) - \nabla \cdot (K_1 \cdot \nabla C_1) + \sigma_1 C_1 = 0; \\ \dfrac{\partial C_2}{\partial t} + \nabla \cdot (VC_2) - \nabla \cdot (K_2 \cdot \nabla C_2) + \sigma_2 C_2 = C_1 f; \end{cases} \quad (1)$$

initial conditions in $\bar{\Omega}$:

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$$C_1(x,0)=0,\ C_2(x,0)=0; \tag{2}$$

and boundary conditions on $\Gamma\times(0,T)$:

$$\begin{aligned} n\cdot(K_1\cdot\nabla C_1)+\lambda_1(C_1-C_{1,\infty})=0;\\ n\cdot(K_2\cdot\nabla C_2)+\lambda_2(C_2-C_{2,\infty})=0. \end{aligned} \tag{3}$$

In (1), (3) V is velocity vector, K_i – diffusivity coefficients, σ_i – coefficients of reaction and f – number of encapsulated drug in each nanoparticle.

Because of a fact that equations (1) are linked only by the presence of an unknown concentration of nanoparticles in the right side of the second equation, it is appropriate to firstly search an approximate solution of the first equation, and then find the solution of the second equation. Further let us consider separately each equation, as operator for them is common:

$$Ac=\nabla\cdot\left(\bar{w}c\right)-\nabla\cdot\left(K\cdot\nabla c\right)+\sigma c. \tag{4}$$

Therefore, the next equation has been considered:

$$\frac{\partial c}{\partial t}+Ac=\tilde{f}; \tag{5}$$

with right sides, initial and boundary conditions, respectively.

3. PROPOSED METHOD

During the first numerical experiment it was found that due to significant advantage of advection over diffusion in a case of actual biological and chemical parameters, the solution obtained by using finite element method with standard linear or quadratic basic functions [6] is unstable. This numerical experiment was conducted using FreeFEM++ – free software created at the university of Pierre and Marie Curie in France [2].

Therefore, such kind of problems with large Peclet number should be solved by using special numerical methods. In this paper we propose to use the modification of standard finite element method based on exponential replacement in formulation of problem (1)-(3) and reverse replacement in variation formulation of the problem.

Let us introduce the substitution $i=1,2$ [4]

$$C_i(x,y,z,t)=U_i(x,y,z,t)\exp\left(\frac{1}{2K_i}\mathbf{rv}-\frac{t}{4K_i}\sum_{j=1}^{3}v_j^2\right), \tag{6}$$

where

$$\mathbf{r}=x\mathbf{i}+y\mathbf{j}+z\mathbf{k};\quad \mathbf{v}=v_1\mathbf{i}+v_2\mathbf{j}+v_3\mathbf{k};\quad \mathbf{rv}=xv_1+yv_2+zv_3. \tag{7}$$

Replacement (6) was used in formulation of the problems and leads to deprivation of advection term. For testing proposed solution simplified problem has been considered. The problem is to find unknown concentration c which satisfies the following equation and boundary conditions:

$$\begin{cases} -K\dfrac{d^2c}{dx^2}+\mathrm{V}_1\dfrac{dc}{dx}+\sigma c=f;\\ D_1\dfrac{dc}{dx}(a)+\lambda_1 c(a)=\psi_1;\\ D_2\dfrac{dc}{dx}(b)+\lambda_2 c(b)=\psi_2. \end{cases} \tag{8}$$

Let us assume that

$$c(x)=u(x)\exp(\frac{V_1}{2K}x). \quad (9)$$

Then after substitution (6) in (8) there were obtained following expressions for the first and second derivatives:

$$\frac{dc}{dx}=\frac{du}{dx}\exp(\frac{V_1}{2K}x)+\frac{V_1}{2K}u\exp(\frac{V_1}{2K}x); \quad (10)$$

$$\frac{d^2c}{dx^2}=\exp(\frac{V_1}{2K}x)(\frac{d^2u}{dx^2}+2\frac{du}{dx}\frac{V_1}{2K}+u(\frac{V_1}{2K})^2); \quad (11)$$

Therefore, a new boundary problem has been obtained in the form

$$\begin{cases} -K\dfrac{d^2u}{dx^2}+Wu=f_1; \\ D_1\dfrac{du}{dx}(a)+\tilde{\lambda}_1u(a)=\tilde{\psi}_1; \\ D_2\dfrac{du}{dx}(b)+\tilde{\lambda}_2u(b)=\tilde{\psi}_2, \end{cases} \quad (12)$$

where respectively coefficients are

$$W=\frac{V_1^2}{4K}+\sigma;\ f_1=f\exp(-\frac{V_1}{2K}x);\ \tilde{\lambda}_i=\lambda_i+\frac{D_iV_1}{2K};\ \tilde{\psi}_i=\psi_i\exp(-\frac{V_1}{2K}x). \quad (13)$$

Let us introduce some space

$$V=\{u(x)\in W_2^{(1)}(\bar{\Omega})\}. \quad (14)$$

Then let us multiply (12) and some function $v(x)\in V$. Variation formulation for problem (12) was constructed [5]. Find such unknown function $u\in V$ that meets the following variational equation:

$$\int_a^b -K\frac{d^2u}{dx^2}vdx+\int_a^b wuvdx=\int_a^b f_1vdx,\quad \forall v\in V. \quad (15)$$

After integration by parts we obtaine

$$\int_a^b K\frac{du}{dx}\frac{dv}{dx}dx-K\frac{du}{dx}v\Big|_a^b+\int_a^b wuvdx=\int_a^b f_1vdx\,. \quad (16)$$

In (16) let us use the inverse substitution

$$u(x)=c(x)\exp(-\frac{V_1}{2K}x)\,. \quad (17)$$

After the division of the segment $[a,b]$ by finite elements the solution on a finite element (19) using linear basis functions (18) [7] was constructed

$$\varphi_{i-1}^h=-\frac{x-x_i}{h};\ \varphi_i^h=\frac{x-x_{i-1}}{h}; \quad (18)$$

$$c_h(x)=c_{i-1}^h\varphi_{i-1}^h(x)\exp(-\frac{V_1}{2K}x)+c_i^h\varphi_i^h(x)\exp(-\frac{V_1}{2K}x). \quad (19)$$

The next denotation has been introduced:

$$(\xi_i^h,\varphi_j^h)\overset{df}{=}\int_{x_{i-1}}^{x_i}(c_j^h(\xi_i^h)'(\varphi_j^h)'+w(\xi_i^h)(\varphi_j^h))dx, \quad (20)$$

where

$$\xi_i^h = \varphi_i^h \exp(-\frac{V_1}{2K}x). \tag{21}$$

The main system of linear algebraic equations of finite element method was obtained

$$\sum_{j=1}^{n} c_j^h (\xi_i^h, \varphi_j^h)_A = (f_1, \varphi_i^h), \quad i = \overline{1,n}. \tag{22}$$

Integrals in matrices of rigidity and mass were calculated analytically. The main system of linear equations for finite element method was solved by adaptive Gauss method.

4. NUMERICAL EXPERIMENTS

For finding approximate solution (19) for a problem (12) several numerical experiments were conducted. For this the software based on .NET Windows Forms Application using Advanced Grapher Application was created.

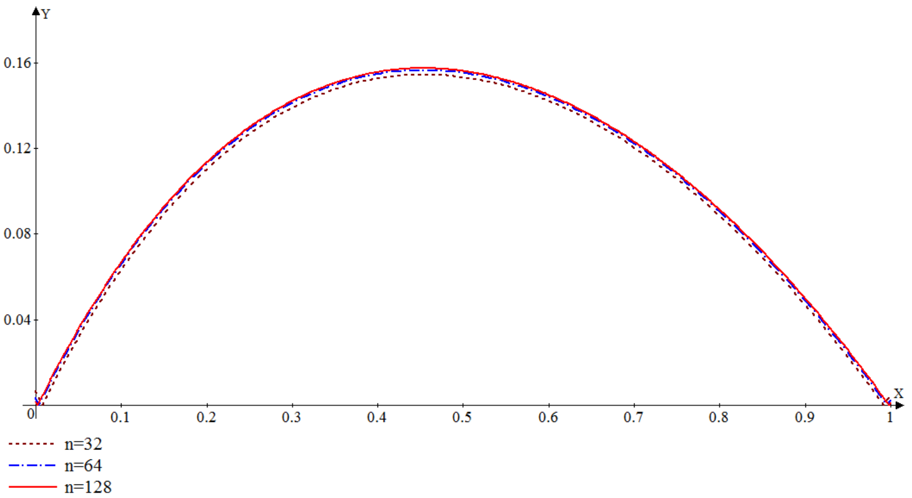

Fig. 1. Concentration of nanoparticles for *Pe* = 1.0

First numerical experiment was conducted for several meshes and Peclet number equals 1.0. On a fig. 1 the stability of solutions for different meshes is demonstrated. Increasing number of finite elements does not much impact on approximation of the solution.

Second numerical experiment was conducted for several meshes and Peclet number equals 100.0. During this numerical experiment results also have been compared with exact solution which is known:

$$c(x) = \left[x - \frac{\exp(\gamma x) - 1}{\exp(\gamma) - 1} \right] \frac{f}{V_1}, \tag{23}$$

where:

$$\gamma = \frac{V_1}{K}; \ \sigma = 0. \tag{24}$$

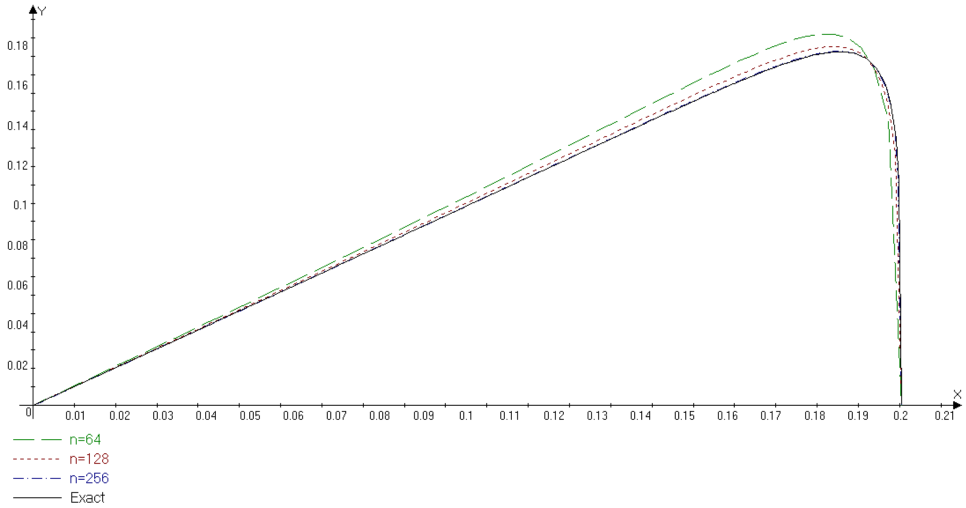

Fig. 2. Concentration of nanoparticles for *Pe* = 100.0

Fig. 2 shows that increasing the number of mesh points leads to improving the approximation to the exact solutions.

Therefore, obtained result for a testing problem (12) shows that using proposed approach in finite element method leads to stability and convergence of approximation.

5. CONCLUSIONS

The mathematical model describing the process of drug delivery in artery wall was considered. After first numerical experiment due to instability of solution obtained by using standard finite element method with quadratic and linear basis functions a new methodology in finite element method was proposed. Numerical experiments for different Peclet numbers has shown that proposed solution gives correct results and could be applied for 2 or 3 dimensional non-stationary problems of advection diffusion due to the specific of the proposed replacement.

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ЕКСПОНЕНЦІАЛЬНА ЗАМІНА В МЕТОДІ СКІНЧЕННИХ ЕЛЕМЕНТІВ ДЛЯ ЗАДАЧ АДВЕКЦІЇ-ДИФУЗІЇ

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Розглянуто математичну модель розповсюдження ліків у стінці артерії під час лікування атеросклерозу, яка є початково-крайовою задачею для системи двох диференціальних рівнянь. Процес розв'язання цієї задачі характеризується такою особливістю, як велике число Пекле. Під час числового експерименту виявили, що використання методу скінченних елементів з лінійними або квадратичними базисними функціями призводить до втрати стійкості розв'язку. Це пов'язано зі специфікою вхідних параметрів задачі, а саме значну перевагу коефіцієнтів адвекції над коефіцієнтами дифузії. Запропоновано використовувати спеціальну експоненціальну заміну всередині методу скінченних елементів.

Ключові слова: адвекція-дифузія, МСЕ, число Пекле, експоненціальна заміна.