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NUMERICAL SOLUTION OF A FRACTIONAL CONVECTION-DIFFUSION EQUATION FOR AIR POLLUTION PREDICTION

Abstract

This paper presents a numerical method for solving the convection-diffusion equation with a fractional-order Caputo derivative to model air pollution in urban environments. The developed finite element scheme accounts for memory effects, offering a more accurate representation of pollutant transport compared to classical models. Stability and convergence of the method are theoretically proven and supported by numerical experiments. The model effectively identifies pollutant accumulation zones and can forecast air quality under various weather conditions. The results have practical value for improving environmental monitoring systems and planning measures to reduce pollution levels.

Keywords: convection-diffusion equation, fractional-order derivatives, pollutant dispersion, finite element method, numerical modeling, convergence, stability.

Introduction

The quality of atmospheric air in urban environments remains one of the most pressing issues of modern times, as air pollution has a significant impact on public health and ecological balance [1–3]. Mathematical modeling of pollutant transport processes is an important tool for predicting the distribution of harmful substances and taking prompt measures to improve the environmental situation. Traditional models based on classical convection-diffusion equations are widely used to describe pollution dynamics [4, 5]. However, as research shows, such models are not always able to adequately account for nonlocal effects and long-memory processes characteristic of turbulent phenomena [6, 7].

To overcome these limitations, models incorporating fractional derivatives, particularly the Caputo derivative, have been increasingly used in recent years, as they allow for the consideration of anomalous diffusion processes and memory effects in the medium [8–10]. Several studies demonstrate

that numerical methods based on fractional calculus provide a more accurate description of pollutant transport dynamics in complex environments [11–13]. Various numerical methods are employed to solve equations with fractional derivatives [14–16]. However, as indicated by the literature review, the finite element method demonstrates high efficiency and is widely used in scientific and engineering studies [17–19].

Unlike classical models based on integer-order derivatives, the proposed method using fractional-order Caputo derivatives accounts for memory effects and anomalous diffusion, making it particularly relevant for modeling air pollution under complex and unstable flow conditions. Thus, compared to alternative approaches, the fractional-order model provides a more realistic representation of pollutant transport dynamics in the atmosphere.

This study proposes a finite element method for solving the convection-diffusion equation with fractional-order derivatives, which takes into account nonlocal memory effects of the medium. An analysis of the stability and convergence of the developed scheme has been conducted, and the results of numerical experiments confirm the expected convergence orders.

Thus, the findings of this study can be used to address the urgent challenge of developing efficient methods for modeling the dispersion of pollutants in the atmosphere, which is of great importance for environmental protection and public health.

Materials and Methods

Problem Formulation. Let us consider the following fractional differential convection-diffusion equation.

Problem 1. In the domain $\bar{\mathbb{Q}} = \bar{\Omega} \times [0, T]$, where $\Omega \subset \mathbb{R}^2$ with a boundary Γ consider the problem

$$\begin{cases} \partial_{0,t}^\alpha \phi + \vec{u} \cdot \nabla \phi - k \nabla^2 \phi = f, & x \in \Omega, \quad t > 0, \\ \phi(x, t) = 0, & x \in \Gamma, \quad t > 0, \\ \phi(x, 0) = 0, & x \in \Omega, \end{cases}$$

where \vec{u} is the wind vector, $k > 0$ is the atmospheric turbulence coefficient and the fractional-order derivative in the sense of Caputo is defined as follows:

$$\partial_{0,t}^\alpha \phi(\cdot, t) = \frac{1}{\Gamma(1-\alpha)} \int_0^t \frac{\partial_t \phi(\cdot, \theta)}{(t-\theta)^\alpha} d\theta, \quad \alpha \in (0,1).$$

Throughout the article, we will adhere to the following assumption:

(A1) Problem 1 has a unique solution with sufficient smoothness for the analysis to be carried out.

Let us define the weak formulation of Problem 1.

Problem 2. Find $\phi : (0, T] \rightarrow H_0^1(\Omega)$, such that for any $v \in H_0^1(\Omega)$:

$$(\partial_{0,t}^\alpha \phi, v) + a(\vec{u}, \phi, v) + k(\nabla \phi, \nabla v) = (f, v), \quad (1)$$

where $\alpha \in (0,1)$, and

$$a(\vec{u}, \phi, v) = \frac{1}{2} \int_\Omega [(\vec{u} \cdot \nabla \phi)v - (\vec{u} \cdot \nabla v)\phi] dx.$$

Semi-Discrete Formulation. We divide the time interval $[0, T]$ by points $t_n = n\tau$, where $\tau > 0$, and $n = 0, 1, \dots, N$, such that $N\tau = T$. Let ϕ^n denote the solution of Problem 2 at time $t = t_n$.

To define the semi-discrete formulation of Problem 1, we use the following approximation formula for the Caputo fractional derivative.

Lemma 1. The discrete analogue $\Delta_\tau^\alpha \phi^n$ of the Caputo fractional derivative $\partial_{0,t}^\alpha \phi(t_n)$ of order $0 < \alpha < 1$ can be expressed as [20]

$$\Delta_\tau^\alpha \phi^n = \sum_{s=1}^n \delta_{n,s}^{(\alpha)} (\phi^s - \phi^{s-1}), \quad (2)$$

where

$$\delta_{n,s}^{(\alpha)} = \frac{\tau^{-\alpha}}{\Gamma(2-\alpha)} [(n-s+1)^{1-\alpha} - (n-s)^{1-\alpha}].$$

For the error term $r_n^{(\alpha)} = \partial_{0,t}^\alpha \phi(t_n) - \Delta_\tau^\alpha \phi(t_n)$, the following estimate holds:

$$|r_n^{(\alpha)}| \leq \frac{5-\alpha}{8(1-\alpha)} \max_{0 \leq t \leq t_n} |\partial_t^2 \phi(t)| \tau^{2-\alpha}.$$

We now present some elementary properties of the coefficients $\delta_{n,s}^{(\alpha)}$.

Lemma 2. The coefficients $\delta_{n,s}^{(\alpha)}$, presented in Lemma 1, satisfy the following properties [18]:

- a) Positivity: $\delta_{n,s}^{(\alpha)} > 0, s = 1, 2, \dots, n$;
- b) Monotonicity: $\delta_{n,s}^{(\alpha)} < \delta_{n,s+1}^{(\alpha)}, s = 1, 2, \dots, n-1$;
- c) Recursive Relation: $\delta_{n,s}^{(\alpha)} = \delta_{n-1,s-1}^{(\alpha)}$;
- d) Summation Property: $\sum_{s=1}^n \delta_{n,s}^{(\alpha)} = \frac{n\tau_n^{-\alpha}}{\Gamma(2-\alpha)}$.

Let (\cdot, \cdot) and $\|\cdot\|$ denote the dot product and norm in $L^2(\Omega)$ for brevity. Let us define the semi-discrete formulation of Problem 1:

Problem 3. Let the solutions $\phi^k \in H_0^1(\Omega)$ be known for $k = 0, 1, \dots, n-1$. Find $\phi^n \in H_0^1(\Omega)$ such that for all $v \in H_0^1(\Omega)$:

$$(\Delta_\tau^\alpha \phi^n, v) + a(\vec{u}, \phi^n, v) + k(\nabla \phi^n, \nabla v) = (f^n, v), \quad (3)$$

where $\alpha \in (0, 1)$.

Fully Discrete Formulation. Let \mathcal{K}_h be a quasiuniform partition of $\bar{\Omega}$. Define the discrete space $V_h \subset H_0^1(\Omega)$. Introduce the projection operator $\Pi_h : H_0^1(\Omega) \rightarrow V_h$ satisfying

$$(\nabla(\Pi_h \phi - \phi), \nabla \phi_h) = 0 \quad \forall \phi \in H_0^1(\Omega), \quad \phi_h \in V_h.$$

The projection operator has the following properties:

$$\|\phi - \Pi_h \phi\| + h \|\phi - \Pi_h \phi\|_{H^1(\Omega)} \leq Ch^2 \|\phi\|_{H^2(\Omega)} \quad \forall \phi \in H_0^1(\Omega) \cap H^2(\Omega). \quad (4)$$

We now define the following problem.

Problem 4. Let the solutions $\phi_h^k \in V_h$, be known for $k = 0, 1, \dots, n-1$, in particular, $\phi_h^0 = \Pi_h \phi_0$. Find $\phi_h^n \in V_h$ satisfying the following identity for any $v_h \in V_h$:

$$(\Delta_\tau^\alpha \phi_h^n, v_h) + a(\vec{u}, \phi_h^n, v_h) + k(\nabla \phi_h^n, \nabla v_h) = (f^n, v_h), \quad (5)$$

where $\alpha \in (0, 1)$.

Results and Discussion

Stability of the Numerical Scheme. Let us proceed to investigate the stability of the method. First, we will provide an auxiliary lemma that will be necessary for the proof of the main theorem.

Lemma 3. For any function $\phi \in L^2(\Omega)$ the following inequality holds [18]:

$$(\Delta_\tau^\alpha \phi^n, \phi^n) \geq \theta_n^{(\alpha)} - \theta_{n-1}^{(\alpha)} - \frac{1}{2} \delta_{n,1}^{(\alpha)} \|\phi^0\|^2,$$

where $\theta_n^{(\alpha)} = \frac{1}{2} \sum_{s=1}^n \delta_{n,s}^{(\alpha)} \|\phi^n\|^2$.

Now, let us prove the main results of this section.

Theorem 1. The discrete scheme (5) is unconditionally stable with respect to the right-hand side, and the following estimate holds:

$$\|\phi_h^n\|^2 + \tau^\alpha \sum_{m=1}^n \|\nabla \phi_h^m\|_{L^2(\Omega)}^2 \leq C \tau^\alpha \sum_{m=1}^n \|f^m\|^2,$$

where $\alpha \in (0,1)$ and $C = \frac{1}{\sigma_L}$.

Proof. Choose $v_h = \phi_h^n$ in (5):

$$(\Delta_\tau^\alpha \phi_h^n, \phi_h^n) + a(\vec{u}, \phi_h^n, \phi_h^n) + k(\nabla \phi_h^n, \nabla \phi_h^n) = (f^n, \phi_h^n). \quad (6)$$

Estimate each term in (6). Using Lemma 3, we obtain:

$$(\Delta_\tau^\alpha \phi_h^n, \phi_h^n) \geq \frac{1}{\tau^\alpha} \left(\theta_n^{(\alpha)} - \theta_{n-1}^{(\alpha)} - \frac{1}{2} \delta_{n,1}^{(\alpha)} \|\phi^0\|^2 \right). \quad (7)$$

Further, it is obvious that $a(\vec{u}, \phi_h^n, \phi_h^n) = 0$. The right-hand side is estimated as follows:

$$(f^n, \phi_h^n) \leq \frac{C^2}{4\varepsilon} \|f^n\|^2 + \varepsilon \|\nabla \phi_h^n\|_{L^2(\Omega)}^2. \quad (8)$$

Taking into account these estimates, we obtain from (6) that

$$\theta_n^{(\alpha)} - \theta_{n-1}^{(\alpha)} + \frac{k}{2} \|\nabla \phi_h^n\|_{L^2(\Omega)}^2 \leq C \|f^n\|^2 + \frac{1}{2} \delta_{n,1}^{(\alpha)} \|\phi^0\|^2.$$

Sum the last inequality over n from 1 to n and consider that $\theta_0^{(\alpha)} = 0$ to obtain

$$\theta_n^{(\alpha)} + \frac{k\tau^\alpha}{2} \sum_{m=1}^n \|\nabla \phi_h^m\|_{L^2(\Omega)}^2 \leq C \tau^\alpha \sum_{m=1}^n \|f^m\|^2,$$

which yields the statement of the theorem.

Convergence of the Scheme. Let us proceed to investigate the convergence of the method.

Theorem 2. Let $\{\phi_h^i\}_{i=0}^N$, where $\phi_h^i \in H_0^1(\Omega)$ be the solution to Problem 4. Then, under the assumption (A1) and for $\alpha \in (0,1)$, the following inequality holds for $\phi_h^n \in H_0^1(\Omega)$:

$$\|\phi(t_n) - \phi_h^n\| + \tau^{\frac{\alpha}{2}} \sum_{m=1}^n \|\nabla(\phi(t_m) - \phi_h^m)\|_{L^2(\Omega)} \leq C \tau^{\frac{\alpha}{2}} (h^l + \tau^{2-\alpha}),$$

where C is a positive constant independent of mesh parameters.

Proof. We introduce the decomposition:

$$\phi(t_n) - \phi_h^n = (\phi(t_n) - \Pi_h \phi^n) + (\Pi_h \phi^n - \phi_h^n) = \psi^n + \xi^n. \quad (9)$$

where ϕ^n is the projection error and ξ^n is the discretization error. Consider the difference of identities (3) and (5), take into account (9) and choose $v_h = \xi^n$ to obtain

$$\begin{aligned} (\Delta_\tau^\alpha \xi^n, \xi^n) + a(\vec{u}, \phi(t_n), \xi^n) - a(\vec{u}, \phi_h^n, \xi^n) + k(\nabla \xi^n, \nabla \xi^n) = \\ = -(\Delta_\tau^\alpha \psi^n, \xi^n) + (r_n^{(\alpha)}, \xi^n). \end{aligned} \quad (10)$$

Estimate the terms in (10) as follows:

$$\begin{aligned} a(\vec{u}, \phi(t_n), \xi^n) - a(\vec{u}, \phi_h^n, \xi^n) \leq C \|\vec{u}\|_{L^2(\Omega)}^2 \|\nabla \psi^n\|_{L^2(\Omega)}^2 + \\ + (\varepsilon_1 + \varepsilon_2) \|\nabla \xi^n\|_{L^2(\Omega)}^2 + C \|\vec{u}\|_{L^2(\Omega)}^2 \|\psi^n\|^2, \end{aligned}$$

$$|(\Delta_\tau^\alpha \psi^n, \xi^n)| \leq C \max_{1 \leq s \leq n} \|\partial_t \psi\|_{L^\infty(t_{s-1}, t_s; L^2(\Omega))}^2 + \varepsilon_4 \|\nabla \xi^n\|_{L^2(\Omega)}^2.$$

Then it follows from (10) that

$$\begin{aligned} \theta_n^{(\alpha)} - \theta_0^{(\alpha)} + \frac{k}{5} \sum_{m=1}^n \|\nabla \xi^m\|_{L^2(\Omega)}^2 \leq \\ \leq C \sum_{m=1}^n \|\vec{u}\|_{L^2(\Omega)}^2 \|\nabla \psi^m\|_{L^2(\Omega)}^2 + C \sum_{m=1}^n \|\vec{u}\|_{L^2(\Omega)}^2 \|\psi^m\|^2 + \\ + C \sum_{m=1}^n \|r^m\|^2 + C \sum_{m=1}^n h^{2l+2}, \end{aligned}$$

which yields the assertion of the theorem.

Computational Experiments. In this section, we present numerical experiments to verify the theoretical estimate. To validate the theoretical convergence estimate established in Theorem 2, a series of computational experiments were conducted using a model problem.

Example 1. Consider the equation:

$$\partial_{0,t}^\alpha \phi + u_1 \frac{\partial \phi}{\partial x} + u_2 \frac{\partial \phi}{\partial y} - k \left(\frac{\partial^2 \phi}{\partial x^2} + \frac{\partial^2 \phi}{\partial y^2} \right) = f, \quad t > 0, \quad (11)$$

where

$$f(x, y, t) = \frac{2t^{2-\alpha}(x-x^2)(y-y^2)}{\Gamma(1-\alpha)(1-\alpha)(2-\alpha)} - t^2((1+2x)(y^2-y) + (1+2y)(x^2-x))$$

with initial and boundary conditions:

$$\phi(x, y, t) = 0, \quad (x, y) \in \Gamma, \quad t > 0 \quad (12)$$

$$\phi(x, y, t) = 0, \quad (x, y) \in \Omega, \quad (13)$$

where $\alpha \in (0, 1)$. The exact solution is $p(x, t) = xy(1-x)(1-y)t^2$.

The goal of this computational experiment is to determine the actual order of convergence with respect to the fractional derivative order α . Several combinations of fractional derivative orders from the set $\{0.1, 0.5, 0.9\}$ were considered in the experiment.

To analyze the dependence of the error order on the spatial step, the time step was fixed as $\tau = h$, while the spatial step h varied from $h = \frac{1}{10}$ to $h = \frac{1}{160}$, decreasing by a factor of two at each stage.

The errors were evaluated using the L_2 -norm for the solution ϕ . Table 1 presents the error values for different fractional derivative orders α and corresponding parameters h and τ . Figure 1 shows the convergence plot of the finite element method in a log-log scale. The results exhibit a straight line, indicating a clear algebraic convergence. The slope of the line corresponds to an empirical convergence rate, consistent with the theoretical prediction for the method and problem considered.

Table 1 – L_2 -errors and convergence orders for Example 1 for cases $\alpha = 0.1, \alpha = 0.5$ and $\alpha = 0.9$

$\tau = h$	$\alpha = 0.1$		$\alpha = 0.5$		$\alpha = 0.9$	
	L^2 -error	Order	L^2 -error	Order	L^2 -error	Order
$\frac{1}{10}$	$1.0297 \cdot 10^{-2}$	-	$8.2755 \cdot 10^{-3}$	-	$7.2457 \cdot 10^{-3}$	-
$\frac{1}{20}$	$5.1843 \cdot 10^{-3}$	$0.99 (\approx 1.05)$	$3.6021 \cdot 10^{-3}$	$1.20 (\approx 1.25)$	$2.7266 \cdot 10^{-3}$	$1.41 (\approx 1.45)$
$\frac{1}{40}$	$2.5922 \cdot 10^{-3}$	$1.00 (\approx 1.05)$	$1.5571 \cdot 10^{-3}$	$1.21 (\approx 1.25)$	$1.0190 \cdot 10^{-3}$	$1.42 (\approx 1.45)$
$\frac{1}{80}$	$1.2694 \cdot 10^{-3}$	$1.03 (\approx 1.05)$	$6.5923 \cdot 10^{-4}$	$1.24 (\approx 1.25)$	$3.7817 \cdot 10^{-4}$	$1.43 (\approx 1.45)$
$\frac{1}{160}$	$6.1308 \cdot 10^{-4}$	$1.05 (\approx 1.05)$	$2.7717 \cdot 10^{-4}$	$1.25 (\approx 1.25)$	$1.3842 \cdot 10^{-4}$	$1.45 (\approx 1.45)$

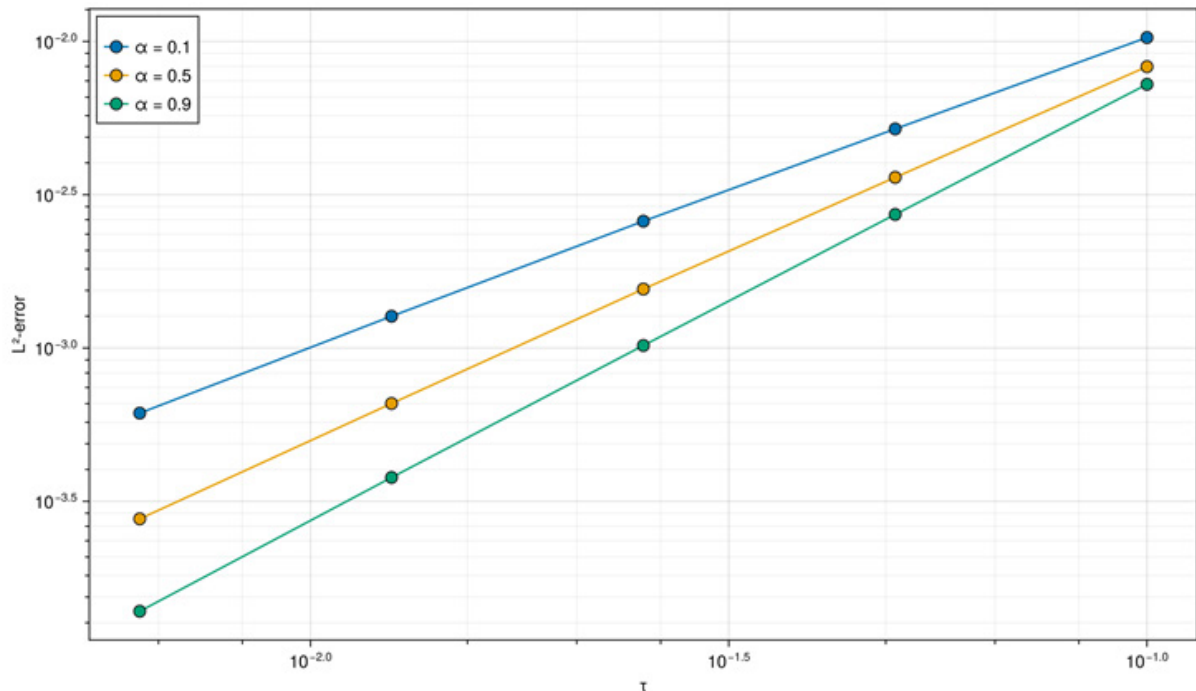
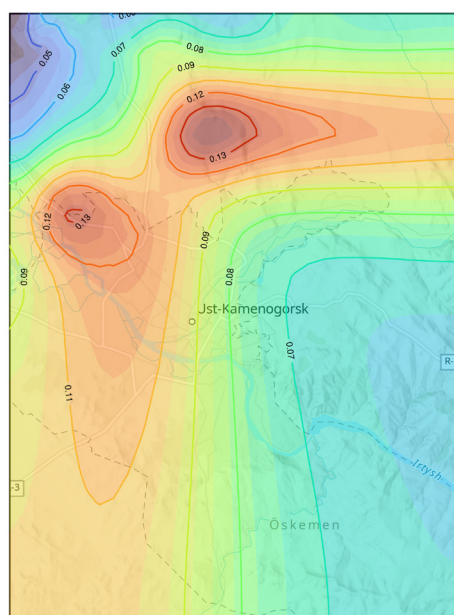


Figure 1 – Convergence plots for Example 1 for cases $\alpha = 0.1, \alpha = 0.5$ and $\alpha = 0.9$

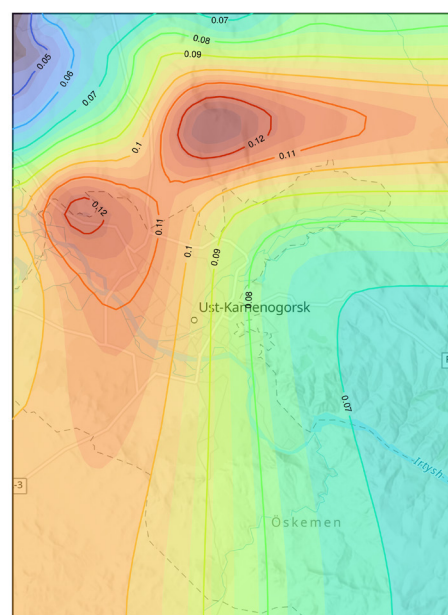
As seen from Table 1, the convergence order strongly depends on the value of α . Higher values of $\alpha = 0.9$ yield the best accuracy and convergence order. Lower values of $\alpha = 0.1$ result in a reduced

convergence order, confirming the sensitivity of the method to the fractional derivative order. Overall, the experiment confirms the theoretical conclusions regarding the convergence of the method and its dependence on α . The computational experiments verified the theoretical convergence estimates established in Theorem 2. The results demonstrate that the method exhibits the expected convergence rate for higher values of α and a decrease in accuracy for lower fractional derivative orders.

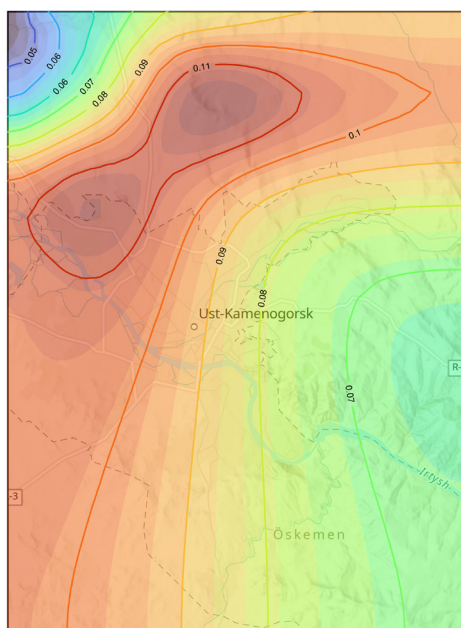
Example 2. Let us consider a more realistic example. In this numerical test, the goal is to predict the dynamics of the SO_2 in the atmosphere based on the proposed fractional differential model on the example of the city of Ust-Kamenogorsk during one day, January 1, 2024.



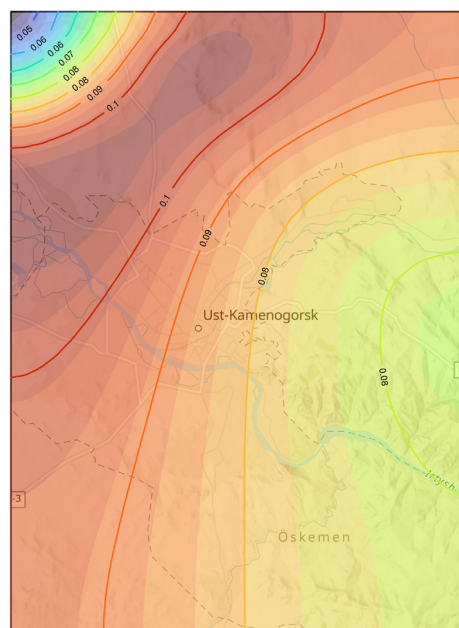
a) Concentration field after 1 hour



b) Concentration field after 2 hours



c) Concentration field after 3 hours



d) Concentration field after 4 hours

Figure 2 – Simulation results of SO_2 distribution for $\alpha = 0.9$

Unlike Problem 1, the boundary conditions of the first kind are replaced by boundary conditions of the second kind, and the right-hand side is selected as the sum of two sources. Computational experiments were carried out for orders of fractional derivatives $\alpha \in \{0.5, 0.6, \dots, 0.9\}$. The modeling results for the case of $\alpha = 0.9$ are shown in Figure 2.

The results show that SO_2 spreads more slowly compared to classical diffusion which is suitable for modeling pollution in urban areas with obstacles and complex wind patterns. Therefore the order α controls the degree of temporal memory: smaller values of α correspond to stronger memory effects and subdiffusive behavior, leading to slower pollutant spread and prolonged atmospheric retention. This is consistent with observed pollutant dynamics in complex urban environments.

Moreover, the proposed scheme has proven itself to be stable for a wide range of time steps.

Conclusion

This study proposed a numerical solution of the convection-diffusion equation with fractional-order derivatives for assessing air quality in urban environments. The developed model takes into account the influence of linear sources of pollutants, transport processes, turbulent mixing, and the memory effect modeled using the Caputo fractional derivative. This approach enabled a more accurate description of the dynamics of pollutant dispersion in complex urban conditions.

The theoretical analysis of the stability and convergence of the proposed finite element scheme confirmed its efficiency and reliability. Numerical experiments demonstrated a high degree of agreement with theoretical results, validating the correctness of the chosen approach.

The developed model proved its applicability for forecasting atmospheric pollution under various weather and infrastructural conditions. It effectively identifies pollutant accumulation zones and helps in planning measures to reduce pollution levels. This makes the model a valuable tool for environmental monitoring and for developing strategies to improve air quality in urban areas.

The obtained results can be used in future research for more complex modeling scenarios, including the consideration of nonlinear pollutant sources, as well as integration with real-time monitoring systems for air quality assessment. Further development of the model will enhance its accuracy and broaden its application in environmental and engineering tasks.

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АУАНЫҢ ЛАСТАНУЫН БОЛЖАУ ҮШІН БӨЛШЕКТІ РЕТТІ КОНВЕКЦИЯ-ДИФфуЗИЯ ТЕҢДЕУІНІҢ САНДЫҚ ШЕШІМІ

Аңдатпа

Бұл мақалада қалалық ортадағы ауаның ластануын модельдеу үшін Капуто мағынасындағы бөлшекті ретті туындылары бар конвекция-диффузия теңдеуін шешудің сандық әдісі ұсынылады. Есептелген ақырлы элементтер сұлбасы жады әсерін ескере отырып, лаптаушы заттардың таралуын дәлірек сипаттауға мүмкіндік

береді. Әдістің орнықтылығы мен жинақтылығы теориялық тұрғыда дәлелденіп, сандық тәжірибелер арқылы расталды. Ұсынылған модель түрлі метеорологиялық жағдайларда ауа сапасын болжауға мүмкіндік береді. Зерттеу нәтижелері экологиялық мониторинг жүйелерін жетілдіруге және ауаның ластануын төмендетуге бағытталған шараларды жоспарлауға практикалық үлес қоса алады.

Тірек сөздер: конвекция-диффузия теңдеуі, бөлшекті ретті туындылар, ластаушы заттардың таралуы, ақырлы элементтер әдісі, сандық модельдеу, жинақтылық, орнықтылық

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ЧИСЛЕННОЕ РЕШЕНИЕ УРАВНЕНИЯ КОНВЕКЦИИ-ДИФФУЗИИ ДРОБНОГО ПОРЯДКА ДЛЯ ПРОГНОЗА ЗАГРЯЗНЕНИЯ ВОЗДУХА

Аннотация

В работе представлен численный метод решения уравнения конвекции-диффузии с производными дробного порядка в смысле Капуто для моделирования загрязнения воздуха в городской среде. Разработанная конечно-элементная схема учитывает эффекты памяти, обеспечивая более точное описание переноса загрязняющих веществ по сравнению с классическими моделями. Теоретически доказаны устойчивость и сходимость метода, что подтверждено численными экспериментами. Модель эффективно определяет зоны накопления загрязнений и позволяет прогнозировать качество воздуха при различных метеоусловиях. Результаты исследования имеют практическое значение для совершенствования систем экологического мониторинга и планирования мер по снижению загрязненности воздуха.

Ключевые слова: уравнение конвекции-диффузии, производные дробного порядка, распространение загрязняющих веществ, метод конечных элементов, численное моделирование, сходимость, устойчивость.

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