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VERIFICATION OF THE HIGH ACCURACY SCHEME TO SOLVE ADVECTION-DIFFUSION-REACTION PROBLEMS

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РЕЗЮМЕ. Розглянуто початково-крайову задачу адвекції-дифузії-реакції з великим числом Пекле. Запропоновано новий альтернативний високо-точний підхід для чисельної апроксимації розв'язку методом скінченних елементів. Розроблене програмне забезпечення з реалізованим методом перевірено за допомогою чисельних розрахунків. Ця схема заснована на застосуванні експоненціальних замінів, а саме прямої у постановці задачі та зворотної у варіаційній постановці після пониження порядку диференціювання. Виведено аналітичні формули для обчислення матриць методу скінченних елементів у разі лінійної дискретизації. Чисельні розрахунки показують високу ефективність запропонованого підходу, експериментально отриманий порядок збіжності підтверджується теоретичними оцінками.

ABSTRACT. The initial-boundary problem of advection-diffusion-reaction with a large Péclet number is considered. A new alternative high accuracy approach for the numerical approximation of the solution by finite element method was proposed. We considered the problem of verification the numerical accuracy of the created software in which the proposed approach is implemented. This scheme is based on applying exponential replacements, direct in the problem formulation, and inverse in the variational formulation, after reducing the order of differentiation. Analytical formulas for calculate matrices of the finite element method in case of linear discretization are derived. Numerical calculations show the high efficiency of the proposed solution, theoretical results are verified by calculating the experimental order of convergence.

1. INTRODUCTION

Numerical modelling of mass transfer processes is an important area of research and is used in biology, medicine, chemical engineering, ecology, hydrology, mining, and others. It is worth noting that mathematical and computer modelling of the process of substance transfer in complex environments [1], [2] deserves special attention. In particular, these models are used to study the problems of biology and medicine (mass transfer in living tissues), ecology (such as the spread of pollution in the atmosphere, surface waters, groundwater, the spread of harmful impurities), chemistry (chemical reactions), meteorology (forecasting weather, climate change forecasting), etc.

The mathematical modelling of advection-diffusion-reaction (ADR) processes has important applications in solving many problems of engineering and mechanics. This is especially actual during scientific researches in biomechanics

Key words. Péclet number; advection-diffusion-reaction; mass transfer; finite element method.

and medicine, e.g., mass transfer in coronary system, blood flow, drug release processes [3]. In many cases, these processes are characterized by a very high-value advective component in the corresponding equations, the so-called problem of large Péclet number. In this case, the solution of the ADR problem is characterized by appearing boundary and inner layers, and applying the classical finite element method (FEM) leads to the loss of stability.

To date, a large number of specialized numerical schemes have been developed to find an approximate solution of the problem with large Péclet numbers [4], [5]. Among the most popular schemes are two approaches in the finite element method: grid thickening [6], [7], [8] and construction of higher-order basis functions [9]. The most significant result can be achieved by a combination of these two approaches. However, the use of such schemes as, for example, adaptive FEM [10], h- and hp-adaptive FEM [11], applying the exponential basis [12], functions-bubbles in FEM [13], discontinuous Galerkin method [14], [15], counter-flow schemes [17], has some specifics. The use of additional meshing points for spatial variables, building complicated basis functions, solving some additional problems might seriously affect the accuracy, and complicate the programming process. In addition to this, in the case of non-stationary processes, an important task is to build a high accuracy stable numerical method, and then time-variable discretization might be simple. Therefore, the construction and analysis of new alternative numerical schemes for finding approximate solutions of ADR problems with high Péclet numbers are important and motivated.

The main goal of this paper is to construct the new scheme of FEM applying to the ADR problem with high Péclet numbers, to perform the theoretical research of its convergence properties. Implementing of these steps will ensure the verification of the developed software and validation of numerical scheme which was proposed in [17]. The new scheme of application of the FEM to ADR problems with a large Péclet number has to have several advantages. First, the method should give a high accuracy at a low numerical cost. Secondly, this scheme has to do not require complicated construction of the grid of division of the area, it's thickening, and the definition of additional nodes, and therefore it has to be convenient to apply in the case of objects of complex shapes, as well as contact problems. The simplicity of method programming and computational costs are also important and useful.

2. SCHEME OF THE EXPONENTIAL REPLACEMENTS

2.1. Problem description. We find such concentration c which satisfies the ADR equation in the bounded limited area Ω with a Lipchitz boundary Γ

$$\frac{\partial c}{\partial t} + P_e (\mathbf{V} \cdot \nabla c) - K \Delta c + \sigma c = f(\mathbf{x}, t); \quad \mathbf{x} \in \Omega, \quad t \in (0, T]; \quad (1)$$

with initial condition

$$c(\mathbf{x}, 0) = c_0; \quad \mathbf{x} \in \bar{\Omega}; \quad (2)$$

and boundary condition

$$K (\boldsymbol{\nu} \cdot \nabla c) + \lambda c = \psi; \quad \mathbf{x} \in \Gamma, \quad t \in (0, T]. \quad (3)$$

In (1) P_e is a Péclet number, $\mathbf{V} = (V_1, V_2)$ is a velocity vector with constant values V_1, V_2 , K - a diffusivity coefficient, σ - a coefficient of the reaction, λ - a coefficient of the mass transfer on the boundary Γ , c_0 - an initial value of the concentration in Ω , $f = f(\mathbf{x}, t) : \Omega \times [0, T] \rightarrow R$, $\psi = \psi(\mathbf{x}, t) : \Gamma \times [0, T] \rightarrow R$ - functions of external sources in Ω , Γ , respectively, T - a final value of time variable t and $0 < T \leq \infty$; $\boldsymbol{\nu} = (l_1, l_2)$ - the vector of normal to the boundary Γ . Coefficients are positive, constant and dimensionless.

2.2. Exponential replacements. We proposed to use a special exponential replacement in the formulation of the problem to eliminate the advection term in the Equation (1). For this purpose let us apply in (1)-(3) the next replacement [18], [21] :

$$c = u \exp\left(\frac{P_e(\mathbf{V} \cdot \mathbf{x})}{2K}\right). \quad (4)$$

For further compactness, we introduce the denotation

$$E_{P_e} \stackrel{\text{def}}{=} \exp\left(\frac{P_e(\mathbf{V} \cdot \mathbf{x})}{2K}\right); E_{P_e}^- \stackrel{\text{def}}{=} \exp\left(-\frac{P_e(\mathbf{V} \cdot \mathbf{x})}{2K}\right).$$

Then, considering the following expressions for derivatives:

$$\begin{aligned} \frac{\partial c}{\partial x_i} &= \frac{\partial u}{\partial x_i} E_{P_e} + \frac{P_e V_i}{2K} u E_{P_e}; \\ \frac{\partial^2 c}{\partial x_i^2} &= \left(\frac{\partial^2 u}{\partial x_i^2} + \frac{P_e V_i}{K} \left(\frac{\partial u}{\partial x_i} + \frac{P_e V_i}{2K} u \right) \right) E_{P_e}; \\ \frac{\partial c}{\partial \nu} &= \left(\frac{\partial u}{\partial \nu} + \frac{P_e}{2K} (\mathbf{V} \cdot \mathbf{l}) u \right) E_{P_e}, \end{aligned}$$

the problem statement (1)-(3) might be equivalent to the problem

$$\frac{\partial u}{\partial t} - K(\Delta u) + \left(P_e^2 \left(\frac{V_1^2 + V_2^2}{4K} \right) + \sigma \right) u = f(\mathbf{x}, t) E_{P_e}^-, \mathbf{x} \in \Omega, t \in (0, T]; \quad (5)$$

$$u(\mathbf{x}, 0) = c_0 E_{P_e}^-; \quad \mathbf{x} \in \bar{\Omega}; \quad (6)$$

$$\beta K \frac{\partial u}{\partial \nu} + \left(\frac{\beta P_e}{2} (\mathbf{V} \cdot \mathbf{l}) + \lambda \right) u = \psi E_{P_e}^-, \quad \mathbf{x} \in \Gamma. \quad (7)$$

In order to get the variation formulation let us introduce the space $W = \{u \in W_2^{(1)}(\Omega)\}$, multiply the initial condition (6) and equation (5) on some function $w \in W$, and integrate over Ω . We will get

$$\begin{aligned} \int_{\Omega} \frac{\partial u}{\partial t} w d\Omega - K \int_{\Omega} \Delta u w d\Omega + \left(P_e^2 \frac{V_1^2 + V_2^2}{4K} + \sigma \right) \int_{\Omega} u w d\Omega &= \\ = \int_{\Omega} f w E_{P_e}^- d\Omega; t \in (0, T], \mathbf{x} \in \Omega; \\ \cdot \int_{\Omega} u(\mathbf{x}, 0) w d\Omega &= \int_{\Omega} c_0 w E_{P_e}^- d\Omega; \quad \mathbf{x} \in \bar{\Omega}. \end{aligned} \quad (8)$$

Let us apply Green's formula to the Laplasian operator in (8)

$$\begin{aligned} \int_{\Omega} \frac{\partial u}{\partial t} w d\Omega + K \left(\int_{\Omega} \nabla u \nabla w d\Omega - \int_{\Gamma} \frac{\partial u}{\partial \nu} w d\Gamma \right) + \\ + \left(P_e^2 \frac{V_1^2 + V_2^2}{4K} + \sigma \right) \int_{\Omega} u w d\Omega = \int_{\Omega} f w E_{P_e}^- d\Omega. \end{aligned} \quad (9)$$

According to the classical procedure of FEM, the next step might be a discretization by spatial variables and constructing iteration process by time variable. However, in this case a new specific problem occurs. Taking into account subintegral expressions in (9) on the left side and on the right side in case of high Péclet number it is obviously that system of linear algebraic equation (SLAE) might have different orders of the right and the left parts. This is due to the last multiplier in integral expression in the right part of (9).

In this case the problem leads to the problem of finding some specific coefficient to solve SLAE numerically with high precision and this is another numerically complicated task. Instead of this we propose to use the inverse exponential replacement in (9) in order to balance its left and right parts

$$u = cE_{P_e}^-.$$

It should be noted that we carry out the inverse replacement after lowering the order of differentiation in the subintegral diffusion expression. Thus, a direct replacement was made in the problem statement, and the reverse one in the variational formulation after the application of the Green's formula. Therefore, the use of direct and inverse substitution does not lead to identical expressions.

Applying inverse replacement we get the following expression for the diffusion component of term (9):

$$K \int_{\Omega} \nabla u \nabla w d\Omega = K \int_{\Omega} \nabla c \nabla w E_{P_e}^- d\Omega - \sum_{i=1,2} \frac{P_e V_i}{2} \int_{\Omega} c \frac{\partial w}{\partial x_i} E_{P_e}^- d\Omega; \quad (10)$$

and taking into account that

$$\int_{\Omega} v \frac{\partial u}{\partial x_i} d\Omega = - \int_{\Omega} u \frac{\partial v}{\partial x_i} d\Omega + \int_{\Gamma} u v l_i d\Gamma, \forall u, v \in W;$$

for the last term in the right part of (10) we will get that

$$\begin{aligned} -\frac{P_e V_i}{2} \int_{\Omega} c \frac{\partial w}{\partial x_i} E_{P_e}^- d\Omega &= \frac{P_e V_i}{2} \int_{\Omega} \frac{\partial c}{\partial x_i} w E_{P_e}^- d\Omega - \\ -\frac{P_e V_i}{2} \int_{\Gamma} c w l_i E_{P_e}^- - \frac{(P_e V_i)^2}{4K} \int_{\Omega} c w E_{P_e}^- d\Omega, i = 1, 2. \end{aligned} \quad (11)$$

From the boundary condition (7) it is easy to make sure that

$$-K \int_{\Gamma} \frac{\partial u}{\partial \nu} w d\Gamma = \int_{\Gamma} \left(\frac{P_e}{2} (\mathbf{V} \cdot \boldsymbol{\nu}) \right) u w d\Gamma + \int_{\Gamma} \frac{\lambda}{\beta} u w d\Gamma - \int_{\Gamma} \frac{\psi}{\beta} E_{P_e}^- w d\Gamma.$$

Therefore, after applying the inverse replacement we will get that

$$-K \int_{\Gamma} \frac{\partial u}{\partial \nu} w d\Gamma = \int_{\Gamma} \left(\frac{P_e}{2} (\mathbf{V} \cdot \boldsymbol{\nu}) \right) w E_{P_e}^- d\Gamma + \quad (12)$$

Finally, by combining expressions (8)-(12), we obtain the following variational formulation: to find such weak solution $c(\mathbf{x}, t) \in L_2(W_2^1(\Omega); 0, T)$ that satisfies

$$\begin{cases} m(c', w) + a(c, w) = l(w) & \forall t \in (0, T); \\ m(c(0) - c_0, w) = 0 & \forall w \in W, \end{cases} \quad (13)$$

$$\begin{aligned} a(c, w) &= K \int_{\Omega} \nabla c \nabla w E_{P_e}^- d\Omega + \int_{\Gamma} \frac{\lambda}{\beta} w E_{P_e}^- d\Gamma + \\ + \sum_{i=1,2} \frac{P_e V_i}{2} \int_{\Omega} \frac{\partial}{\partial x_i} w E_{P_e}^- d\Omega + \sigma \int_{\Omega} c w E_{P_e}^- d\Omega; \end{aligned} \quad (14)$$

$$l(w) = \int_{\Omega} fwE_{P_e}^- d\Omega + \int_{\Gamma} \frac{\psi}{\beta} wE_{P_e}^- d\Gamma.$$

Thus, the use of exponential substitutions leads to the appearance of exponential weights in sub-integral expressions, with both sides of the integral equation. In addition, there is a halving in the constant factors of the advective term, compared with the use of classical exponential weights.

2.3. Discretization. In proposing to conduct theoretical research about convergence and the order of convergence of the proposed scheme, next step is a spatial discretization of the problem. For this, we propose to use a spatial discretization based on linear basis functions. In case of the initial-boundary value plane problem, for some parameter of meshing $h \in \mathbb{R}$, let us introduce a finite-dimensional subspace $W_h \subset W$ of dimension N with a linear basis $\{\varphi_i^h\}$, and use a semi-discrete representation

$$c_h(\mathbf{x}, t) = \sum_{j=1}^N c_j(t) \varphi_j^h(\mathbf{x}). \quad (15)$$

Thus, from (13) we get its approximate formulation

$$\begin{cases} m(c_h', w_h) + a(c_h, w_h) = l(w_h); & \forall w_h \in W_h; \\ m(c_h(0) - c_0, w_h) = 0. \end{cases} \quad (16)$$

Then, taking the approximate solution (15) into (16), and, by the Galerkin method, substituting the basic functions $\{\varphi_i^h\}$ instead of arbitrary functions w_h , we get the Cauchy problem for the ODE

$$\begin{cases} MC'(t) + AC(t) = L(t), & t \in (0, T]; \\ MC(0) = P, \end{cases} \quad (17)$$

where

$$m_{ij} = m(\varphi_i^h, \varphi_j^h); a_{ij} = a(\varphi_i^h, \varphi_j^h); l_i(t) = l(\varphi_i^h); p_i = m(c_0, \varphi_i^h); \\ M = \{m_{ij}\}; A = \{a_{ij}\}; C(t) = \{C_i(t)\}; L(t) = \{l_i(t)\}; P = \{p_i\}.$$

By using the Crank-Nicolson scheme to sample the time variable in a step $\delta = t_{j+1} - t_j$, we obtain the following one-step recurrent scheme in terms of increments $\Delta C = C^{j+1} - C^j$:

$$\begin{cases} M\Delta + \frac{1}{2}\delta A\Delta C = \delta F^{j+\frac{1}{2}} - \delta AC^j, \\ MC^0 = P. \end{cases} \quad (18)$$

It should be noted that the scheme of applying exponential replacements in FEM has a computational feature. The coefficients of corresponding SLAE consist of sums of integrals, which contain exponential multipliers in integrands.

Therefore, analytical formulas for calculating these integrals are derived. As an alternative, we recommend calculating integrals using special IOST quadrature with high orders of convergence. This quadrature is based on Gaussian quadrature, described and tested on exponential functions in [19], [20]. This

might be very useful for any order of basic functions in FEM, not only linear one.

On the other hand, this scheme does not require complicated construction of the grid of division of the area, it's thickening, and the definition of additional nodes, and therefore it is convenient to apply in the case of objects of complex shapes.

3. NUMERICAL RESULTS AND VERIFICATION

A number of numerical experiments were conducted to find approximate solutions of the ADR problems using the exponential replacements scheme in the FEM. For this goal, C# high-level software was created on the base of object-oriented techniques.

3.1. Convergence. We consider the stationary two-dimensional case of the ADR problem and compare the results obtained with classical FEM and the exponential replacements scheme in FEM.

The area Ω is defined as a single square and on its boundary Γ a homogeneous Dirichlet condition is specified. Coefficients are set as the following:

$$P_e = 100, K = 1, V_1 = 1, V_2 = 1, \sigma = 1, f = 1; 0, 1[]$$

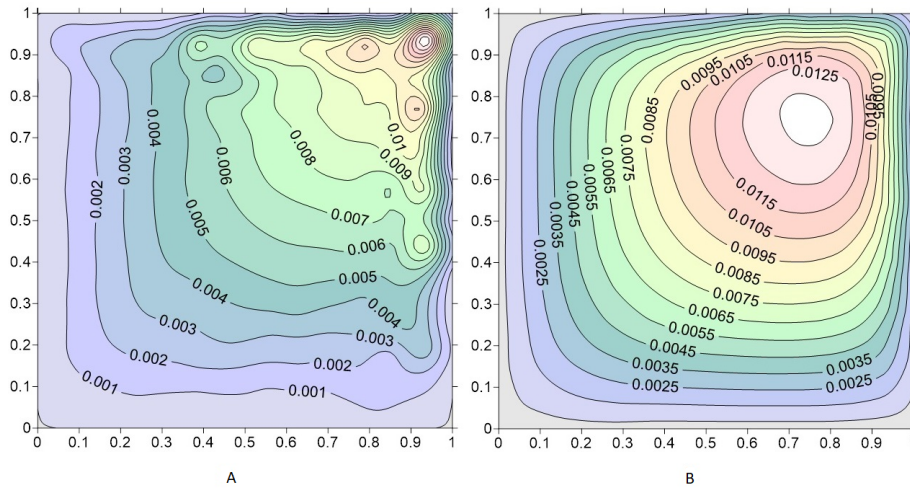


FIG. 1. Approximations by linear FEM (A) and the scheme of exponential substitutions (B)

Number of triangular finite elements on Figure 1 (A), (B) $N = 300$. As can be seen from the Figure 1 (A) with taking high Péclet number, the approximation loses stability and oscillation appears in the upper right corner of the area Ω . It is known that the thickening of the grid does not give the desired result for the approximate solution. On the other hand, as can be seen from Figures 1 (B), the proposed exponential replacements scheme in FEM overcomes the disadvantage of the loss of approximation stability. Oscillation does not occur;

the approximation is smooth and stable with the increase in the number of finite elements. The appearance of the approximations corresponds to the physical interpretation of the ADR process.

3.2. Stability. The high accuracy of the proposed scheme is very useful, in particular, in the case of finding an approximate solution of the nonstationary ADR problem, as it provides stability of approximation by spatial variables. In this numerical experiment, the Crank-Nicolson scheme (18) is used. For further analysis of the approximation behaviour and stability of the proposed scheme, we consider the graphs of changes in concentrations with increasing time variable at a fixed point in the region.

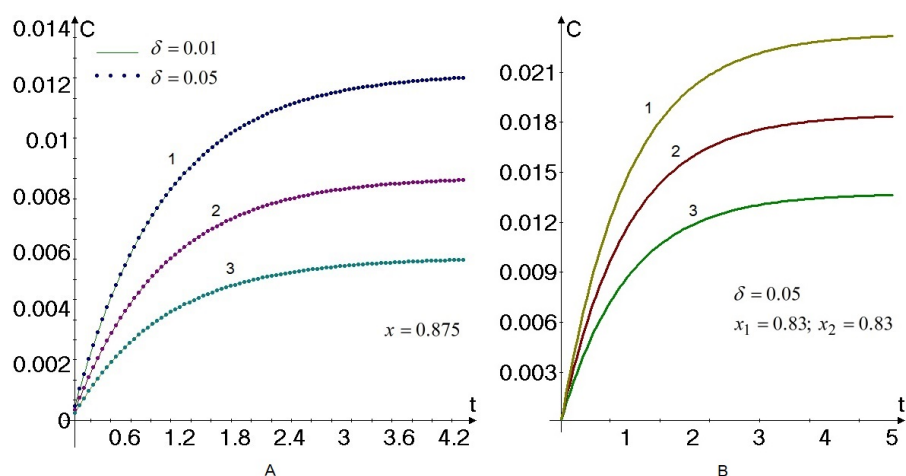


FIG. 2. Changes of concentrations in time at fixed points for one-dimensional (A) and two-dimensional (B) non-stationary ADR problems

Figure 2 shows graphs of changes in the desired concentration over time at fixed points in the region for one-dimensional (A) and two-dimensional case (B). Figure 2 (A) demonstrates plots of approximate solutions for different Péclet numbers and different steps over the time variable. Curve 1 corresponds to $P_e = 70$, Curve 2 - to $P_e = 100$, and Curve 3 - to $P_e = 150$. Number of finite elements $n = 128$. As can be seen from this graph, with the decreasing of the step by the time variable the approximate solutions are stable. With the growth of the time variable, the process becomes stationary. It is also worth noting that the maximum values of the desired concentration at the point $x = 0.875$ decrease with increasing Péclet number. The numerical result corresponds to the nature of the process, as well as the fact that with an increasing number P_e , numerical solutions reach stationary behaviour faster. Figure 2 (B) demonstrates the plots of approximate solutions for different Péclet numbers at a fixed point $P = (0.83, 0.83)$ of the region Ω . Curve 1 corresponds to $P_e = 50$, Curve 2 - to $P_e = 70$, and Curve 3 - to $P_e = 100$. The initial and

boundary conditions are set to zero. The coefficients and the right part are chosen as follows:

$$K = 1, V_1 = V_2 = 1; \sigma = 1, f(t) = 1 - e^{-t}.$$

The step by the time variable $\delta = 0.05$, number of finite elements $N = 308$. Figure 2 (B) shows that with the increase of the advection coefficient, the maximum of the solution decreases, and the process degenerates into a stationary one faster, which corresponds to the nature of the phenomenon. It is worth noting the high stability of approximations at a fixed point; the graphs in all three cases are definitely smooth.

Results show that the approximations are smooth, stable, no oscillation occurs. Since the scheme of exponential replacements proposed in this paper has high accuracy, the error does not accumulate when discretizing over the time variable.

4. CONCLUSIONS

This work was devoted to the development of the new scheme of applying FEM to the singular-perturbed problems of ADR. The formulation of the initial boundary value problem of ADR in an incompressible medium has been considered. The applying scheme of exponential replacements has led to a modification of the ADR variational problem in comparison with the classical approach.

We carried out the theoretical studies regarding the existence and uniqueness of the solution of the weak formulation of the problem, as well as of the order of convergence of the proposed method. A comparison with a priori estimates of the error using the classical FEM was done and the significant advantages of the exponential replacement method have shown. We described the application of this method to the initial-boundary-value problem of ADR, as well as time-domain sampling according to Crank-Nicolson schemes. Numerical calculations have shown the high efficiency of the proposed method, and verification by calculating the experimental order of convergence of the exponential replacement scheme has confirmed the results of theoretical studies.

The obtained theoretical results and the results of numerical experiments presented in the paper make it possible to state that the developed numerical scheme and implemented software satisfies the verification requirements.

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