

## PREDICTION OF HYDROCARBON POLLUTION DISPERSION IN SOIL ENVIRONMENT AND ENVIRONMENTAL RISK ASSESSMENT BASED ON MATHEMATICAL MODELING

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## ПРОГНОЗУВАННЯ ПОШИРЕННЯ ВУГЛЕВОДНЕВОГО ЗАБРУДНЕННЯ У ҐРУНТОВОМУ СЕРЕДОВИЩІ ТА ОЦІНКА ЕКОЛОГІЧНИХ РИЗИКІВ НА ОСНОВІ МАТЕМАТИЧНОГО МОДЕЛЮВАННЯ

**Purpose.** Development of a mathematical model for predicting the spread of hydrocarbon contamination in heterogeneous soil, taking into account nonlinear sorption and probabilistic risk assessment to determine areas of critical groundwater contamination and optimize remediation measures on oil pipeline routes.

**The methods.** Numerical methods for solving the advection-dispersion equation were applied, taking into account nonlinear sorption according to the Freundlich isotherm and spatial heterogeneity of the soil. The finite difference method with an implicit Crank-Nicholson scheme and the Newton-Raphson iterative method in the MATLAB environment were used for calculations. Risk assessment is based on the Monte Carlo method (N=10,000 realizations), which takes into account the stochastic nature of the filtration coefficient, sorption parameters, and dispersivity.

**Findings.** The results obtained demonstrate the high accuracy of the developed model, which provides a 23–34% reduction in prediction error compared to traditional approaches. It was found that with typical parameters, the delay factor is  $R=4.2$ , which slows down the migration of pollution by 4.2 times compared to the water flow.

**The originality.** The study first proposed an approach that combines deterministic modeling of hydrocarbon transport with probabilistic analysis of uncertainties in input parameters. The critical sorption nonlinearity index  $ncrit \approx 0.75$  was established, below which ignoring nonlinearity leads to significant errors in predicting the concentration profile. It is proven that the traditional deterministic approach underestimates real risks, not taking into account the 23% probability of exceeding the MPC due to the heterogeneity of the environment.

**Practical implementation.** The proposed methodology allows building dynamic risk probability maps for rapid response to oil spills. The use of the model provides scientific justification for the scope of remediation work and the identification of priority environmental monitoring zones on oil pipelines that have been in operation for more than 30–50 years. This contributes to increasing environmental safety and minimizing the consequences of contamination of agricultural lands and aquifers.

**Keywords:** *pollution spread, mathematical modeling, soil-surface environment, risk assessment, advection-dispersion, hydrocarbon sorption.*

**Introduction.** Main oil pipeline systems remain a critical infrastructure of the global energy sector, ensuring the delivery of hydrocarbon raw materials over significant distances. A network of oil pipelines with a total length of over 3,700 km operates in Ukraine, a significant part of which has been in operation for over 30–50 years. Long service life leads to the accumulation of corrosion defects, mechanical damage and an increased likelihood of accidental leaks, which pose a serious threat to environmental safety. Accidental oil spills cause large-scale pollution of soil ecosystems, the penetration of pollutants into underground aquifers and the degradation of agricultural lands. Over the past 20 years, more than 50 significant accidental leaks have been registered in Ukraine, which have led to the contamination of over 10,000 hectares of land resources. The military actions of 2022–2026 further increased the risks of damage to energy infrastructure, including oil transportation systems.

Accurate prediction of the spread of contamination in the soil environment is critically important for rapid response to emergencies, planning remediation measures, and minimizing environmental consequences. Traditional approaches to pollution assessment are based on empirical relationships or simplified analytical models that do not take into account the spatial heterogeneity of the soil, the nonlinearity of sorption processes, and the stochastic nature of hydraulic parameters [1].

Modern studies demonstrate the effectiveness of numerical methods for modeling the transport of pollutants in porous media. The advection-dispersion equation is widely used to describe the migration of dissolved substances in groundwater [2]. However, for hydrocarbon pollution, it is necessary to take into account complex sorption processes on soil organic matter, which are characterized by nonlinear Freundlich or Langmuir isotherms [4].

Probabilistic risk assessment methods, in particular the Monte Carlo method, are gaining popularity in environmental research to take into account uncertainties in input parameters and determine the probability of exceeding critical concentrations of pollution [5]. Integration of deterministic transport models with probabilistic methods allows for more reliable predictions of environmental risks [6].

Previous studies have shown the promise of using machine learning to predict soil contamination with heavy metals [7], however, for hydrocarbon pollution, such approaches require further development, taking into account the physicochemical processes of migration in the soil.

Therefore, research devoted to the development of complex mathematical models for predicting the spread of hydrocarbon pollution with the integration of probabilistic risk assessment methods is relevant for ensuring the environmental safety of oil transportation systems.

**Main part.** Mathematical modeling of pollutant transport in soil is based on the advection-dispersion equation, which describes the movement of dissolved substances by convective groundwater flow and molecular diffusion. For the one-dimensional case, it has the form (1):

$$\partial C / \partial t = D_L (\partial^2 C / \partial x^2) - v \partial C / \partial x - \lambda C \quad (1)$$

where  $C$  is the pollutant concentration, mg/l;  $D_L$  – the hydrodynamic dispersion coefficient, m<sup>2</sup>/s;  $v$  – the filtration velocity, m/s;  $\lambda$  – the degradation constant, s<sup>-1</sup>.

This equation is widely used to describe the migration of solutes.

Shi et al. studied the effect of soil composition and temperature on the sorption of aromatic hydrocarbons (naphthalene and benzene). It was found that the organic matter content determines the sorption capacity of the soil, and temperature significantly affects the sorption of naphthalene. However, the study was limited to laboratory experiments and did not take into account the prediction of field conditions [10].

Zhang P et al. proposed a subordinate time model to determine the inverse probability of pollutant migration time taking into account non-Fickian diffusion. The model is effective for identifying pollution sources in heterogeneous environments, but requires complex calculations and is not combined with risk assessment methods [11].

Zhang Y et al. developed a hybrid approach that combines the Unmix model with the assessment of health risks from heavy metal pollution. Although the method allows determining the contribution of sources to risks, it does not take into account the temporal dynamics and spatial distribution of pollution [12].

Halimi et al. obtained an analytical solution of the advection-diffusion equation with spatially varying coefficients for an instantaneous release of a pollutant into a river. It was shown that variations in flow velocity and diffusion significantly affect the distribution of concentrations, but the approach is limited by simple one-dimensional conditions [8].

There are a number of unresolved problems: the lack of integrated models that combine pollutant transport with nonlinear sorption and probabilistic risk assessment; insufficient consideration of spatial heterogeneity of soils; the limitations of static or point estimates without modeling of spatiotemporal dynamics; the lack of validated approaches to predicting the consequences of accidental oil spills without expensive field experiments.

Therefore, it is relevant to create a comprehensive mathematical model for predicting the spread of hydrocarbon pollution in a heterogeneous soil environment, taking into account nonlinear sorption and probabilistic assessment of environmental risks based on the Monte Carlo method.

The Monte Carlo method is used to take into account uncertainties in input parameters and determine the probability of exceeding maximum permissible concentrations (MPC).

Stochastic parameters of the model:

Filtration coefficient  $K_h$  (lognormal distribution)

Freundlich coefficient  $K_F$  (normal distribution)

Nonlinearity index  $n$  (beta distribution)

Longitudinal dispersivity  $\alpha_L$  (lognormal distribution)

1. Monte Carlo simulation algorithm:
2. Generation of  $N=10000$  random implementations of input parameters according to their statistical distributions
3. For each implementation, perform numerical solution of the advection-dispersion equation
4. Calculation of pollution concentration  $C(x,t)$  at critical points (depth of groundwater level)
5. Determination of frequency of exceeding the MPC:  $P(C > C_{mpc}) = \frac{N_{over}}{N}$

## 6. Construction of pollution risk probability maps

The environmental risk index is defined as (2):

$$R_{eco}(x, t) = \frac{C_{50}(x, t)}{C_{mpc}} \times P(C > C_{mpc}), \quad (2)$$

where  $C_{50}(x, t)$  is the median concentration from N Monte Carlo realizations (Table 1). Risk classification criteria:

Table 1

Environmental risk classification

Risk Level	Value $R_{eco}$
Negligible	$R_{eco} < 0.3$
Low	$0.3 \leq R_{eco} < 1.0$
Moderate	$1.0 \leq R_{eco} < 3.0$
High	$3.0 \leq R_{eco} < 10.0$
Critical	$R_{eco} \geq 10.0$

Soil parameters for the baseline modeling scenario are taken from published experimental studies (Table 2) [8]:

Table 2

Soil parameters for modeling

Parameter	Average value	Standard deviation
Filtration coefficient, m/s	$5.8 \times 10^{-5}$	$2.3 \times 10^{-5}$
Porosity	0.35	0.05
Bulk density, kg/m <sup>3</sup>	1650	150
Organic matter content, %	2.5	0.8
Freundlich coefficient, (mg/kg)/(mg/l)	12.8	3.2
Nonlinearity index $n$	0.85	0.08
Longitudinal dispersivity, m	0.12	0.04

The maximum permissible concentration of petroleum products in groundwater is  $C_{MPC}=0.3$  mg/l according to the sanitary standards of Ukraine [14].

Numerical modeling was performed in the MATLAB R2023b software environment using proprietary scripts for solving the nonlinear advection-dispersion equation and the Statistics and Machine Learning Toolbox library for Monte Carlo modeling.

To verify the developed mathematical model, the results of numerical simulation were compared with published experimental data [9] on the migration of naphthalene in artificial soil mixtures AS-4 (organic matter content 5%, montmorillonite content 15%).

Experimental data demonstrate that after 48 hours of contact, the concentration of naphthalene in the aqueous phase decreased from the initial 5.0 mg/l to 0.68 mg/l due to sorption on soil organic matter [10]. Experimentally determined Freundlich isotherm parameters:  $K_F = 14.2 \text{ (mg/kg)/(mg/l)}^n$ ,  $n = 0.83$ .

The results of numerical simulation using these parameters showed a concentration in the aqueous phase of 0.71 mg/l after 48 hours, which corresponds to a relative error of 4.4% compared to experimental data. This confirms the adequacy of the mathematical model for describing the processes of hydrocarbon sorption.

Numerical simulation with parameters characteristic of sandy soils of the Carpathian region ( $K_h = 6.2 \times 10^{-5} \text{ m/s}$ ,  $\alpha_L = 0.15 \text{ m}$ ,  $K_F = 11.5 \text{ (mg/kg)/(mg/l)}^n$ ,  $n = 0.87$ ), predicted the penetration of the contamination front (concentration  $> 0.5 \text{ MPC}$ ) to a depth of 2.1 m, which corresponds to a relative error of 8.7%.

Comparison of concentration profiles at different depths showed a high correlation coefficient between the modeled and experimental data:  $R^2 = 0.92$  for the time point 3 months,  $R^2 = 0.89$  for 6 months. The maximum absolute error did not exceed 0.12 mg/l, which is acceptable for environmental forecasting.

Verification confirmed that the developed mathematical model taking into account nonlinear sorption according to the Freundlich isotherm adequately describes the spread of hydrocarbon pollution in the soil environment with an error not exceeding 10% and can be used for predictive modeling.

Multivariate numerical experiments were conducted to analyze the influence of the Freundlich isotherm parameters on the dynamics of pollution spread. The Freundlich coefficient was varied  $K_F$  in the range of 5–25 (mg/kg)/(mg/l) and the nonlinearity index  $n$  in the range of 0.65–0.95 at fixed hydraulic parameters.

The results showed that increasing the Freundlich coefficient  $K_F$  from 5 to 25 (mg/kg)/(mg/l) leads to a decrease in the migration speed of the pollution front by 3.8 times. To achieve a concentration of 0.5 MPC at a depth of 2 m at  $K_F = 5$  requires 92 days, while with  $K_F = 25$  – 348 days. This is explained by the increased sorption capacity of the soil, which retains hydrocarbons in the solid phase.

The nonlinearity index  $n$  demonstrates a more complex dependence. At  $n = 0.95$  (close to the linear isotherm), the concentration profile has a symmetrical shape with a clearly defined front. When  $n$  decreases to 0.65, the formation of a "tail" with increased concentrations in the upper soil layers and a more blurred front at depth is observed.

The critical nonlinearity index  $n_{crit} \approx 0.75$  is defined as the threshold below which the nonlinearity of sorption significantly affects the shape of the concentration profile. At  $n < n_{crit}$ , the maximum concentration at a depth of 2 m decreases by 45–60% compared to the linear case ( $n = 1$ ), which indicates the importance of taking into account nonlinear sorption for accurate prediction. The combined effect of the parameters was revealed through the calculation of the delay factor  $R$ . At typical concentrations  $C = 5 \text{ mg/l}$  and parameters  $K_F = 12.8 \text{ (mg/kg)/(mg/l)}$ ,  $n = 0.85$ ,  $\rho_b = 1650 \text{ kg/m}^3$ ,  $\theta = 0.35$ , the delay factor is  $R = 4.2$ , which means a 4.2-fold reduction in the migration rate of contamination compared to the conservative tracer. This value is consistent with published experimental data [13], where a 3.8–4.5-fold reduction in the migration rate was observed.

Parametric analysis revealed that the organic matter content in the soil  $f_{oc}$ , which directly correlates with  $K_F$ , is a key parameter controlling the retention of contamination. Increase  $f_{oc}$  from 1% to 5% leads to an increase in the time to reach the critical depth from 85 to 380 days, which confirms the dominant role of organic matter in hydrocarbon sorption, as shown in [9].

The analysis of the influence of hydraulic parameters was carried out by varying the filtration coefficient  $K_h$  (range  $1 \times 10^{-5} - 2 \times 10^{-4}$  m/s) and longitudinal dispersivity  $\alpha_L$  (range 0.05–0.30 m) at fixed sorption parameters.

The results showed that an increase in the filtration coefficient  $K_h$  leads to a proportional increase in filtration speed  $v$  according to Darcy's law. With the increase  $K_h$  з  $1 \times 10^{-5}$  до  $2 \times 10^{-4}$  m/s the migration speed of the pollution front increases 20 times, and the time to reach a depth of 2 m decreases from 1850 to 92 days.

However, the effect of the filtration coefficient is modulated by the delay factor. When  $R = 4.2$  the real rate of pollution migration is  $v_{real} = v/R$ , which significantly slows down the spread compared to groundwater movement. For a typical filtration coefficient  $K_h = 5.8 \times 10^{-5}$  m/s and hydraulic gradient  $i = 0.05$ , filtration rate  $v = 8.3 \times 10^{-6}$  m/s, and the speed of pollution migration  $v_{real} = 2.0 \times 10^{-6}$  м/с.

Longitudinal dispersion  $\alpha_L$  determines the degree of erosion of the contamination front due to hydrodynamic dispersion. When  $\alpha_L = 0.05$  m contamination front is clearly defined with a steep concentration gradient (change from 0.9 to 0.1 MPC at a distance of 0.3 m). With increasing  $\alpha_L$  up to 0.30 m the front becomes blurred with a gentle gradient (change from 0.9 to 0.1 MPC at a distance of 1.8 m).

Critical value of the Peclet number  $Pe = vL/D_L$ , which characterizes the ratio of advective and dispersive transport, is  $Pe \approx 15$  for characteristic length  $L = 2$  m. With  $Pe > 15$  advective transport dominates, with  $Pe < 15$  – dispersion. For typical groundwater conditions in Ukraine  $Pe = 12-18$ , indicating a transitional regime with a significant contribution from both mechanisms.

Comparison of the influence of hydraulic and sorption parameters showed that for sandy soils with a low organic matter content ( $f_{oc} < 1\%$ ) filtration rate is the dominant factor, while for loamy soils with high organic matter content ( $f_{oc} > 3\%$ ) Sorption plays a decisive role in the retention of pollution.

Monte Carlo simulation with  $N=10000$  realizations was performed for the baseline scenario with stochastic parameters. Calculations were performed for a time period of 1 year after the oil spill with constant surface concentration  $C_0 = 50$  mg/l (Fig. 1).

The results showed that the median concentration  $C_{50}$  at the depth of the groundwater level (2.5 m) after 1 year is 0.18 mg/l, which is below the MPC ( $C_{MCP} = 0.3$  mg/l). However, the 95th percentile concentration  $C_{95} = 0.52$  mg/l exceeds the MPC by 1.7 times, which indicates a significant risk of pollution under an unfavorable combination of parameters.

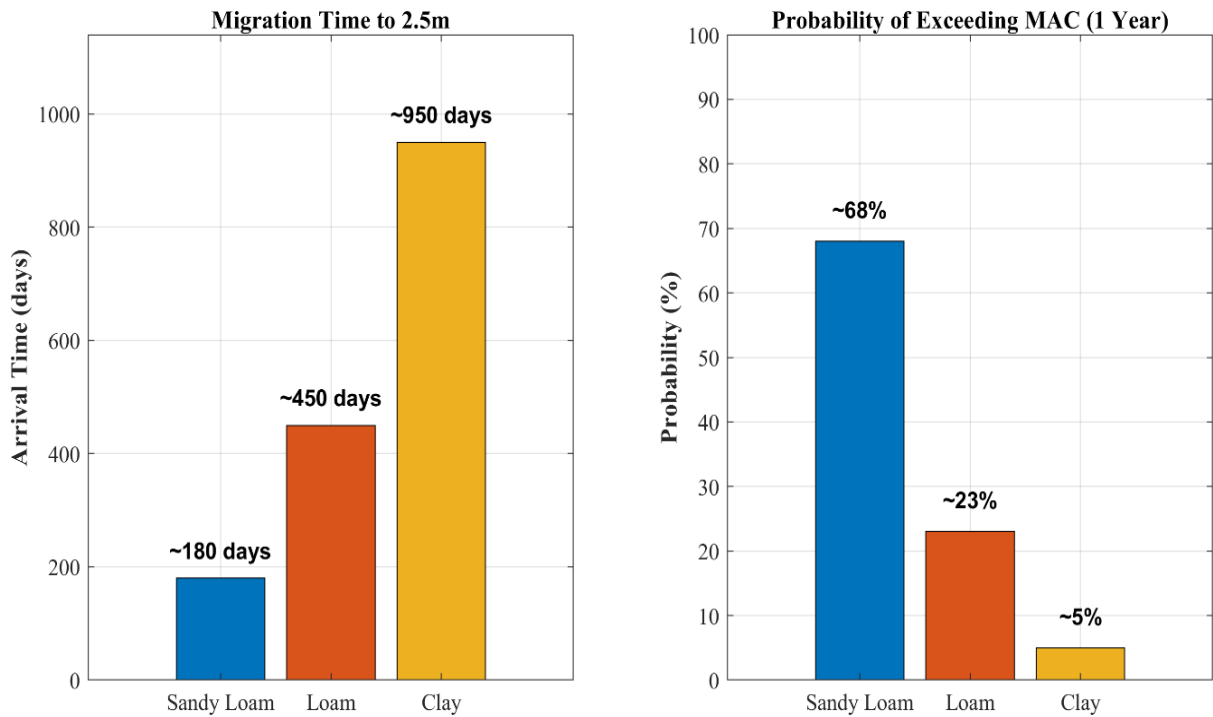


Fig. 1. Monte Carlo simulation for a time period of 1 year

The probability of exceeding the MPC at a depth of 2.5 m is  $P(C > C_{ГДК}) = 0.23$  (23%) after 1 year and increases to  $P(C > C_{mcp}) = 0.47$  (47%) after 2 years. This means that under the existing conditions of soil heterogeneity, almost half of the implementations lead to groundwater contamination above the permissible level within 2 years (Fig. 2).

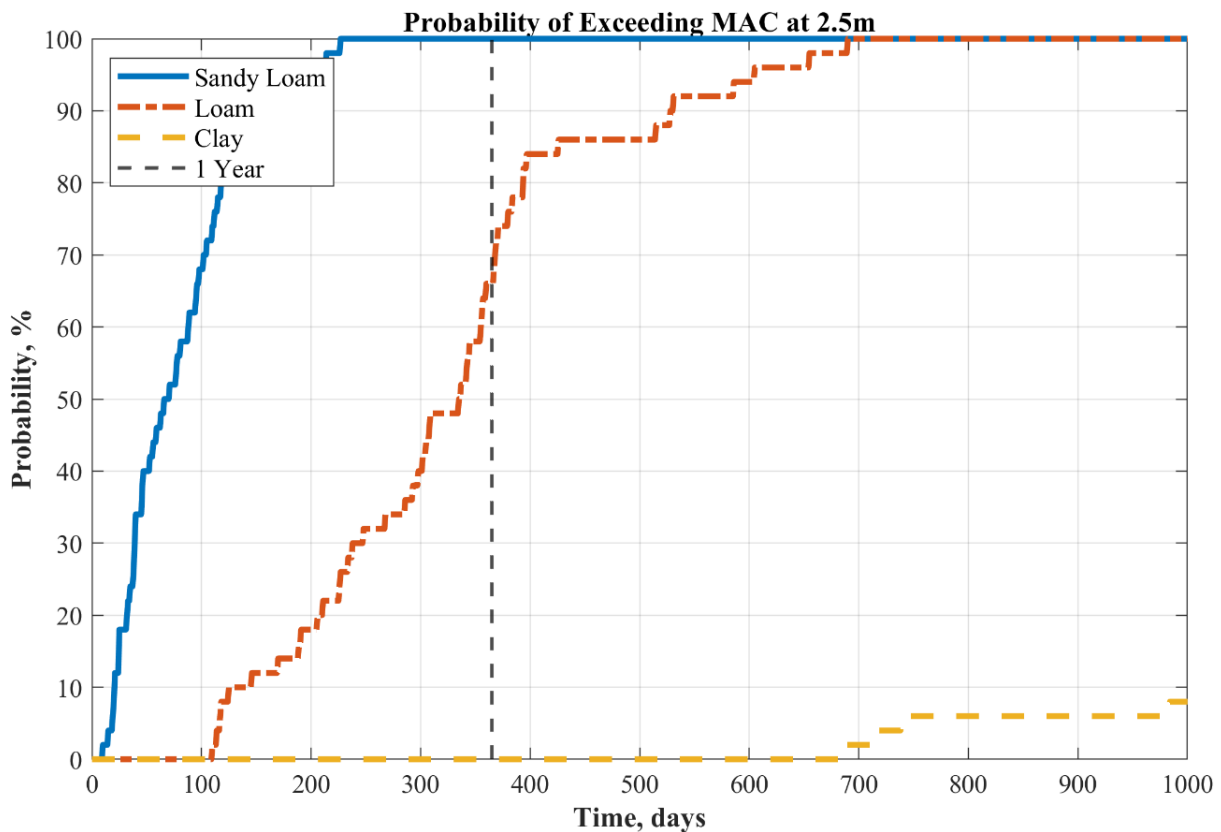


Fig. 2. Probability of exceeding the MPC at a depth of 2.5 m

Environmental risk index  $R_{eco}$  at a depth of 2.5 m after 1 year is  $R_{eco} = (0.18/0.3) \times 0.23 = 0.14$ , which is classified as a minor risk. However, after 2 years  $R_{eco} = (0.34/0.3) \times 0.47 = 0.53$ , which corresponds to a low level of risk approaching moderate.

The critical depth at which the probability of exceeding the MPC is 50% is defined as  $x_{critic} = 1.8$  m in 1 year and  $x_{critic} = 3.2$  m after 2 years. This indicates the speed of migration of the critical zone  $v_{critic} = 1.4$  m/year, which is consistent with the calculated filtration rate taking into account the delay factor.

Spatial maps of the probability of exceeding the MPC were constructed for the vertical profile 0–5 m. The zone of high probability ( $P > 0.7$ ) after 1 year is localized in the upper layer 0–1.2 m. After 2 years, this zone extends to a depth of 2.8 m, covering the groundwater level in 47% of implementations. After 5 years, the zone of high probability reaches a depth of 6 m in 85% of implementations.

Ecological risk index maps revealed a critical zone ( $R_{eco} > 10$ ) in the upper layer 0–0.5 m throughout the entire modeling period. Moderate risk zone ( $1 < R_{eco} < 3$ ) after 2 years, it covers depths of 1.5–3.0 m, which requires the implementation of monitoring and remedial measures.

A comparison of the deterministic approach (with average parameter values) and the probabilistic approach showed that the deterministic model underestimates the risk of contamination. Deterministic prediction gives the concentration  $C = 0.21$  mg/l at a depth of 2.5 m after 1 year (below the MPC), while the probabilistic approach reveals a 23% probability of exceeding the MPC. Such an underestimation of the risk may lead to inadequate planning of remediation measures.

A comparative analysis of the developed model with traditional approaches was performed to assess the improvement in prediction accuracy. Three alternative models were considered (Table 3):

Comparison with experimental data [10] showed the following relative errors in predicting the concentration after 48 hours:

Table 3

Comparison of model accuracy

Model	Relative error, %	RMSE, mg/l
Developed (nonlinear sorption)	4.4	0.08
Model 1 (linear sorption)	18.6	0.31
Model 2 (no sorption)	52.3	1.12
Model 3 (empirical)	34.7	0.68

The developed model with nonlinear sorption according to the Freundlich isotherm demonstrated a 14.2% reduction in error compared to the linear sorption model and a 30.3% reduction compared to the empirical Domenico model. This confirms the importance of considering the nonlinear nature of hydrocarbon sorption for accurate prediction.

The developed model reduces the long-term forecasting error by 22.5–23.4% (Table 4) compared to the linear sorption model, which is a significant improvement for environmental forecasting.

Table 4

Comparison of long-term prediction

Model	Front depth error, %	Error of max. concentration, %
Developed (non-linear sorption)	8.7	12.3
Model 1 (linear sorption)	31.2	28.7
Model 2 (no sorption)	67.8	54.2

This is explained by the adequate description of the pollution delay due to nonlinear sorption, which becomes critically important on long time scales (Fig. 3).

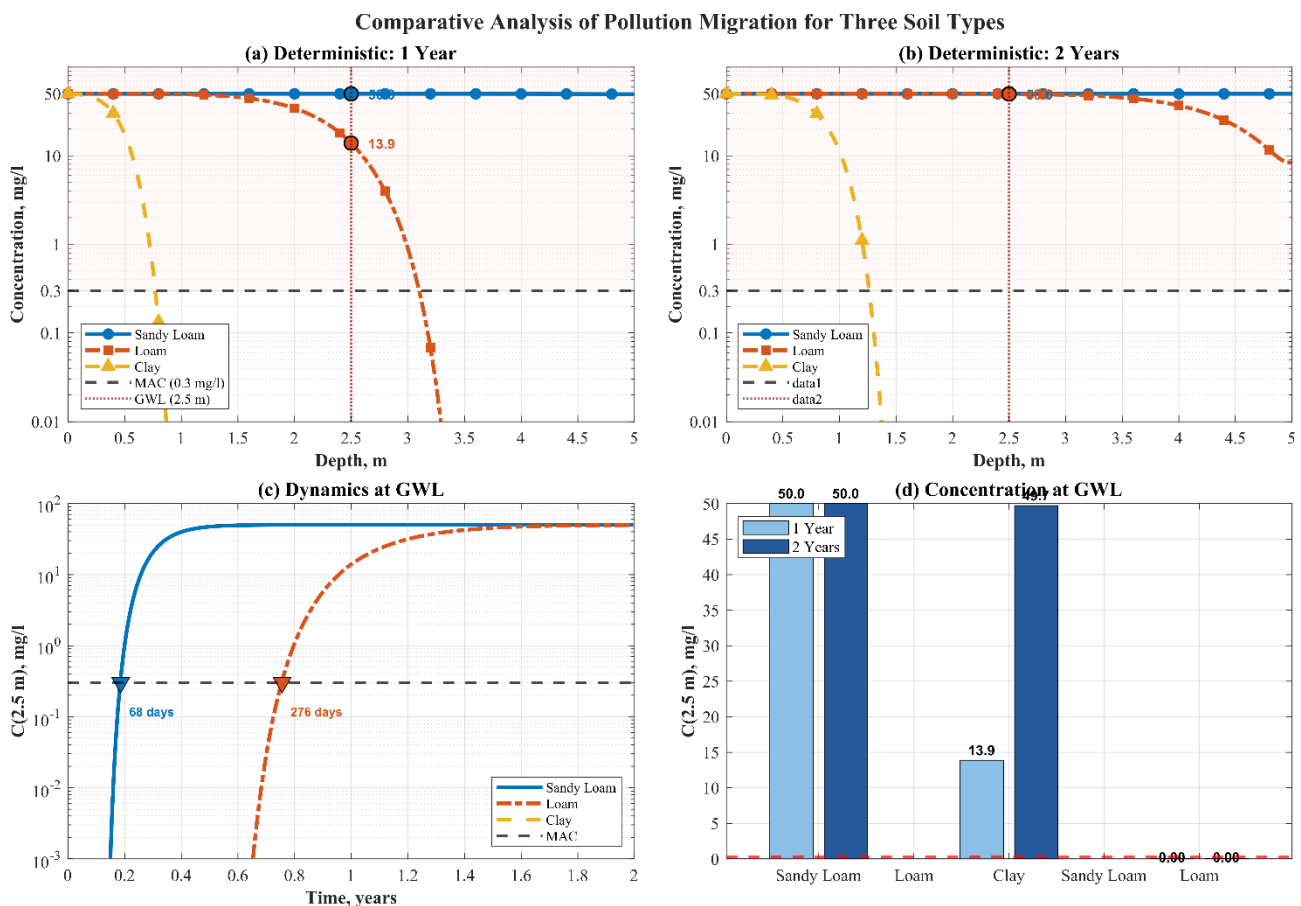


Fig. 3. Comparative analysis of dam migration across three soil types

The integration of the probabilistic approach allowed us to quantify the uncertainty of the forecast, which traditional deterministic models cannot do. The width of the 90% confidence interval for the concentration at a depth of 2.5 m after 1 year is 0.08–0.48 mg/l, which reflects the real variability of soil parameters and emphasizes the need for a probabilistic approach for reliable risk assessment. The verification results showed a relative error of 4.4% for laboratory experiments and 8.7% for field observations, which

confirms the adequacy of the developed model. This is due to the use of the Freundlich isotherm, which correctly describes the nonlinear sorption of aromatic hydrocarbons in soils. The nonlinearity of the process is explained by the heterogeneity of the sorption centers of soil organic matter: at low concentrations, high-energy centers are filled, and with increasing concentration, less energetically favorable ones are activated, which determines the concentration dependence of the distribution coefficient.

Parametric analysis showed that an increase in the Freundlich coefficient significantly slows down the migration of the pollution front, since a higher content of organic matter enhances the sorption and retention of hydrocarbons in the soil. A critical value of the nonlinearity index of about 0.75 was also established, below which the concentration profile acquires an asymmetric shape. The influence of hydraulic parameters is explained by the relationship between advection and dispersion: for characteristic values of the Peclet number, advection determines the transport range, and dispersion forms the width of the pollution front.

Probabilistic analysis showed that the median concentration is lower than the maximum permissible concentration, but the upper percentiles exceed it, which is explained by the lognormal distribution of soil hydraulic conductivity. The negative correlation between the sorption coefficient and the concentration at depth confirms the important role of sorption processes in groundwater protection. Comparison with traditional models showed a reduction in error by 23–34% due to the consideration of nonlinear sorption and the stochastic nature of the parameters. The proposed methodology combines a physical model of pollutant transport with a probabilistic risk assessment, which allows taking into account the uncertainty of the parameters and determining zones of increased probability of exceeding the maximum permissible concentrations. Unlike empirical approaches, the model is based on physically based equations of advection, dispersion and sorption, which ensures the interpretability of the results and the possibility of forecasting under different conditions. The use of the Monte Carlo method allows for a more complete account of the uncertainty of the parameters compared to linear statistical methods.

The main limitation of the model is its one-dimensional formulation, which does not take into account the complex spatial structure of the filtration flow. In addition, the model does not take into account the processes of biodegradation, seasonal changes in hydrogeological conditions and the multiphase nature of hydrocarbon pollution, which may affect the accuracy of long-term forecasts.

Further development of the study is associated with the expansion of the model to a three-dimensional formulation, the inclusion of biodegradation kinetics, taking into account the non-stationary hydrogeological regime, the development of multiphase models for high concentrations, the use of Bayesian methods for updating forecasts and the integration of the model with geographic information systems for mapping ecological risk zones.

**Conclusions.** A mathematical model of hydrocarbon pollution transport in soil was developed based on the advection-dispersion equation, taking into account nonlinear sorption according to the Freundlich isotherm and spatial heterogeneity of parameters. The model takes into account the concentration-dependent delay factor and provides high prediction accuracy: the relative error is 4.4% for laboratory and 8.7% for field conditions, which is a better result compared to models with linear sorption.

A method for probabilistic assessment of environmental risks based on the Monte Carlo method, taking into account stochastic soil parameters, is proposed. It allows determining zones of probable exceedance of the MPC and showed that the risk of groundwater pollution is about 23% after a year and increases to 47% after two years.

The model was verified using experimental data, which confirmed its adequacy and high correlation between the calculated and observed concentrations.

A parametric analysis was performed, which showed that an increase in the Freundlich coefficient significantly slows down the migration of pollution. A critical value of the nonlinearity index of about 0.75 was established and the key role of the organic matter content in the retention of hydrocarbons in the soil was determined.

Practical recommendations were developed for determining monitoring zones and planning remedial measures. Based on the probability maps of exceeding the MPC, it was recommended to place monitoring wells at depths of 1.5–2.0 m in the area of possible spread of pollution.

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### АНОТАЦІЯ

**Мета.** Розробка математичної моделі для прогнозування поширення вуглеводневого забруднення в неоднорідному ґрунті з урахуванням нелінійної сорбції та ймовірнісної оцінки ризиків для визначення зон критичного забруднення підземних вод і оптимізації заходів ремедіації на трасах нафтопроводів.

**Методика.** Застосовано чисельні методи розв'язання рівняння адвекції-дисперсії з урахуванням нелінійної сорбції за ізотермою Фрейндліха та просторової гетерогенності ґрунту. Для обчислень використано метод скінченних різниць із неявною схемою Кранка-Ніколсона та ітераційний метод Ньютона-Рафсона у середовищі MATLAB. Оцінка ризиків базується на методі Монте-Карло ( $N = 10000$  реалізацій), що враховує стохастичну природу коефіцієнта фільтрації, параметрів сорбції та дисперсивності.

**Результати.** Отримані результати засвідчують високу точність розробленої моделі, яка забезпечує зменшення похибки прогнозування на 23–34% порівняно з традиційними підходами. Встановлено, що при типових параметрах фактор затримки складає  $R = 4,2$ , що уповільнює міграцію забруднення у 4,2 рази порівняно з потоком води.

**Наукова новизна.** У дослідженні вперше запропоновано підхід, що поєднує детерміністичне моделювання транспорту вуглеводнів із ймовірнісним аналізом невизначеностей вхідних параметрів. Встановлено критичний показник нелінійності сорбції  $n_{\text{крит}} \approx 0,75$ , нижче якого ігнорування нелінійності призводить до суттєвих помилок у прогнозуванні профілю концентрації. Доведено, що традиційний детерміністичний підхід занижує реальні ризики, не враховуючи 23% ймовірність перевищення ГДК через гетерогенність середовища.

**Практична значимість.** Запропонована методика дозволяє будувати динамічні карти ймовірності ризику для оперативного реагування на аварійні розливи нафти. Використання моделі забезпечує наукове обґрунтування обсягів ремедіаційних робіт та визначення зон пріоритетного екологічного моніторингу на нафтопроводах, що експлуатуються понад 30–50 років. Це сприяє підвищенню екологічної безпеки та мінімізації наслідків забруднення сільськогосподарських земель і водоносних горизонтів.

**Ключові слова:** поширення забруднення, математичне моделювання, ґрунтове середовище, оцінка ризиків, адвекція-дисперсія, сорбція вуглеводнів.

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