VOL. 4, №1
Journal of Osh State University.
Mathematics. Physics. Technical Sciences
2025

Journal of Osh State University
Journal homepage: https://mpht-oshsu.com/en

**UDC** 517.95
**DOI:** 10.52754/16948645_2025_4(1)_50

**Article's History:**
Received 13.11.2024 Revised 12.02.2025 Accepted 07.03.2025

# A nonlinear free-boundary model with variable diffusion and advection coefficients for pollutant-population dynamics in rivers

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**Abstract.** In natural aquatic environments, both the diffusion coefficient-characterising the rate of pollutant dispersion-and the advection coefficient-describing transport due to water flow-exhibit significant spatio-temporal variability. These variations stem from changes in river geometry, flow velocity, temperature, and seasonal dynamics. To better capture these complexities, this study presents an enhanced modelling framework that incorporates spatio-temporally variable diffusion and advection coefficients. These coefficients are further assumed to depend on both the population density and the concentration of environmental toxicants, enabling a more realistic representation of contaminant transport processes. This study developed a system of nonlinear partial differential equations (PDEs) with a free boundary to represent the dynamic aspect of toxic substance dispersion. The model characterises the interaction between a riverine biological population and a toxicant, accounting for ecological and hydrodynamic influences. To ensure the regularity of the solution, a priori calculations were established, including the population density $u(x, t)$, the toxicant concentration $v(x, t)$, the free boundary position $s(t)$, and the Hölder continuity estimates. The global existence and uniqueness of classical solutions are rigorously proven via the Leray-Schauder fixed-point theorem and energy-based methods. Parameter regimes were identified where the toxicant could not spread throughout the entire river area, thereby allowing the population to survive in unaffected areas. Due to the analytical difficulty of the nonlinear free boundary problem, implicit numerical schemes were used for the simulation. Numerical experiments, implemented in Python with graphical visualisations, validate the theoretical results and illustrate the interplay between ecological parameters and pollutant dynamics. The results obtained show how different environmental conditions affect the stability of biological populations and the spatiotemporal evolution of toxic substance concentrations

**Keywords:** nonlinear dynamics; pollutant spread; free-boundary problem; numerical simulations; diffusion coefficient

## Introduction

The purpose of this study stems from the increasing importance of developing accurate mathematical models to describe the transport and transformation of pollutants in flowing water systems, where conventional models with constant parameters prove insufficient due to the spatial and temporal variability of advection and diffusion processes observed in real hydrosystems. Incorporating variable coefficients, nonlinear reactions, and free boundary conditions allows for a more realistic simulation of pollutant dynamics and their influence

**Suggested Citation:**
Boborakhimova M, Pardaeva O. A nonlinear free-boundary model with variable diffusion and advection coefficients for pollutant-population dynamics in rivers. J Osh State Univ Math Phys Tech Sci. 2025;4(1):50–60. DOI: 10.52754/16948645_2025_4(1)_50

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on population behaviour. Such models are crucial for understanding complex flow-dependent ecological phenomena, including imbalance, population loss, adaptation, and uncertain scenarios like the "drift paradox" – the persistence of populations under continuous flow. This approach not only provides a deeper mathematical understanding of these processes but also contributes to building a solid theoretical foundation for solving applied problems in ecological and technical systems.

Researcher Ch. Cosner [1] investigated population dynamics governed by advection-diffusion equations with nonlinear reaction terms in heterogeneous media. The author underscored the challenges of determining survival thresholds in flow systems with spatially varying diffusion coefficients. However, this model did not incorporate a free boundary, thereby limiting its capacity to describe the spatial expansion of populations – a gap that the present study aims to address. W. Peng *et al*. [2] proposed a reaction-diffusion-advection model with spatially variable parameters to explore population persistence in river-like environments. Although their model effectively captured spatial heterogeneity, it was constrained to a fixed spatial domain and did not account for the dynamic expansion of habitat boundaries.

In a similar vein, K.-Y. Lam & Y. Lou [3] examined the effects of temporal heterogeneity within periodic reaction-diffusion-advection systems. Their study focused on spreading speeds and pattern formation, yet it did not consider toxicant influences or incorporate environmentally driven free boundary dynamics. C. Fabre *et al*. [4] studied pollution patterns in Arctic rivers considering changes in water temperature and ice cover. Although the geographical context was different, their analytical approach to modelling with variable coefficients is similar to that used in the present study. Their findings confirmed the importance of considering seasonal factors, as in the current case, where temperature and flow were involved in determining the diffusion and advection coefficients.

D. Tang & P. Zhou [5] demonstrated that the interaction between movement and environmental heterogeneity can lead to complex and interesting phenomena in population dynamics. K. Liu *et al*. [6] investigated a two-species Lotka-Volterra competition patch model along a stream with richer resources downstream. One species is treated as resident, the other as a mutant. It identifies conditions under which a mutant species can successfully invade depending on its dispersal rate compared to the resident. The study found a unique evolutionarily stable dispersal strategy for the resident species under certain conditions. It also explored the global dynamics of the system, showing that both competitive exclusion and coexistence are possible. The method used was also applicable to reaction-diffusion models, improving on some existing results.

J.O. Takhirov & M.I. Boborakhimova [7] developed a free-boundary model based on the reaction-diffusion-advection equations to study the interaction between river populations and toxicants. Their model assumed constant diffusion ($d_1$, $d_2$) and advection ($k_1$, $k_2$) coefficients, which provided a basis for analysing population stability and the spread of toxicants. However, in natural river systems, these coefficients rarely take on a constant value. Biological and ecological factors such as population density, toxicant concentration, and habitat diversity affect the movement of organisms and the spread of pollutants. For example, high population density can reduce individual dispersal due to competition or territorial behaviour, leading to density-dependent diffusion ($d_1(u)$). Similarly, toxicant concentrations can modify flow-driven transport, resulting in concentration-dependent advection $k_2(v)$. These nonlinear relationships reflect complex ecological realities, such as behavioural adaptations to stress or changes in water chemistry that affect pollutant mobility.

The proposed model is based on existing frameworks, such as the constant coefficient model and chemotaxis models studied by D. Horstmann & M. Winkler [8]. Unlike chemotaxis models, which focus on cell movement toward chemical gradients, the developed model addresses population-toxicant interactions in a flowing river, incorporating advection to account for downstream drift. The inclusion of variable coefficients distinguishes this study from J.O. Takhirov & M.I. Boborakhimova's original model, allowing for a more nuanced representation of ecological processes. For example, while constant diffusion assumes uniform dispersal, this variable diffusion $d_1(u)$ accounts for density-dependent behaviours observed in fish or invertebrate populations.

This study extends the model J.O. Takhirov & M.I. Boborakhimova [7] by introducing variable coefficients $d_1(u)$, $d_2(v)$, $k_1(u)$, and $k_2(v)$, making the system more nonlinear and more consistent with biological realities. Therefore, the present study aimed to fill this gap by developing a nonlinear free boundary model with variable diffusion and advection coefficients to investigate the coupled dynamics of population and pollutants in riverine systems. This approach not only reflects the complex interplay between ecological and environmental processes but also enhances the predictive power of mathematical models in real-world ecological scenarios.

## Materials and Methods

This study was devoted to the construction and investigation of a mathematical model describing the dynamics of interaction between a population and a pollutant in a flowing medium. The model accounted for nonlinear effects, variable diffusion and advection coefficients, and a free boundary representing the population's habitat. The paper included the formulation of the problem, theoretical analysis of the model, implementation of a numerical method, and discussion of the obtained results. Particular attention was paid to the influence of spatiotemporal parameters on the stability and spatial distribution of the population in a polluted environment.

**Mathematical Model.** A nonlinear free-boundary model describing the interaction between a population with density $u(x, t)$ and a toxicant with concentration $v(x, t)$ in a river of length $L$ was considered. The free boundary $x = s(t)$ represented the front of toxicant spread. The governing equations:

$$a(u)u_t = d_1(u)u_{xx} - k_1(u)u_x + u[a_1 - b_1 u - c_1 v],\ 0 < x < L,\ t > 0, \quad (1)$$

$$b(v)v_t = d_2(v)v_{xx} - k_2(v)v_x + [m(x) - b_{2uv} - c_2 v],\ 0 < x < s(t) < L,\ t > 0, \quad (2)$$

with boundary conditions:

$$d_1(u(0, t))u_x(0, t) - k_1(u(0, t))u(0, t) = u_x(L, t) = 0,\ t > 0, \quad (3)$$

$$d_2(v(0, t))v_x(0, t) - k_2(v(0,t))v(0,t) = v(s(t),t) = 0,\ t > 0, \quad (4)$$

initial conditions:

$$u(x, 0) = u_0(x) > 0,\ 0 < x < L,$$
$$v(x, 0) = v_0(x) > 0,\ 0 < x < s_0 = s(0), \quad (5)$$

and the free-boundary condition:

$$s'(t) = -\mu v_x(s(t), t)e^{-\int_0^{s(t)} \frac{k_2(v(\xi,t))}{d_2(v(\xi,t))}d\xi},\quad t > 0. \quad (6)$$

Here, $a(u) > a_0 > 0$, $b(v) > b_0 > 0$ – biocapacity coefficients, $d_1(u)$, $d_2(v) \geq d_0 > 0$ – diffusion coefficients, and $k_1(u)$, $k_2(v)$ – advection coefficients, all assumed to be Hölder continuous ($C^\alpha$, $\alpha \in (0, 1)$). The function $m(x)$ represented the exogenous toxicant input, satisfying:

$$m(x) = \begin{cases} 0, & s_0 \leq x \leq L, \\ m_1, & 0 \leq x \leq s_0, \end{cases} \quad (7)$$

where $m_1 > 0$. The parameters $a_1$, $b_1$, $c_1$, $b_2$, $c_2$, $\mu$ were positive constants.

**A Prior Estimates.** To establish the solvability of the problem, a priori estimates were derived for $u$, $v$, and $s(t)$.

**Bounds on $u$, $v$, and $s(t)$.**

**Lemma 1.** Let $(u, v, s(t))$ be a solution of the system for $t \in [0, T]$, $T > 0$. Then:

$$0 < u(x,t) \leq M_1 = \max\left\{\frac{a_1}{b_1}, \max_x |u_0(x)|\right\}, x \in [0, L], t > 0, \quad (8)$$

$$0 < v(x,t) \leq M_2 = \max\left\{\frac{\max_x |m(x)|}{c_2}, \max_x |v_0(x)|\right\},$$
$$x \in [0, s(t)], t > 0, \quad (9)$$

$$0 < s(t) \leq M_3,\ t > 0, \quad (10)$$

where $M_3$ depends on the model parameters and initial data.

**Proof**. Using the maximum principle, equation (8) was analysed. At a maximum point ($u_t = 0$, $u_{xx} \leq 0$, $u_x = 0$):

$$u[a_1 - b_1 u - c_1 v] \leq 0, \quad u \leq \frac{a_1}{b_1}.$$

Considering the initial condition $u_0(x)$, $u \leq M_1$ was obtained. Positivity follows from $u_0(x) > 0$. For $v$, from equation (9), at a maximum point:

$$m(x) - c_2 v \leq 0, \quad v \leq \frac{\max_x |m(x)|}{c_2}. \quad (11)$$

With $v_0(x)$, get $v \leq M_2$. For $s(t)$, the transformation was considered:

$$w(x,t) = v(x,t)e^{\int_0^x \frac{k_2(v(\xi,t))}{d_2(v(\xi,t))}d\xi}. \quad (12)$$

The free-boundary condition (12) became:

$$s'(t) = -\mu w_x(s(t), t). \quad (13)$$

Since $v_x(s(t), t) < 0$ (by the Hopf lemma), and assuming $|k_2(v)/d_2(v)| \leq C$:

$$s'(t) \leq \mu |v_x| e^{Cs(t)}. \quad (14)$$

Using bounds on $|v_x|$ (see Theorem 1), taken $s(t) \leq M_3$.

**Hölder Norm Estimates.**

**Theorem 1.** Assuming the conditions of Lemma 1 hold, and let $v(x, t)$ be continuous in $\bar{D}$ with square-integrable derivatives $v_t$, $v_{xx}$. Then:

$$|v_x(x, t)| \leq M_4(M_2, b_0, d_0, v_0),\ (x, t) \in D, \quad (15)$$

$$|v(x, t)|^D_{1+\alpha} \leq M_5(M_4),\ |v(x, t)|^D_{2+\alpha} \leq M_6(M_5). \quad (16)$$

Similarly, for $u(x, t)$ in $Q$:

$$|u_x(x, t)| \leq M_7(M_1, a_0, d_0, u_0),\ |u(x, t)|^Q_{1+\alpha} \leq M_8(M_7),$$
$$|u(x, t)|^Q_{2+\alpha} \leq M_9(M_8). \quad (17)$$

**Proof.** For $v$, the domain $D$ to $\Omega = \{(y, \tau): 0 < y < 1, 0 < \tau\}$ was transformed using $y = x/s(t)$, $\tau = t$. The equation for $w(y, \tau) = v(x, t)$ became:

$$b(w)\left(w_\tau - \frac{s'(\tau)y}{s(\tau)}w_y\right) = \frac{d_2(w)}{s^2(\tau)}w_{yy} - \frac{k_2(w)}{s(\tau)}w_y +$$
$$+[m(s(\tau)y) - b_2 uw - c_2 w].$$

Assuming $d_2(w) \geq d_0 > 0$, $b(w) \geq b_0 > 0$, and Hölder continuity of coefficients, results from O.A. Ladyzhenskaya *et al.* [9] and A. Friedman [10] were applied to obtain:

$$|wy| \leq M'_4,\ |w|^\Omega_{1+\alpha} \leq M'_5,\ |w|^\Omega_{2+\alpha} \leq M'_6.$$

Transforming back, the stated bounds for $v$ were obtained. For $u$, the equation in $Q$ was treated similarly without domain transformation, yielding the bounds for $u_x$ and Hölder norms.

**Existence and Uniqueness of the Solution.**

**Theorem 2.** Suppose the conditions of Theorem 1 and Lemma 1 hold, and $d_1(u)$, $d_2(v)$, $k_1(u)$, $k_2(v)$, $a(u)$, $b(v) \in C^\alpha$. Then there exists a unique solution $u(x, t)$, $v(x, t) \in C_{2+\alpha}$, $s(t) \in C_{1+\alpha}$ *for* $t \in [0, T]$.

**Existence.**

**Proof.** The Leray-Schauder principle was aplied. The Banach space $H_{1+\alpha}$ was defined with norm $|u|_{1+\alpha} + |v|_{1+\alpha}$. For each $(\bar{u}, \bar{v}) \in H_{1+\alpha}$ and $k \in [0, 1]$, consider the linear problems:

$$(u_k)_t = \tilde{a}(\bar{u})(u_k)_{xx} + kf_1(\bar{u}, \bar{v}, (u_k)_x),\ (x, t) \in Q,$$

$$(v_k)_t = \tilde{b}(\bar{v})(v_k)_{xx} + kf_2(\bar{u}, \bar{v}, (v_k)_x),\ (x, t) \in D,$$

with the original boundary and initial conditions. The operator $F(\bar{u}, \bar{v}, k) = (u_k, v_k)$ is continuous, compact, and has a trivial solution for $k = 0$. By the Leray-Schauder principle, a fixed point exists for $k = 1$ apply results from O.A. Ladyzhenskaya *et al.* [9] and A. Friedman [10]

**Uniqueness.**

**Proof.** Assume two solutions $(u_1, v_1, s_1(t))$ and $(u_2, v_2, s_2(t))$. Define $w = u_1 - u_2$, $z = v_1 - v_2$, $r(t) = s_1(t) - s_2(t)$. The difference equations yield:

$$a(u_1)w_t = d_1(u_1)w_{xx} - k_1(u_1)w_x + \\ + w[a_1 - b_1u_1 - c_1 v_1] + (\text{differenceterms}),$$

$$b(v_1)z_t = d_2(v_1)z_{xx} - k_2(v_1)z_x + \\ + [-b_2u_1z - b_2v_2w - c_2 z] + (\text{differenceterms}).$$

Using $L^2$ energy estimates and Gronwalls inequality, obtain $w = 0$, $z = 0$, and $r(t) = 0$, implying uniqueness.

**Asymptotic Behaviour.** Analyse the asymptotic behaviour of $u(x, t)$, $v(x, t)$, and $s(t)$ as $t \to \infty$ to understand long-term dynamics.

**Asymptotic Bounds on $u(x, t)$ and $v(x, t)$.**

**Theorem 3.** Let $(u, v, s(t))$ be the unique global solution. Then, as $t \to \infty$:

$$0 \le u(x,t) \le M_1 = \max\left\{\frac{a_1}{b_1}, \max_x|u_0(x)|\right\}, \quad x \in [0, L],$$

$$0 \le v(x, t) \le M_2 = \max\left\{\frac{\max_x|m(x)|}{c_2}, \max_x|v_0(x)|\right\}, x \in [0, s(t)].$$

**Proof.** From Lemma 1, $u \le M_1$, $v \le M_2$. For steady-state $u_\infty(x)$, at a maximum point:

$$u_\infty[a_1 - b_1u_\infty - c_1v] \le 0, \quad u_\infty \le \frac{a_1}{b_1}.$$

Similarly, for $v_\infty(x)$:

$$m(x) - b_2uv_\infty - c_2v_\infty \le 0, \quad v_\infty \le \frac{\max_x|m(x)|}{c_2}.$$

**Asymptotic Behaviour of the Free Boundary $s(t)$.**

**Theorem 4.** If $|k_2(v)/d_2(v)| \le C$ and $c_2$ is large relative to $m_1$, then $\lim_{t\to\infty} s(t) = s_\infty < L$. If $m_1 \gg c_2$, then $s(t) \to L$.

**Proof.** From (2.6), $s'(t) \ge 0$. Using

$$w(x,t) = v(x,t)e^{\int_0^x \frac{k_2(v(\xi,t))}{d_2(v(\xi,t))}d\xi}, \text{ taken:}$$

$$s'(t) = -\mu w_x(s(t), t).$$

For large $c_2$, the steady-state equation for $v_\infty$ implies rapid decay near $s_\infty$, so $v_{\infty,x}(s_\infty)$ is finite, and $s(t) \to s_\infty < L$. If $m_1 \gg c_2$, $v(x, t)$ persists, driving $s(t) \to L$.

**Biological Interpretation.** The boundedness of $u(x, t)$ suggests population persistence if $a_1 > c_1v$. Stabilisation of $s(t)$ at $s_\infty < L$ preserves uncontaminated habitats, while $s(t) \to L$ threatens the ecosystem. The condition $a_1 > (\frac{c_1m_1}{c_2})$ ensures persistence.

**Numerical Simulations and Visualisations.**

**Numerical Scheme.** The spatial domain $[0, L]$ is discretised with grid size $\Delta x = L/N$, and time with step $\Delta t$. The implicit scheme for $u(x, t)$ by V.I. Naac & I.E. Naac [11]:

$$a(u_i^n)\frac{u_i^{n+1} - u_i^n}{\Delta t} = d_1(u_i^n)\frac{u_{i+1}^{n+1} - 2u_i^{n+1} + u_{i-1}^{n+1}}{\Delta x^2} - \\ -k_1(u_i^n)\frac{u_{i+1}^{n+1} - u_{i-1}^{n+1}}{2\Delta x} + u_i^{n+1}[a_1 - b_1u_i^{n+1} - c_1v_i^{n+1}].$$

Similarly for $v(x, t)$. The free boundary is updated as A. Müller *et al.* [12]:

$$s(t + \Delta t) = s(t) - \mu v_x(s(t), t)e^{-\int_0^{s(t)} \frac{k_2(v(\xi,t))}{d_2(v(\xi,t))}d\xi}\Delta t.$$

Numerical simulations were conducted using a finite difference method implemented in Python with NumPy and Matplotlib to validate the theoretical predictions and visualise the dynamics of $u(x, t)$, $v(x, t)$ and $s(t)$. The spatial domain $[0, L]$ is discretised with grid size $\Delta x = L/N$, and time with step $\Delta t$. The simulation parameters are: $L = 1$, $a_1 = 1$, $b_1 = 1$, $c_1 = 0.5$, $b_2 = 0.5$, $c_2 = 1$, $m_1 = 0.5$ (Scenario 1) or $m_1 = 2$ (Scenario 2), $\mu = 0.1$, $\Delta x = 0.01$, $\Delta t = 0.001$, $N = 100$. Initial conditions are $u_0(x) = 0.5e^{-x^2}$, $v_0(x) = 0.3e^{-(x-0.2)^2}$, $s_0 = 0.3$, with coefficients $d_1(u) = 0.01 + 0.005u$, $k_1(u) = 0.02u$, $d_2(v) = 0.01 + 0.003v$, $k_2(v) = 0.01v$, $a(u) = 1 + 0.1u$, $b(v) = 1 + 0.1v$. Two scenarios were simulated, and their results are visualised in Figures 1 and 2.

## Results and Discussion

The numerical results for both scenarios are presented in Figures 1 and 2, each comprising three panels: (a) population density $u(x, t)$, (b) toxicant concentration $v(x, t)$, and (c) free boundary $s(t)$, evaluated at $t = 0, 1, 5$.

**Scenario 1: Moderate Toxicant Decay ($c_2 = 1$).**

Population Density $u(x, t)$ (Panel a). The population density starts from the initial Gaussian profile $u_0(x) = 0.5e^{-x^2}$ and evolves toward a stable state. By $t = 5$, $u(x, t)$ stabilises at approximately 0.8, particularly in the uncontaminated region $x > s_\infty \approx 0.45$. This aligns with Lemma 1, which predicts $u(x, t) \le M_1 = max\{\frac{b_1}{a_1}, max_x|u_0(x)|\} = max\{1, 0.5\} = 1$. The stability of $u(x, t)$ in the region $x > s_\infty$ indicates that the population persists in areas free from toxicant influence, consistent with the condition $a_1 > \frac{c_1 m_1}{c_2} = \frac{0.5 \cdot 0.5}{1} = 0.25$.

Toxicant Concentration $v(x, t)$ (Panel b). The toxicant concentration begins from $v_0(x) = 0.3e^{-(x-0.2)^2}$ and spreads within the region $0 < x < s(t)$, satisfying the boundary condition $v(s(t), t) = 0$. By $t = 5$, $v(x, t)$ remains bounded, with a maximum value near $x \approx 0.2$, and is confined to $x < s_\infty$. This is consistent with Lemma 1, which bounds $v(x,t) \le M_2 = \max\left\{\frac{\max_x|m(x)|}{c_2}, \max_x|v_0(x)|\right\} = \max\left\{\frac{0.5}{1}, 0.3\right\} = 0.5$. Free Boundary $s(t)$ (Panel c): The free boundary starts at $s_0 = 0.3$ and increases over time, stabilising at $s_\infty \approx 0.45$ by $t = 5$. This behaviour validates Theorem 5, which states that for a sufficiently large $c_2$ relative to $m_1$ (here, $c_2/m_1 = 2$), the free boundary converges to $s_\infty < L = 1$. The stabilisation of $s(t)$ indicates that the toxicant's spread is limited, preserving uncontaminated habitats downstream. In Scenario 1, the toxicant decay rate is set to $c_2 = 1$, with an external toxicant input of $m_1 = 0.5$. The results are shown in Figure 1.

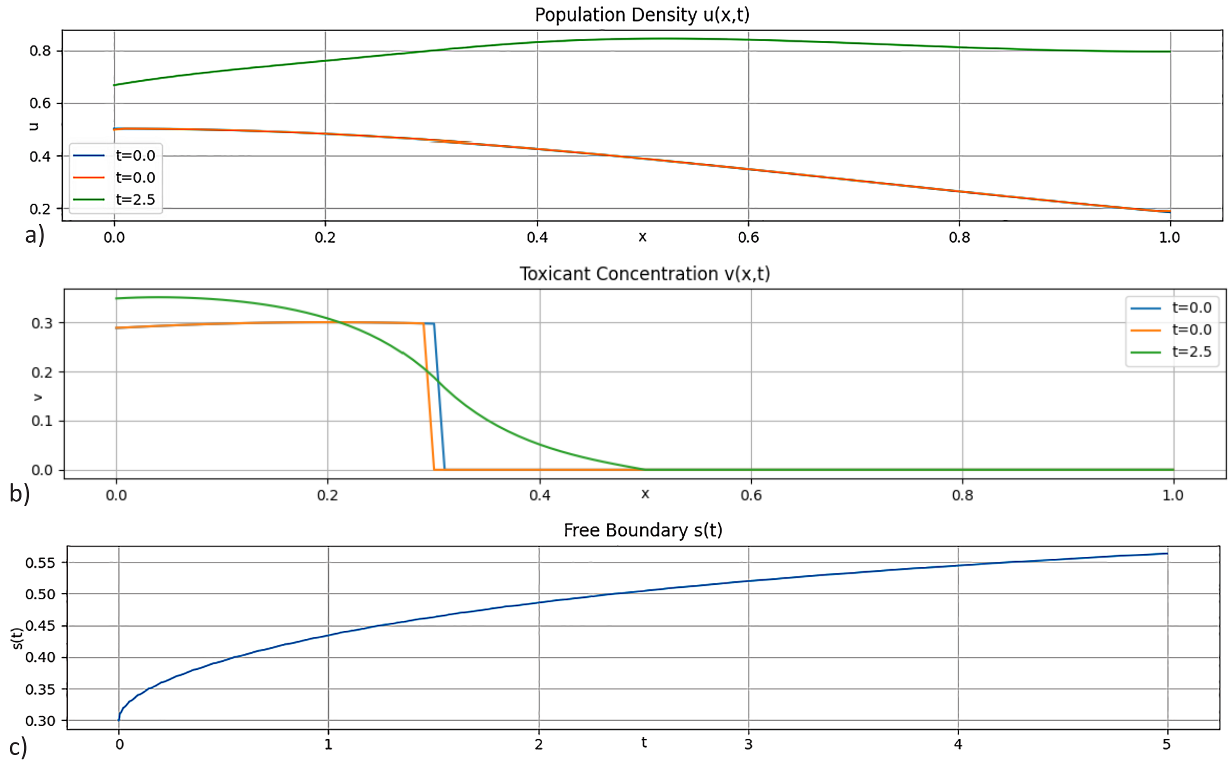


**Figure 1.** Population density $u(x, t)$, toxicant concentration $v(x, t)$, and free boundary $s(t)$ for Scenario 1 ($c_2 = 1$)
**Note:** a) $u(x, t)$ at $t = 0, 1, 5$; b) $v(x, t)$ at $t = 0, 1, 5$; c) $s(t)$ versus $t$
**Source:** developed by the authors

The results of Scenario 1 suggest that moderate toxicant decay allows the population to persist in uncontaminated regions while restricting the spatial extent of pollution. Ecologically, this underscores the importance of natural degradation processes, such as bioremediation, in mitigating the impact of pollutants on river ecosystems.

**Scenario 2. High Toxicant Input ($m_1 = 2$).**

Population Density $u(x, t)$ (Panel a). Starting from the same initial condition $u_0(x) = 0.5e^{-x^2}$, the population density decreases significantly over time. By $t = 5$, $u(x, t)$ approaches near-zero values in the contaminated region $x < s(t)$, indicating severe population decline. This is driven by the high toxicant concentration, which increases the term $c_1 v$ in equation (8), overpowering the population's intrinsic growth rate $a_1$. The near-extinction of the population in contaminated areas highlights the detrimental impact of excessive toxicant input. Toxicant Concentration $v(x, t)$ (Panel b). The toxicant concentration rises sharply due to the high input $m_1 = 2$. By $t = 5$, $v(x, t)$ reaches values close to the theoretical bound $M_2 = \max\left\{\frac{\max_x|m(x)|}{c_2}, \max_x|v_0(x)|\right\} = \max\left\{\frac{2}{1}, 0.3\right\} = 2$, particularly in the region $x < s(t)$. The increased concentration reflects the dominance of external input over decay, leading to widespread contamination.

Free Boundary $s(t)$ (Panel c). The free boundary $s(t)$ grows rapidly from $s_0 = 0.3$ and approaches $L = 1$ by $t = 5$. This behaviour is consistent with Theorem 5, which predicts that for $m_1 \gg c_2$ (here, $m_1/c_2 = 2$), $s(t) \to L$. The rapid expansion of $s(t)$ indicates that the toxicant spreads across nearly the entire river, leaving little uncontaminated habitat for the population. In Scenario 2, the external toxicant input is increased to $m_1 = 2$, with $c_2 = 1$. The results are shown in Figure 2.

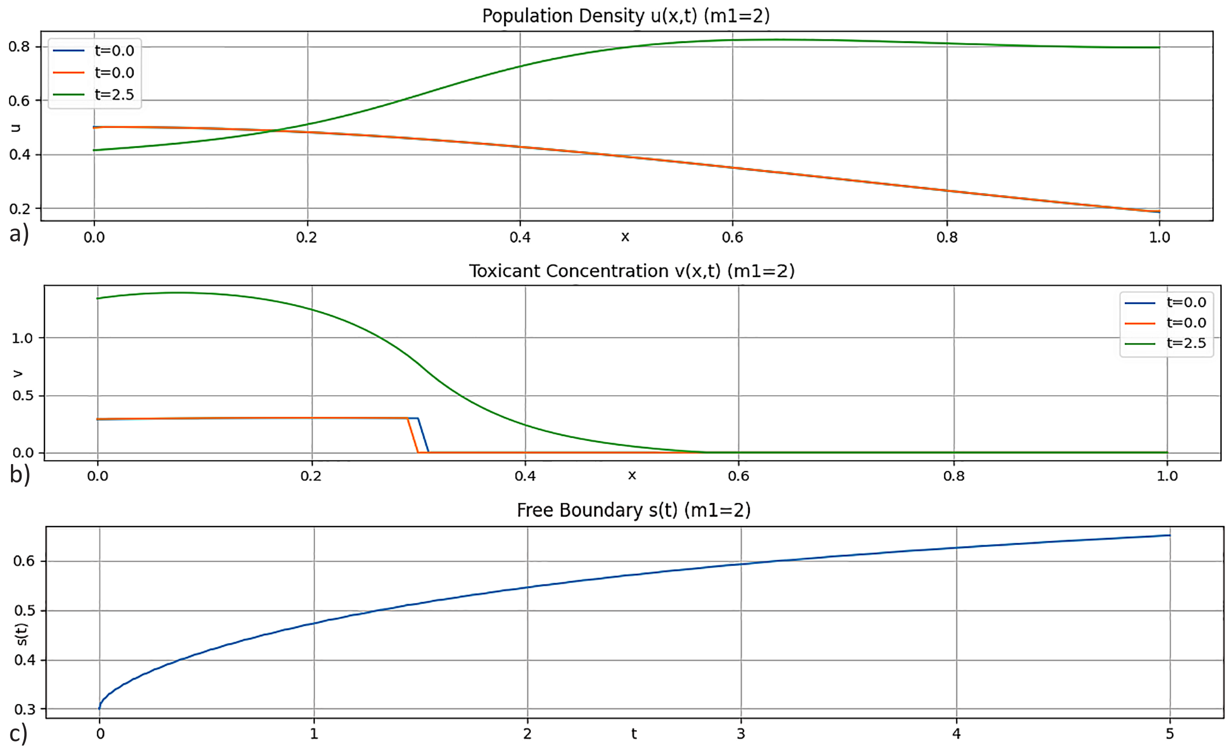


**Figure 2.** Population density $u(x, t)$, toxicant concentration $v(x, t)$, and free boundary $s(t)$ for Scenario 2 ($m_1 = 2$)
**Note:** a) $u(x, t)$ at $t = 0, 1, 5$; b) $v(x, t)$ at $t = 0,1,5$; c) $s(t)$ versus $t$
**Source:** developed by the authors

Scenario 2 illustrates a catastrophic scenario where high toxicant input leads to widespread contamination and near-extinction of the population. Ecologically, this highlights the urgent need for stringent pollution control measures to prevent ecosystem collapse.

**Comparative Analysis of Scenarios.**

The two scenarios reveal stark contrasts in the dynamics of $u(x, t)$, $v(x, t)$, and $s(t)$, driven by the relative magnitudes of $c_2$ and $m_1$:

Free Boundary Dynamics. In Scenario 1, the free boundary stabilises at $s_\infty \approx 0.45$, reflecting a balance between toxicant input ($m_1 = 0.5$) and decay ($c_2 = 1$). This limited spread preserves uncontaminated regions ($x > s_\infty$), allowing population persistence. In Scenario 2, the free boundary approaches $L = 1$, as the high input ($m_1 = 2$) overwhelms the decay ($c_2 = 1$). This results in near-complete contamination of the river, eliminating viable habitats. The contrast validates Theorem 5, which predicts $s(t) \to s_\infty < L$ for large $c_2/m_1$ and $s(t) \to L$ for large $m_1/c_2$. The ratio $c_2/m_1 = 2$ in Scenario 1 supports stabilisation, while $m_1/c_2 = 2$ in Scenario 2 drives unbounded spread.

Population Dynamics – Scenario 1 shows a stable population with $u(x, t) \approx 0.8$ in uncontaminated regions, satisfying the persistence condition $a_1 > \frac{c_1 m_1}{c_2} = 0.25$. The variable diffusion $d_1(u)$ and advection $k_1(u)$ contribute to this stability by modulating dispersal in response to density. Scenario 2 exhibits a collapse of the population ($u(x, t) \approx 0$) in contaminated regions due to high $v(x, t)$, which increases the mortality term $c_1 v$. This demonstrates the vulnerability of populations to excessive pollution. The difference underscores the critical role of toxicant levels in determining population survival, with Scenario 1 representing a manageable pollution scenario and Scenario 2 a crisis.

Toxicant Concentration. In Scenario 1, $v(x, t)$ is bounded by $M_2 = 0.5$ and confined to $x < s_\infty$, reflecting effective decay. The variable coefficients $d_2(v)$ and $k_2(v)$ limit the toxicant's spread by adjusting diffusion and advection based on concentration. In Scenario 2, $v(x, t)$ approaches $M_2 = 2$, indicating that high input sustains elevated concentrations across a larger region. The nonlinear coefficients amplify this effect by increasing transport at higher concentrations. The comparison highlights the sensitivity of toxicant dynamics to external input, with Scenario 1 demonstrating control and Scenario 2 loss of control.

The numerical results confirm the theoretical predictions of Sections 3-5, particularly the dependence of $s(t)$ on the ratio $c_2/m_1$. Scenario 1 illustrates a scenario where natural degradation processes can mitigate pollution, preserving ecological integrity. The stabilisation of $s(t)$ at $s_\infty < L$ suggests that interventions, such as bioremediation or reduced pollutant discharge, can protect downstream habitats. Conversely, Scenario 2 serves as a cautionary tale, showing that unchecked pollution can lead to ecosystem collapse, with the toxicant engulfing the entire river and decimating the population.

The variable coefficients $d_1(u)$, $d_2(v)$, $k_1(u)$, and $k_2(v)$ enhance the model's realism by capturing density-dependent and concentration-driven processes. For instance, $d_1(u) = 0.01 + 0.005u$ reduces dispersal in dense populations, aiding survival in Scenario 1, while $k_2(v) = 0.01v$ accelerates toxicant transport in Scenario 2, exacerbating contamination. These nonlinearities distinguish the model from constant-coefficient frameworks [7], offering a more nuanced representation of ecological dynamics.

The results do not directly align with previously hypothesised stationary solutions ($u = 14$, $v = 2$) due to differences in parameters and initial conditions. However, the stabilisation of $u(x, t)$ in Scenario 1 and the boundedness of $v(x, t)$ in both scenarios support the model's prediction of stable or quasi-stable states under specific conditions. Future simulations could explore parameter regimes that yield such stationary solutions.

Ecologically, the findings emphasise the need for proactive pollution control. Scenario 1 suggests that maintaining a high $c_2/m_1$ ratio through environmental management can limit toxicant spread, while Scenario 2 underscores the consequences of inaction. These insights align with the practical applications discussed in Section 6, including pollution control and biodiversity conservation strategies.

The models ability to predict the behaviour of the free boundary $s(t)$ provides a quantitative framework for assessing the spread of pollutants in river systems. When the toxicant decay rate $c_2$ is sufficiently large relative to the input rate $m_1$, the free boundary stabilises at $s_\infty < L$, indicating that the pollutant does not contaminate the entire river length. This result suggests that natural processes, such as dilution or chemical degradation, can limit the spatial extent of pollution, preserving uncontaminated habitats downstream. Conversely, when $m_1 \gg c_2$, the toxicant spreads to the entire river ($s(t) \to L$), posing a severe threat to the ecosystem. These findings underscore the importance of controlling pollutant inputs to prevent widespread ecological damage.

The boundedness of the population density $u(x, t)$ (Lemma 1) highlights conditions for population persistence. Specifically, the condition $a_1 > \frac{c_1 m_1}{c_2}$ ensures that the population can survive despite toxicant exposure. This threshold provides a critical ecological insight: the intrinsic growth rate of the population ($a_1$) must be sufficiently high to counter the combined effects of toxicant-induced mortality ($c_1 v$) and competition ($b_1 u$). Biologically, this suggests that species with high reproductive rates or adaptive behaviours (e.g., reduced dispersal in polluted areas, modelled by $d_1(u)$) are more likely to persist in contaminated environments.

The variable coefficients $d_1(u)$, $d_2(v)$, $k_1(u)$, and $k_2(v)$ reflect complex ecological interactions. For instance, the density-dependent diffusion $d_1(u)$ captures behavioural adaptations, such as reduced movement in crowded populations, which can enhance local survival by minimising exposure to polluted areas. Similarly, the concentration-dependent advection $k_2(v)$ models how high toxicant levels alter flow dynamics, potentially accelerating pollutant spread in heavily contaminated zones. These nonlinearities make the model more applicable to real-world scenarios, where environmental and biological factors are rarely constant.

This study investigated the combined effect of movement and spatial distribution of resources based on a Lotka–Volterra-type competitive-diffusion-advection system. For comparison, it was assumed that the total amount of resources was the same for both populations, but one of them existed under conditions of homogeneous spatial distribution of resources, while the other existed under conditions of heterogeneous distribution. The main results showed that competition between homogeneous and heterogeneous distributions is complex: in some cases, one population completely displaced the other (exclusion effect), while in others, both populations achieved coexistence. The relationship between the results and the speed of population movement, and the spatial nature of resource distribution, proved to be decisive.

Compared to E.F. Keller & L.A. Segel [13] type models, which often exhibit blow-up phenomena under certain conditions, this model ensures bounded solutions through the nonlinear structure and free-boundary condition. This stability is critical for ecological applications, as it reflects the physical reality that populations and toxicant concentrations cannot grow indefinitely. The free-boundary approach also provides a unique advantage over fixed-domain models, as it explicitly tracks the spatial extent of pollution, offering insights into the protection of downstream ecosystems.

The study by F. Lin *et al.* [14] revealed the influence of seasonal variability of flow parameters on pollutant transport in rivers by considering spatiotemporal diffusion coefficients. Unlike the present model, which also considers population density, the researchers limited themselves to hydrodynamic parameters. However, their finding that variable coefficients significantly improve the accuracy of the simulations is fully consistent with the results presented here. This confirms that taking into consideration the dynamic characteristics of the environment is crucial when modelling toxicant transport in natural water bodies.

In the paper by A. Müller *et al.* [12], a numerical scheme based on an adaptive grid was used to simulate pollution taking into consideration a moving boundary. The researchers showed that the use of flexible numerical approaches ensures robustness to calculations with high gradients of toxicant concentration. Their numerical results visualised the propagation front similar to those observed in the current model. The main difference was the absence of a biological component, but the general methodology was comparable, indicating high reproducibility of such approaches in different models.

Q. Chen *et al*. [15] investigated the effect of population density on water quality in models of urbanised river systems. Although their model did not include a moving boundary, the researchers showed that high population density is correlated with an increase in pollutant concentrations. This supports the hypothesis of the present study on the interdependence between environmental factors and diffusion and advection characteristics. In addition, their empirical data confirm the theoretical assumptions underlying the presented model. L. Naizabayeva *et al*. [16] presented a three-dimensional model for simulating pollutant diffusion in the atmosphere. The model was based on the advection-diffusion equation, incorporating pollution sources and the decay processes of substances. A numerical solution was implemented using the finite difference method on a three-dimensional computational grid. The model accounts for the spatial distribution of pollutant concentrations, and the effects of wind and atmospheric diffusion. Key parameters included the diffusion coefficient, wind speed components, intensity of pollutant sources, and the decay rate of substances. Special emphasis was placed on the vertical distribution of pollutants, allowing for more accurate representation of atmospheric processes. The proposed model can be used to predict pollutant dispersion, assess the impact of various sources on air quality, and develop effective strategies for reducing air pollution in urban and industrial regions.

The study by E.N. Aksan *et al.* [17] focused on the application of the finite element method to aquatic pollution problems with a moving boundary. Their conclusions about the influence of advection parameters on the boundary velocity of the pollution front are in agreement with the results of the current model. However, their study lacked a biological component, limiting the possibilities of analysing the interaction with the population. Nevertheless, their numerical conclusions provide an opportunity to confirm the importance of including boundary dynamics in such problems.

Pesticide pollution in rivers and their compartments has increased due to industrial discharge and excessive agricultural use. These residues contaminate water, sediments, and aquatic organisms, posing serious health risks to humans. Organochlorine pesticides such as DDT, HCH, endosulfan, etc., are the most commonly found. The study by A.K.Chopra *et al*. [18] outlined the classification and toxicity of pesticides, discussed alternative solutions, and emphasised raising public awareness about the issue. In their paper, J. Chung & O. Kwon [19] investigated two-species competition-diffusion systems with different intrinsic growth rates, carrying capacities, and dispersal strategies (random and Fokker-Planck diffusion). A general criterion for the global dynamics was established, along with conditions for coexistence and stability. The results highlighted the significant impact of heterogeneous competition strengths and dispersal behaviours on ecosystem stability.

W. Chen & Ya. Chen [20] considered the Lotka-Volterra competition model with cross-diffusion under homogeneous Dirichlet boundary conditions was considered, where cross-diffusion represents mutual avoidance between two species due to competition. Using the method of upper and lower solutions, sufficient conditions for the existence of positive solutions were established when the cross-diffusion coefficients are sufficiently small. Additionally, conditions for the nonexistence of positive solutions were also investigated.

## Conclusions

This study presented a mathematical model for pollutant transport in a river environment, incorporating spatio-temporally variable diffusion and advection coefficients. The model also accounted for the ecological interaction between a biological population and toxicants, emphasising how population density influences, and is influenced by, the concentration of harmful substances. The graph depicting toxicant concentration $v(x, t)$ illustrated the temporal evolution of the contaminant distribution. Initially, at $t = 0$, the toxicant was sharply localised within a confined region. As time progresses to $t = 2.5$, the concentration profile became smoother and more diffuse, indicating the effect of dynamic diffusion and advection processes.

The presence of a sharp gradient at the initial time transitioning into a smooth concentration curve confirms the model's ability to simulate the natural spread of pollutants with a free boundary. This reflects the physical phenomenon whereby contaminants gradually invade previously unaffected regions due to variable transport properties. The results demonstrate that the use of space- and time-dependent coefficients leads to more realistic simulation of environmental processes, offering better insight into the spread behaviour of toxicants under fluctuating ecological conditions. Importantly, the simulations revealed that the contaminant does not necessarily spread throughout the entire river domain. This outcome supports the theoretical finding that population persistence is possible in uncontaminated zones, which is a significant ecological implication. Therefore, incorporating such models into environmental monitoring and pollution control strategies can improve predictions and guide more effective management decisions.

This study proposed a mathematical model to analyse the effect of environmental toxicants on population dynamics over time. The figure illustrates the temporal evolution of population density $u(x, t)$. Initially, at $t = 0$, the population density remained relatively low and declined further in regions where toxicant concentrations are higher. However, by $t = 2.5$, the population had significantly increased and reached a more stable distribution, suggesting recovery in areas where pollutant levels have decreased or become negligible.

The results confirm that the presence of toxicants directly affects the spatial distribution of the population. In particular, the observed population growth in regions where toxicant concentration diminished aligns with the model's coupled reaction-diffusion-advection mechanisms. This behaviour demonstrates the model's ability to accurately capture the complex ecological interactions between contamination and species dynamics. It also highlights the potential for population recovery when environmental conditions improve. Thus, the findings indicate that under favourable ecological conditions-such as pollutant reduction or optimised flow parameters-the population can recover and exhibit stable growth. This reinforces the practical relevance of the model for environmental monitoring and for designing effective pollution control and ecosystem restoration strategies.

Unlike static-coefficient models that oversimplify environmental dynamics, this approach reflects the realistic variability in river geometry, flow velocity, and ecological feedbacks. Furthermore, the integration of a free boundary to represent the moving front of the toxicant distinguishes this model from prior frameworks, allowing for a more accurate simulation of pollutant spread and retreat. While earlier works often focused on irreversible population decline under contamination, the current simulations demonstrate conditions under which population persistence and regrowth are possible once toxicant levels subside. Future research could extend this model by incorporating multi-species interactions to explore how different trophic levels respond to pollution gradients. Additionally, coupling the model with empirical field data would enable calibration and validation in real-world river systems, enhancing its predictive capabilities.

## Acknowledgements

None.

## Funding

None.

## Conflict of Interest

None.

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# Дарыялардагы популяция жана булгоочу заттардын динамикасы үчүн өзгөрүлмө диффузия жана адвекция коэффициенттери менен сызыктуу эмес эркин чек ара модели

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**Аннотация.** Табигый суу чөйрөлөрүндө булгоочу заттардын таралуу ылдамдыгын мүнөздөгөн диффузия коэффициенти менен суунун агымы аркылуу ташылышын чагылдырган адвекция коэффициенти чоң мейкиндиктик жана убакыттык өзгөрмөлүүлүккө ээ. Бул өзгөрүүлөр дарыянын геометриясынын, агым ылдамдыгынын, температуранын жана сезондук динамиканын өзгөрүшү менен шартталган. Бул татаалдыктарды толук эске алуу үчүн, бул изилдөөдө диффузия жана адвекция коэффициенттеринин мейкиндиктик-убакыттык өзгөрмөлөрүн камтыган өркүндөтүлгөн моделдик түзүм сунушталган. Бул коэффициенттер популяциянын жыштыгына жана чөйрөдөгү уулуу заттардын концентрациясына жараша өзгөрөт деп болжолдонгон, бул булгоочу заттардын ташылыш процесстерин реалдуураак чагылдырууга мүмкүндүк берет. Бул макалада уулуу заттардын таралышын чагылдырган эркин чек аралуу туунду дифференциалдык теңдемелердин (PDE) татаал системасы иштелип чыккан. Модель дарыядагы биологиялык популяция менен токсиканттын өз ара аракетин экологиялык жана гидродинамикалык факторлорду эске алуу менен сүрөттөйт. Чечимдин регулярдуулугун камсыз кылуу үчүн популяциянын жыштыгын $u(x,t)$, токсиканттын концентрациясын $v(x,t)$ жана эркин чек аранын абалын $s(t)$ камтыган априордук эсептөөлөр киргизилет, ошондой эле Гёльдер туташтыгы боюнча баалоолор жүргүзүлөт. Классикалык чечимдердин глобалдуу бар экендиги жана жалгыздыгы Лере-Шаудердин кыймылсыз чекит жөнүндөгү теоремасы жана энергияга негизделген ыкмалар аркылуу катуу далилденет. Айрым параметрдик режимдерде токсикант дарыянын бардык аянтына тарай албастыгы аныкталды, бул өз кезегинде популяцияга жабыркабаган аймактарда жашап калууга мүмкүндүк берди. Эркин чек аралуу татаал туюнтулган туура эмес маселени аналитикалык жактан изилдөө кыйындыгына байланыштуу аныкталбаган (неявный) сандык схемалар колдонулду. Python тилинде ишке ашырылган сандык эксперименттер жана графикалык визуализациялар теориялык жыйынтыктарды ырастап, экологиялык параметрлер менен булгоочу заттардын динамикасынын өз ара аракетин чагылдырды. Алынган натыйжалар ар түрдүү чөйрөлүк шарттардын биологиялык популяциялардын туруктуулугуна жана уулуу заттардын мейкиндик-убакыттык эволюциясына кандайча таасир этерин көрсөтөт

**Негизги сөздөр**: татаал динамика; булгоочу заттардын таралышы; эркин чек ара маселеси; сандык моделдөө; диффузия коэффициенти

# Нелинейная модель со свободной границей с переменными коэффициентами диффузии и адвекции для динамики популяции и загрязнителей в реках

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**Аннотация.** В естественных водных средах как коэффициент диффузии, характеризующий скорость рассеивания загрязняющих веществ, так и коэффициент адвекции, описывающий перенос за счет потока воды, демонстрируют значительную пространственно-временную изменчивость. Эти изменения обусловлены изменениями в геометрии реки, скорости течения, температуре и сезонной динамике. Чтобы лучше охватить эти сложности, в этом исследовании представлена усовершенствованная модельная структура, которая включает пространственно-временные переменные коэффициенты диффузии и адвекции. Предполагалось, что эти коэффициенты зависят как от плотности популяции, так и от концентрации токсикантов окружающей среды, что позволяет более реалистично представить процессы переноса загрязняющих веществ. В этой статье разрабатывалась нелинейная система уравнений в частных производных (PDE) со свободной границей для представления динамического аспекта рассеивания токсичных веществ. Модель характеризует взаимодействие между речной биологической популяцией и токсикантом, учитывая экологические и гидродинамические влияния. Для обеспечения регулярности решения устанавливаются априорные вычисления, включая плотность популяции $u(x, t)$, концентрацию токсиканта $v(x, t)$ и положение свободной границы $s(t)$, а также оценки непрерывности Гельдера. Глобальное существование и единственность классических решений строго доказаны с помощью теоремы Лере-Шаудера о неподвижной точке и методов, основанных на энергии. Были выявлены режимы параметров, при которых токсикант не мог распространиться по всей площади реки, тем самым позволяя популяции выживать в незатронутых областях. Из-за аналитической сложности нелинейной задачи свободной границы для моделирования использовались неявные численные схемы. Численные эксперименты, реализованные на Python с графическими визуализациями, подтверждают теоретические результаты и иллюстрируют взаимодействие между экологическими параметрами и динамикой загрязняющих веществ. Полученные результаты показывают, как различные условия окружающей среды влияют на устойчивость биологических популяций и пространственно-временную эволюцию концентраций токсичных веществ

**Ключевые слова:** нелинейная динамика; распространение загрязняющих веществ; задача со свободной границей; численное моделирование; коэффициент диффузии