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NUMERICAL SOLUTION OF ONE-DIMENSIONAL DISPERSION EQUATION IN HOMOGENEOUS POROUS MEDIUM BY MODIFIED FINITE ELEMENT METHOD

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This article discusses the mathematical modeling of the longitudinal dispersion phenomenon in a homogeneous porous medium and its solution using the modified finite element method. Also, the theorem about existence and uniqueness, and stability of nonlinear system that arose in the numerical scheme, by utilizing nonlinear functional analysis and the Banach fixed point theorem are proved. Finally, illustrations are added to show the efficacy of the derived method.

Keywords: Burger's equation; porous medium; finite element scheme.

Introduction

Longitudinal dispersion in a porous medium is an important concept in studying fluid flow and solute transport through porous materials such as soils, aquifers, and reservoirs. Problems like predicting the spread of pollutants and their concentration at various distances from the source, optimizing EOR methods to maximize the recovery of oil, predicting nutrients and fertilizer in the soil, and many problems related to hydrology and environment engineering [1–6]. The longitudinal dispersion phenomenon has a long historical background. Adolf Fick [7] given Fick's laws of diffusion, laid the groundwork for understanding the dispersion of solutes in the medium. Prandtl introduces the concept of the boundary layer which helped to understand the velocity profiles in fluid flow and its implications on the solute transport which became a foundation for the longitudinal dispersion phenomenon. Taylor showed that in laminar flow the combination of molecular diffusion and shear flow leads to enhanced dispersion of solutes now known as Taylor dispersion [8]. Aris [9] extended Taylor's work by giving mathematical techniques to derive the dispersion coefficient by considering velocity profiles and boundary conditions. Bear [1] formulated a general model for dispersion in porous media, recognizing the role of both molecular diffusion and mechanical dispersion. Bear and Bachmat [1] published a foundational text that includes detailed discussions on the mechanisms and mathematical modeling of dispersion in porous media.

A mathematical model derived by Bear is nothing but a Burger's equation which is a second-order nonlinear partial differential equation and it is difficult to find an analytic solution [29–31]. Many researchers developed finite difference as well as finite element schemes to find a solution to this Burgers' equation. The finite difference scheme for the Burgers' equation is found in the monographs [10, 11]. Borana et al [12] implemented a finite difference scheme to study the longitudinal dispersion in a porous medium. On the other hand, the finite element method (FEM) is a powerful numerical technique widely used for solving partial differential equations (PDEs). It has become an essential tool in various fields such as structural mechanics, fluid dynamics, and porous media flow [25–28]. This method was initially conceptualized in the 1940s and 1950s to meet the needs of the aerospace industry, FEM gained prominence through the pioneering work of Richard Courant, who utilized piecewise linear approximations to solve torsion problems [13]. The formal development of FEM is credited to engineers and mathematicians such as Argyris and Clough. Clough's seminar paper in 1960 [14] introduced the term "finite element" and laid the groundwork for its widespread adoption in engineering analysis. Over the decades, FEM has undergone significant advancements [32, 33]. In the 1970s and 1980s, the development of efficient computational algorithms and the increasing availability of computer resources facilitated the method's application to more complex problems [22–24]. The versatility of FEM in handling complex geometries and boundary conditions has made it a preferred choice for solving a wide range of engineering problems [15, 20, 21].

In recent years, FEM has been extended to solve nonlinear PDEs, such as Berger's equation, which describes various physical phenomena in porous media [16–19]. The ongoing improvements in finite element formulations and computational techniques continue to expand the applicability and efficiency of FEM in scientific and engineering research. This manuscript focuses on modifying a finite element scheme to solve the one-dimensional Berger's equation, which governs the phenomena of diffusion in homogeneous porous media. Berger's equation, a type of nonlinear PDE, poses significant challenges due to its nonlinearity and the complexity of the medium.

The paper is structured as follows: Section 1 discusses the problem definition, Mathematical formulation of the problem is discussed in Section 2. Section 3 discusses the Numerical Scheme to convert nonlinear PDE into a nonlinear system of ODEs. Qualitative properties are discussed in Section 4. An illustration and its error analysis are found in Secion 5 followed by the conclusion.

1. Problem Definition

In a homogeneous porous medium, miscible displacement describes a two-phase flow where the phases are completely soluble in each other, thus negating the effects of capillary forces. Under conditions of complete miscibility, the miscible flow of contaminated or saline water and fresh water can be approximated locally as a single-phase fluid obeying Darcy's law. Considering the longitudinal dispersion of the contaminant or saline water with concentration $C(x, t)$ flowing in the x-direction, the medium is initially saturated with fresh water.

Several essential basic assumptions are made:

(i) **No Mass Transfer Between Phases**: There is no exchange of mass between the solid and liquid phases.

(ii) **Solute Transport**: The solute transport across any fixed plane, due to microscopic velocity variations within the flow tube, can be quantitatively expressed as the product of a dispersion coefficient and the concentration gradient.

(iii) **Directional Dispersion**: The miscible flow occurs both longitudinally and transversely, but the dispersion effect is more pronounced in the direction of flow than in the transverse direction.

(iv) **One-Dimensional Treatment**: For simplicity, the dispersion phenomena are treated in one dimension, thereby ignoring the radial or transverse components of dispersion.

This treatment allows for a more straightforward analysis and modeling of the dispersion process, focusing on the predominant direction of flow.

2. Mathematical Formulation

If the fluid is incompressible then the equation of continuity is given by

$$\frac{\partial \rho}{\partial t} + div \cdot (\rho \bar{V}) = 0, \tag{1}$$

where ρ is the density of mixture and $\bar{V}$ is the pore seepage velocity vector [1].

The equation of diffusion for a fluid flow through a homogeneous porous medium, without increasing or decreasing the dispersing material is given by

$$\frac{\partial C}{\partial t} + div(C\bar{V}) = \nabla \cdot \left[\rho \; \bar{D} \; div \left(\frac{C}{\rho}\right)\right], \tag{2}$$

where C is the concentration of the fluid A into the other host fluid B, D is the tensor coefficient of dispersion having unit $length^2/time$ having nine components D_{ij}.

If the flow is laminar in homogeneous porous medium ρ consider as constant, leads to $div \cdot (\bar{V}) = 0$, the equation (2) becomes

$$\frac{\partial C}{\partial t} + \bar{V} \cdot \nabla C = div[\bar{D} \cdot divC]. \tag{3}$$

When the seepage velocity $\bar{V}$ is along $x-$ axis then coefficient of longitudinal dispersion $D_{11} = D_L = \frac{L}{C_0^2}$ and other Dij's are zero. Therefore, equation (3) becomes,

$$\frac{\partial C}{\partial t} + u\frac{\partial C}{\partial x} = D_L \frac{\partial^2 C}{\partial x^2}, \tag{4}$$

where, u is the component of flow velocity $\bar{V}$ along the x-axis is given by $u = \frac{C(x,t)}{C_0}$. Since the concentration of the contaminated water at the surface $x = 0$ is considerably high and constant, one can take $C_0 = 1$. Therefore the equation (4) becomes,

$$\frac{\partial C}{\partial t} + C\frac{\partial C}{\partial x} = D_L \frac{\partial^2 C}{\partial x^2} \tag{5}$$

The equation (5) describes the longitudinal hydrodynamic dispersion of miscible contaminants or saline water flowing through the homogeneous porous medium.

3. Numerical Scheme

This section develops a numerical scheme to solve the one-dimensional dispersion phenomenon in a homogeneous porous medium, governed by Berger's equation [12].

$$\frac{\partial C}{\partial t} + C\frac{\partial C}{\partial x} - D^2 \frac{\partial^2 C}{\partial x^2} = 0, \tag{6}$$

where C is the concentration of fluid A in the other host fluid B (i.e. C is the mass of fluid A per unit volume of the mixture) and $D = D_L$.

Dividing the spatial domain $[0, L]$ into N subdomain and equating weighted residue over each element

$$R = \int_0^{h_e} W^e \left[\frac{\partial C}{\partial t} + C \frac{\partial C}{\partial y} - D^2 \frac{\partial^2 C}{\partial y^2} \right] d\bar{y} = 0, \tag{7}$$

where, W^e is the weight function of y and y is temporary variable over the e^{th} element $[0, h_e]$.

Assuming the solution of the form $C^e(y,t) = \sum_{j=1}^{M} C_j^e(t)\phi_j^e(y)$ over e^{th} element and plugging it into equation (7), the equation becomes

$$\int_0^{h_e} W^e \left[\left(\sum_{j=1}^{M} \frac{dC_j^e}{dt} \phi_j^e \right) + \left(\sum_{j=1}^{M} C_j^e \phi_j^e \right) \left(\sum_{j=1}^{M} C_j^e \frac{d\phi_j^e}{dy} \right) - D^2 \left(\sum_{j=1}^{M} C_j^e \frac{d^2\phi_j^e}{dy^2} \right) \right] dy = 0 \tag{8}$$

and taking weak formulation of the equation (8),

$$\begin{aligned} \int_0^{h_e} \left[\left(\sum_{j=1}^{M} \frac{dC_j^e}{dt} W^e \phi_j^e \right) + W^e \left(\sum_{j=1}^{M} C_j^e \phi_j^e \right) \left(\sum_{j=1}^{M} C_j^e \frac{d\phi_j^e}{dy} \right) + D^2 \left(\sum_{j=1}^{M} C_j^e \frac{dW^e}{dy} \frac{d\phi_j^e}{dy} \right) \right] dy \\ = \left[D^2 W^e \sum_{j=1}^{M} C_j^e \frac{d\phi_j^e}{dy} \right]_0^{h_e}. \end{aligned} \tag{9}$$

Choosing $W_i^e = \phi_i^e$ for each $i = 1, 2, \cdots M$ and integrating over $[0, h_e]$ the equation (9) becomes:

$$\begin{aligned} \sum_{j=1}^{M} \frac{dC_j^e}{dt} \int_0^{h_e} \phi_i^e \phi_j^e dy + \sum_{j=1}^{M} \sum_{k=1}^{M} C_j^e C_k^e \int_0^{h_e} \phi_i^e \phi_j^e \frac{d\phi_k^e}{dy} dy + \sum_{k=1}^{M} C_j^e \int_0^{h_e} D^2 \frac{d\phi_i^e}{dy} \frac{d\phi_j^e}{dy} dy \\ = \left[D^2 \phi_i^e \sum_{j=1}^{M} C_j^e \frac{d\phi_j^e}{dy} \right]_0^{h_e} \end{aligned} \tag{10}$$

Considering $\mathcal{M}^{(e)} = \left(\int_0^{h_e} \phi_i^e \phi_j^e dy \right)_{M \times M}$, $\mathcal{L}^{(e)} = \left(\int_0^{h_e} \phi_i^e \phi_j^e \frac{d\phi_k^e}{dy} dy \right)_{M \times M}$, $\mathcal{K}^{(e)} = \left(\int_0^{h_e} D^2 \frac{d\phi_i^e}{dy} \frac{d\phi_j^e}{dy} dy \right)_{M \times M}$ and $\mathcal{B}^{(e)} = \left(\left[D^2 \phi_i^e \sum_{j=1}^{M} \frac{d\phi_j^e}{dy} \right]_0^{h_e} \right)_{M \times M}$ the system can be rewritten as

$$\mathcal{M}^{(e)} \frac{dU^{(e)}}{dt} + (U^{(e)})^T \mathcal{L} U^{(e)} + \mathcal{K} U^{(e)} = \mathcal{B}^{(e)} U^{(e)}, \tag{11}$$

where $U^{(e)} = \left(C_i^e \right)_{M \times 1}$.

Assembling the system over the entire domain $[0, L]$ using the principle of continuity, and applying boundary conditions, the system (11) becomes:

$$\mathcal{M} \frac{dU}{dt} + U^T \mathcal{L} U + \mathcal{K} U = \mathcal{B} U. \tag{12}$$

The system (12) is a nonlinear system of ordinary differential equations with constant coefficients. Note that dimensions of matrices $\mathcal{M}, \mathcal{L}, \mathcal{K}$ and $\mathcal{B}$ depend on the boundary conditions.

4. Qualitative Properties

This section is devoted to the qualitative analysis, including the existence, uniqueness, and stability of solutions for the system (12).

Theorem 1. *If the matrix $\mathcal{M}$ is non-singular and $\Phi(t)$ is the continuous and bounded transition matrix of the linear system $\frac{dU}{dt} = \mathcal{M}^{-1}\mathcal{K}U$, then the system (12) has a unique solution over the finite interval $[0, T_0]$ with the initial condition $U(0) = U_0$.*

Proof. The system (12) can be rewritten as

$$\mathcal{M}\frac{dU}{dt} = -\mathcal{K}U - U^T\mathcal{L}U + \mathcal{B}U. \tag{13}$$

Since $\mathcal{M}$ is non-singular and $\Phi(t)$ is the transition matrix generated by the operator $-\mathcal{M}^{-1}\mathcal{K}$, the mild solution is given by

$$U(t) = \Phi(t)U(0) + \int_0^t \Phi(t,s)\mathcal{M}^{-1}\big[-U^T\mathcal{L}U + \mathcal{B}U\big]ds. \tag{14}$$

The mild solution (14) is of the form

$$U(t) = \Phi(t)U(0) + \int_0^t \Phi(t,s)\mathcal{M}^{-1}\mathcal{F}(s, U(s))ds \tag{15}$$

having the first part $U^T\mathcal{L}U$ of $\mathcal{F}$ is Lipchitz continuous with respect to U over the finite interval and second part $\mathcal{B}U$ is linear in U. Therefore by generalized fixed point theorem, the system (13) has a unique mild solution over the finite interval $[0, T]$. Moreover, $\mathcal{F}$ is differentiable over t and U therefore the mild solution (14) is solution of the (13) and the following algorithm

$$U_1(t) = \Phi(t)U_0 - \int_0^t \Phi(t,s)\mathcal{M}^{-1}\big[U_0^T\mathcal{L}U_0 + \mathcal{B}U_0\big]ds \tag{16}$$

and

$$U_{n+1}(t) = \Phi(t)U(0) - \int_0^t \Phi(t,s)\mathcal{M}^{-1}\big[U_n^T(t)\mathcal{L}U_n(t) + \mathcal{B}U_n(t)\big]ds \tag{17}$$

converges to the solution of the system (13).

□

The next theorem discusses the stability of the system (12).

Theorem 2. *If the matrix $\mathcal{M}$ is non-singular and $\Phi(t)$ is the continuous and bounded transition matrix of the linear system $\frac{dU}{dt} = \mathcal{M}^{-1}\mathcal{K}U$, then the system (12) is stable.*

Proof. The nonlinear part of the equation (13) $U^T\mathcal{L}U$ is Lipschitz continuous concerning U (differentiable in U and bounded domain in the finite domain) and $\mathcal{B}$ is linear operator therefore the system (13) is stable.

□

5. Numerical Implimentation

This section discusses the solution of one-dimensional Berger's equation

$$\frac{\partial C}{\partial t} + C\frac{\partial C}{\partial x} - \frac{\partial^2 C}{\partial x^2} = 0, \quad 0 < x < 1,\ t > 0 \tag{18}$$

with boundary condition

$$C(0,t) = \frac{1}{2}\left[1 - tanh\left(-\frac{t}{8}\right)\right], \quad C(0,t) = \frac{1}{2}\left[1 - tanh\left(\frac{1-2t}{4}\right)\right], t > 0 \tag{19}$$

and initial condition

$$C(x,0) = \frac{1}{2}\left[1 - tanh\left(\frac{x}{4}\right)\right]. \tag{20}$$

Dividing the spatial domain into N elements and considering Langrangian interpolating polynomials $\phi_1^{(e)} = (1 - \frac{y}{h_e})$ and $\phi_2^{(e)} = \frac{y}{h}$, a system of two time-differential equations for each element is given by

$$\mathcal{M}^{(e)}\frac{dU^{(e)}}{dt} = -\mathcal{K}U^{(e)} - (U^{(e)})^T\mathcal{L}U^{(e)} + \mathcal{B}^{(e)}U^{(e)} \tag{21}$$

where $\mathcal{M}^{(e)} = \frac{h_e}{6}\begin{bmatrix} 2 & 1 \\ 1 & 2 \end{bmatrix}$, $\mathcal{K}^{(e)} = \frac{1}{h_e}\begin{bmatrix} 1 & -1 \\ -1 & 1 \end{bmatrix}$ and $\mathcal{B}^{(e)} = \begin{bmatrix} b_{11} & 0 \\ 0 & b_{22} \end{bmatrix}$. Assembling by adding the forces, the system takes the form

$$\mathcal{M}\frac{dU}{dt} = -\mathcal{K}U - U^T\mathcal{L}U + \mathcal{B}U. \tag{22}$$

where $\mathcal{M} = \frac{h}{6}\begin{bmatrix} 2 & 1 & 0 & 0 & \cdots & 0 & 0 \\ 1 & 4 & 1 & 0 & \cdots & 0 & 0 \\ 0 & 1 & 4 & 1 & \cdots & 0 & 0 \\ \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\ \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\ 0 & 0 & 0 & 0 & \cdots & 1 & 2 \end{bmatrix}$,

$$\mathcal{K} = \frac{1}{h}\begin{bmatrix} 1 & -1 & 0 & 0 & \cdots & 0 & 0 \\ -1 & 2 & -1 & 0 & \cdots & 0 & 0 \\ 0 & -1 & 2 & -1 & \cdots & 0 & 0 \\ \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\ \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\ 0 & 0 & 0 & 0 & \cdots & -1 & 1 \end{bmatrix},$$

$U^T\mathcal{L}U = \frac{1}{6}\begin{bmatrix} -2C_1 + C_1C_2 + C_2^2 \\ -C_1^2 + C_1C_2 + C_2C_3 + C_3^2 \\ \cdots\cdots\cdots \\ \cdots\cdots\cdots \\ -C_{N-1}^2 + C_{N-1}C_N + C_NC_{N+1} + C_{N+1}^2 \end{bmatrix}$ and $\mathcal{B} = \begin{bmatrix} Q_{11} \\ 0 \\ 0 \\ \cdots \\ Q_{N+1} \end{bmatrix}$ and the Dirichlet boundary condition, C_1 and C_{N+1} are known and to find $C_2, C_3, \cdots, C_N$, extract the system by eliminating the rows and column from the system (22) and the new will be of the form

$$\mathcal{M}_1\frac{dU_1}{dt} = -\mathcal{K}_1U_1 - U_1^T\mathcal{L}_1U_1 + \mathcal{B}_1U_1. \tag{23}$$

where $U_1 = \begin{bmatrix} C_2 \\ C_3 \\ . \\ . \\ . \\ C_N \end{bmatrix}$, $\mathcal{M}_1 = \frac{h}{6}\begin{bmatrix} 4 & 1 & 0 & \cdots & 0 \\ 1 & 4 & 1 & \cdots & 0 \\ \cdots & \cdots & \cdots & \cdots & \cdots \\ \cdots & \cdots & \cdots & \cdots & \cdots \\ 0 & 0 & 0 & \cdots & 4 \end{bmatrix}$,

$\mathcal{K}_1 = \frac{1}{h}\begin{bmatrix} 2 & -1 & 0 & \cdots & 0 \\ -1 & 2 & -1 & \cdots & 0 \\ \cdots & \cdots & \cdots & \cdots & \cdots \\ \cdots & \cdots & \cdots & \cdots & \cdots \\ 0 & 0 & \cdots & -1 & 2 \end{bmatrix}$, $U_1^T\mathcal{L}_1U_1 = \begin{bmatrix} -C_1^2 + C_1C_2 + C_2C_3 + C_3^2 \\ \cdots\cdots\cdots \\ \cdots\cdots\cdots \\ -C_{N-2}^2 + C_{N-2}C_{N-1} + C_{N-1}C_N + C_N^2 \end{bmatrix}$

and $\mathcal{B}_1 = \begin{bmatrix} 0 \\ 0 \\ \cdots \\ 0 \end{bmatrix}$. Since, the matrix $-\mathcal{M}_1$ is invertible and the matrix $-\mathcal{M}_1^{-1}\mathcal{K}_1$ generates the bounded transition matrix $\Phi(t)$, therefore, the solution of system (23) has unique and stable. Solving these $N-1$ nonlinear equations using the algorithm given by (16) and (17), the value of C is obtained at each $t > 0$ shown in the figure 1. The exact solution of the equation (18), with boundary conditions (19) and initial condition (20) is given by

$$C(x,t) = \frac{1}{2}\left[1 - tanh\left(\frac{x-2t}{4}\right)\right]. \tag{24}$$

Figure 2 shows the plot of the exact solution. The table below shows the error between the exact solution and the solution by the modified finite element scheme.

Conclusion

This work modified the traditional finite element scheme and implemented it to study the longitudinal dispersion phenomenon governed by Burgers' equation. This work also discusses the qualitative properties like the existence, uniqueness, and stability of the solution of the Burgers' equation. Comparing the modified finite element scheme (by taking two iterations) with the exact solution we found the error is of order 10^{-2} shown in the table.

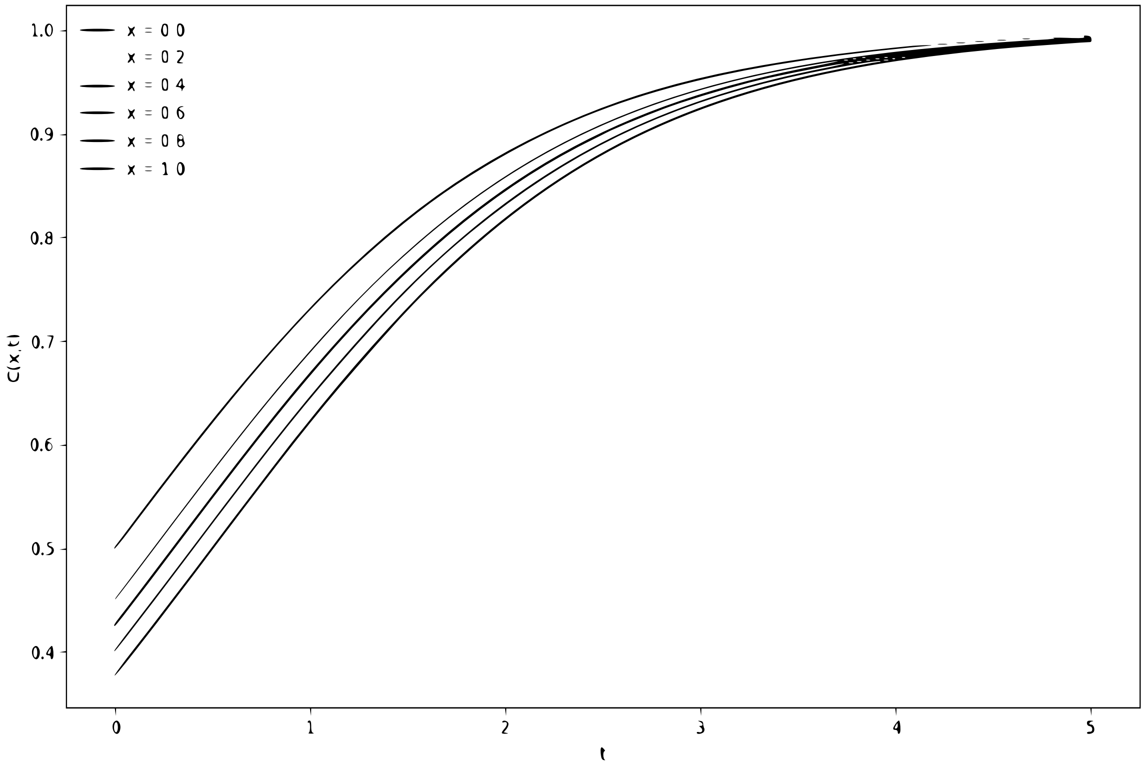

Fig. 1. Approximate concentration $C(x,t)$

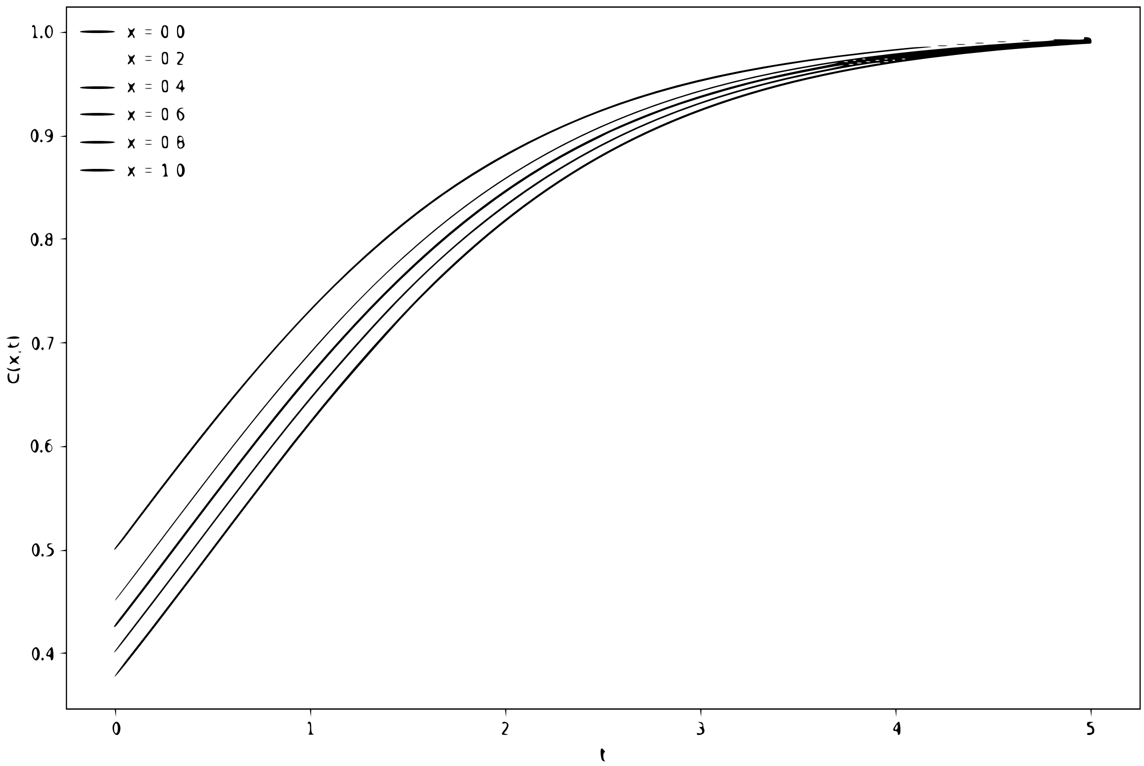

Fig. 2. Exact Concentration $C(x,t)$

Table 1

Error $E(x, t)$

t	$x = 0.0$	$x = 0.2$	$x = 0.4$	$x = 0.6$	$x = 0.8$	$x = 1.0$
0.0	0.02497918	0.0248548	0.02460851	0.02424514	0.02377167	0.02377540
0.1	0.02497918	0.02497918	0.0248548	0.02460851	0.02424514	0.02401312
0.2	0.02485481	0.02497918	0.02497918	0.0248548	0.02460851	0.02425557
0.3	0.02460851	0.02485481	0.02497918	0.02497918	0.0248548	0.02450166
0.4	0.02424514	0.02460851	0.02485481	0.02497918	0.02497918	0.02475021
0.5	0.02377167	0.02424514	0.02460851	0.02485481	0.02497918	0.025
0.6	0.02319697	0.02377167	0.02424514	0.02460851	0.02485481	0.025249791
0.7	0.02253146	0.02319697	0.02377167	0.02424514	0.02460851	0.02549833
0.8	0.02178671	0.02253146	0.02319697	0.02377167	0.02424514	0.02574442
0.9	0.02097502	0.02178670	0.02253146	0.02319697	0.02377167	0.02598687
1.0	0.02010907	0.02097502	0.02178670	0.02253146	0.02319697	0.02622459

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ЧИСЛЕННОЕ РЕШЕНИЕ ОДНОМЕРНОГО УРАВНЕНИЯ ДИСПЕРСИИ В ОДНОРОДНОЙ ПОРИСТОЙ СРЕДЕ МОДИФИЦИРОВАННЫМ МЕТОДОМ КОНЕЧНЫХ ЭЛЕМЕНТОВ

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В этой статье обсуждается математическое моделирование явления продольной дисперсии в однородной пористой среде и его решение с использованием модифицированного метода конечных элементов. Кроме того, доказаны теоремы существования и единственности, устойчивости нелинейной системы, возникающей в численной схеме, с использованием нелинейного функционального анализа и теоремы Банаха о неподвижной точке. Наконец, добавлены иллюстрации, показывающие эффективность полученного метода.

Ключевые слова: уравнение Бюргерса; пористая среда; метод конечных элементов.

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