

Solving Groundwater Pollutant Transport Model by Physics-Informed Neural Networks

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Abstract. In response to the issue in traditional groundwater pollutant transport models where the convection velocity is treated as a constant, making it difficult to describe actual non-uniform transport processes, this paper establishes an improved diffusion-convection-reaction model that considers the convection velocity as a function of both time and space. Based on this governing equation, a Physics-Informed Neural Network (PINN) framework is constructed to solve the model. The partial differential equations and initial/boundary conditions are embedded into the network training process to solve for the spatiotemporal distribution of pollutant concentrations. The model is validated through vertical infiltration experiments in a soil column. The results show that the pollutant transport trends predicted by the model are in good agreement with the experimental observations, demonstrating the effectiveness of the proposed model and methodology.

Keywords: Groundwater pollution, Diffusion-convection-reaction model, Variable convection velocity, Physics-Informed Neural Network, Pollutant transport

1. Introduction and goal

With the rapid development of science and technology, the demand for rare earths is constantly increasing. Countries with rich rare earth resources exploit them in large quantities, and the heavy metals spread towards surroundings. The issue of groundwater and soil heavy metal pollution has become increasingly prominent. Heavy metals can accumulate through the food chain, posing long-term threats to both ecosystem stability and human health. Heavy metals and organic pollutants generated during mineral extraction and smelting processes often exist in complex forms. Their transport behavior is influenced by multiple factors, including rainfall infiltration, groundwater hydrodynamic conditions, and soil composition, resulting in significant uncertainty in the extent and intensity of pollution. Due to the heterogeneous structure and dynamic adsorption-desorption characteristics of natural porous media, traditional models have clear limitations in describing the retention and reaction pathways of heavy metals in complex pore structures. Therefore, there is an urgent need for more efficient and physically-constrained new modeling methods.

In recent years, scholars worldwide have conducted extensive research on groundwater pollution transport modeling and pollution source identification. Traditional physical models often rely on finite element methods and finite difference methods for forward simulations, but they are highly sensitive to parameter accuracy in inverse problems. Gorelick et al. [1] proposed a method

combining linear programming and solute transport modeling for pollution source identification in their paper *Identifying Sources of Groundwater Pollution: An Optimization Approach*. This method is theoretically feasible, but errors can be significantly amplified when there is uncertainty in hydrogeological parameters. To enhance the solving capability, researchers have gradually introduced evolutionary optimization concepts. Aral et al. [2] coupled genetic algorithms with simulation models to identify multiple pollution sources, improving global search capability. Later, Zhang et al. [3] optimized monitoring well placement schemes based on Bayesian theory and information entropy, improving the reliability of pollution source parameter identification. Although these methods alleviate the problem of traditional optimization methods getting stuck in local optima to some extent, they still rely on high-precision physical parameters and require considerable computational resources.

In the field of dynamic data fusion, data assimilation techniques have gradually been applied to groundwater pollution prediction. To address the particle degradation issue commonly encountered in traditional particle filtering, Yin et al. [4] proposed an intelligent enhanced particle filtering method, which improves the particle resampling process by introducing intelligent optimization strategies. Wang et al. [5] combined ensemble Kalman filtering with optimization algorithms to construct a hybrid data assimilation framework, enhancing the solving capability for high-dimensional nonlinear problems. However, these methods are still built upon existing physical model structures, making it difficult to fundamentally improve the model's ability to represent complex coupled processes.

With the development of artificial intelligence technologies, deep neural networks have gradually been applied to groundwater pollution modeling. The deep residual network proposed by He et al. [6] provided an efficient function approximation tool for complex nonlinear systems, and structures such as ED-LSTM have also been used for time series prediction of pollution processes [7]. In addition, Tompson et al. [8] applied convolutional neural networks to solve geophysical problems, while Gao et al. [9] conducted a systematic review of the intelligent advancements in groundwater numerical simulations. These data-driven models have advantages in computational efficiency and nonlinear fitting, but due to the lack of explicit physical constraints from the governing equations, they may produce results that violate basic principles such as mass conservation under conditions of boundary changes or data scarcity, limiting their reliable application in practical engineering.

To compensate for the lack of physical consistency in pure data-driven models, Raissi et al. [10] first proposed PINN in 2017 and further refined the framework in 2019 [11]. By embedding partial differential equations into the loss function, this approach enables a deep integration of physical laws and the neural network training process. Subsequently, Goswami et al. [12] enhanced the prediction accuracy of PINN under unknown boundary conditions by incorporating transfer learning strategies, and Lauzon [13] built a groundwater flow surrogate model based on the U-Net architecture, improving the model's adaptability to complex boundary conditions. These studies demonstrate the significant potential of PINN in addressing groundwater pollution problems where physical information is known but observational data are limited.

However, existing studies are mostly based on steady-state or simplified flow field assumptions, and the description of the temporal and spatial variations of groundwater convection velocity remains insufficient. To address this issue, this paper introduces a spatiotemporal varying convection velocity term within the framework of the diffusion-convection-reaction equation, constructing a new control model for heavy metal transport in groundwater. A solution method based on PINN will integrate physical constraints and data collaboration. The model will be validated through vertical

infiltration experiments, and the results can show whether this method can effectively characterize the dynamic transport process of heavy metals in porous media.

2. Variable convection pollutant transport model

In traditional models, the convection velocity is typically assumed to be constant. However, during the vertical migration of groundwater pollutants, the pollutants sink under the influence of gravity and encounter resistance due to interactions with the sandy soil medium. This resistance is inversely proportional to the permeability and can be assumed to be directly proportional to the migration velocity. Therefore, in this study, the convection velocity is treated as a variable, with the assumption that it changes as a function of the migration location.

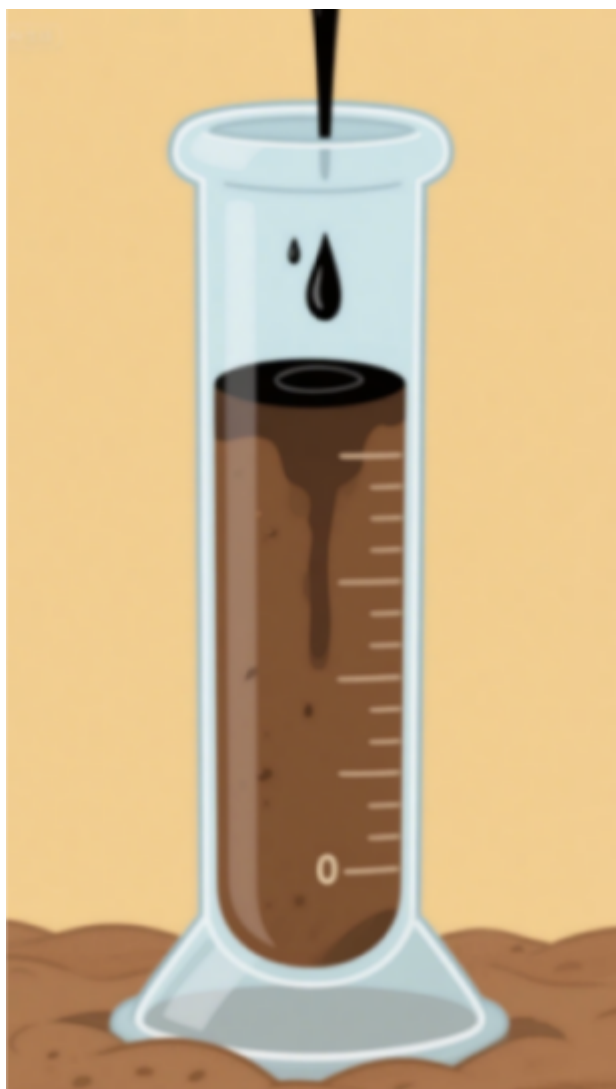


Figure 1. One-dimensional model of downward vertical migration

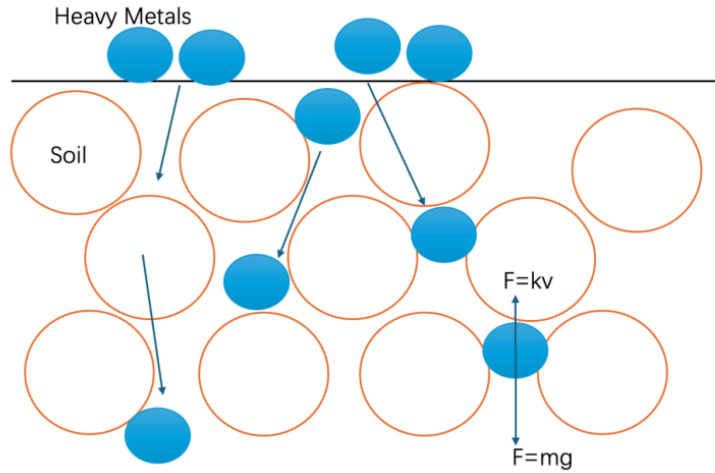


Figure 2. Enlarged model of heavy metal downward migration forces

As the convection velocity increases, the resistance experienced by the pollutants also increases. Under the condition, transport of pollutants can be described by Equation 1:

$$\frac{\partial C}{\partial t} - D \frac{\partial^2 C}{\partial x^2} + v \frac{\partial C}{\partial x} - C = 0 \quad (1)$$

Derived from Newton's second law of motion:

$$mg - kv = m \frac{\partial^2 x}{\partial t^2} \quad (2)$$

the expression for the pollutant position x and velocity v can be obtained as Equation 3:

$$x = -\frac{m}{k} \left[\ln\left(g - \frac{vk}{m}\right)v - \left(g - \frac{vk}{m}\right)\left(\ln\left(g - \frac{vk}{m}\right) - 1\right) \right] \quad (3)$$

Where v , m , k and g represent the convection velocity, mass, resistance, and gravitational acceleration of the pollutant, respectively. Since Equation (3) is a transcendental equation and cannot be solved analytically, a graphical fitting method is used to obtain the relationship between convection velocity and resistance, as shown in the following equation 4:

$$v = -0.1649x + 1.853 \quad (4)$$

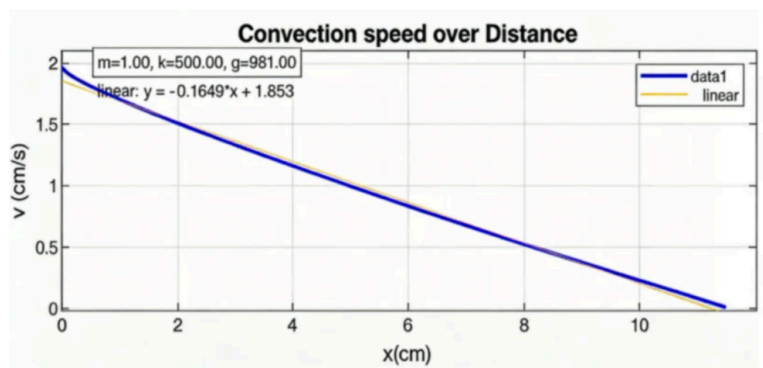


Figure 3. Relationship between advection velocity and position variable

By substituting Equation 4 into Equation 1, the new convection-diffusion-reaction model can be obtained as Equation 5:

$$\frac{\partial C}{\partial t} - D \frac{\partial^2 C}{\partial x^2} + (1.853 - 0.1649x) \frac{\partial C}{\partial x} - C = 0 \quad (5)$$

3. Solution method based on Physics-Informed Neural Networks

PINN differs from traditional neural networks in that their advantage lies in incorporating prior physical knowledge of the problem in the form of differential equations into the network training. Introducing physical information not only improves prediction accuracy under conditions of limited measurement data but also regularizes noisy measurement data, allowing the network to learn the true underlying signal of the system rather than the noise. Assuming that the measurement data θ_{meas} contains noise, the existing data is used to predict the future state of the system θ_{pred} . The feedforward artificial neural network is trained by minimizing the mean square error between the predicted values and the measured values to predict the unobserved values.

The loss function of PINN typically consists of three components: the physics-informed loss $L_{Physics}$, which quantifies whether the network's predictions satisfy the differential equations; the initial and boundary condition loss L_{Conds} ; and the optional measurement data loss L_{Data} . Among these, the physics-informed loss term calculates the residual of the differential equations in the domain using automatic differentiation or numerical differentiation techniques, and can be considered an unsupervised loss, allowing the network to be trained at unobserved points.

Since its introduction in 2017, PINN has given rise to several variants, including: Bayesian PINN (BPINN), used for uncertainty quantification; Variational PINN (VPINN), which incorporates the weak form of partial differential equations into the loss function; and First-Order Formulation PINN (FO PINN), which is faster and more accurate in solving higher-order PDEs.

As shown in Figure 4, this study uses MATLAB and the Deep Learning Toolbox to implement PINN training and testing. This includes constructing or importing the neural network architecture, defining the physics-informed loss function using automatic differentiation, training with the ADAM gradient optimization algorithm, and presenting the results through MATLAB visualization tools.

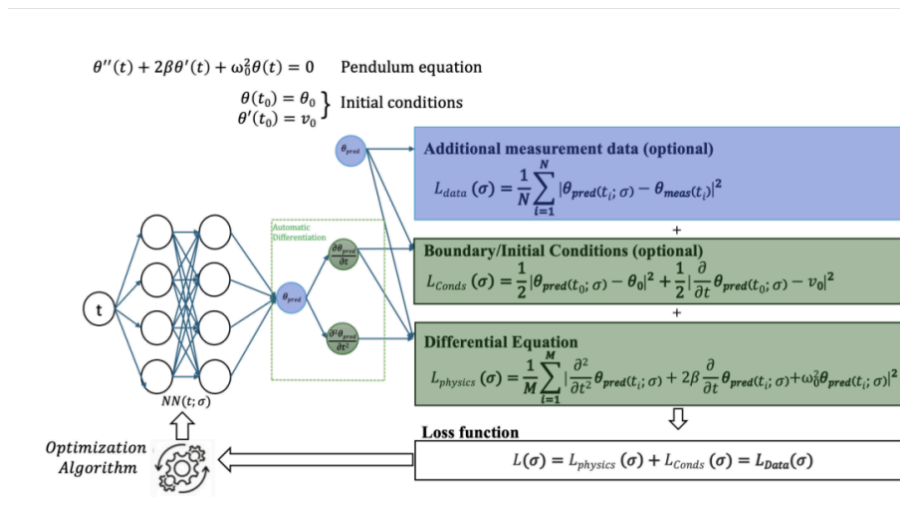


Figure 4. Schematic of the PINN for solving diffusion-convection differential equations [14]

Based on the principles of PINN, this study solves the newly derived model. The solution results are shown in Figure 5 and Figure 6, where the corresponding diffusion coefficients D are 0.001, 0.01, and 0.1 cm^2/s , respectively.

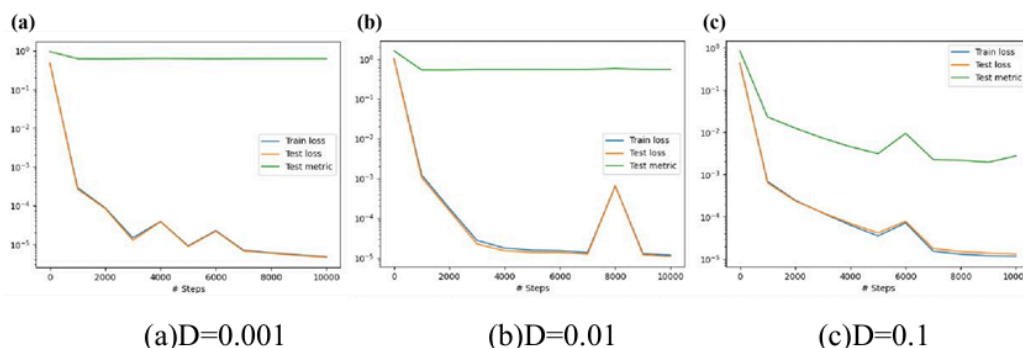


Figure 5. Variation of the loss function with iteration steps during PINN training

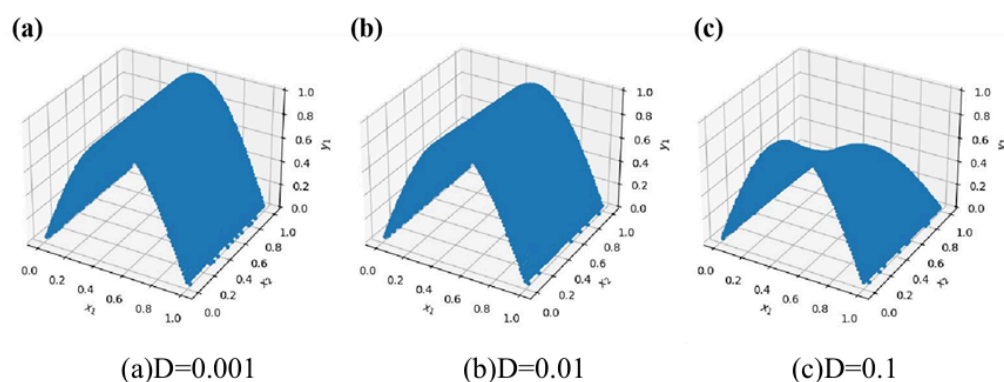


Figure 6. Variation of pollutant concentration with spatial location and time calculated by the PINN model

4. Experimental design and analysis

To validate the derived physical model, this study selects potassium permanganate and lanthanum oxide solution as heavy metal surrogates to study their migration behavior in different soil media. The experiment is divided into two parts: first, examining the variation of pollutant diffusion distance with time by using sandy soil, loam soil, clay soil, and mixed soil as the media; and second, investigating the effect of different resistance on the diffusion velocity using also sandy soil, loam soil, and clay soil as the media. After adding the pollutant solution to the soil, the diffusion of the solution is observed, and the diffusion distance is recorded to obtain pollutant migration data, which is then compared with the results from the PINN solution for analysis. Traditional machine-learning methods are also applied to verify if PINN model are more accurate and efficient.

4.1. Pollutant diffusion distance-time experiment

To study the variation of diffusion velocity of pollutants over time, this study conducted a diffusion distance-time experiment. Potassium permanganate and lanthanum oxide were added to water to form solution with 10% concentration. Soils (sandy, loam, clay, and mixed soil) are kept at same

initial height and the pollutant solution was applied to the surface of each medium. The diffusion distance downward over time was recorded to obtain pollutant migration data. Figure 7 shows the diffusion process of potassium permanganate in different soil media, while Figure 8 displays the diffusion of lanthanum oxide in each soil.



Figure 7. Diffusion experiment of potassium permanganate in different soil media



Figure 8. Diffusion experiment of lanthanum oxide in different soil media

4.2. Pollutant diffusion distance-media experiment

To study the effect of different resistance on pollutant diffusion velocity, this study conducted a diffusion distance-media experiment. Potassium permanganate and lanthanum oxide solutions were used as pollutants, and sandy soil, loam, and clay were used as media. The vertical diffusion height of the pollutant solution was observed in a graduated cylinder, varying with the type of medium. During the experiment, equal volumes of pollutant solution were added to different media, and the

diffusion height of the pollutant in each medium was recorded to obtain migration data under different resistance environments. The experimental results indicate that the pollutants diffuse fastest in sandy soil, followed by loam, and slowest in clay, demonstrating the significant regulatory effect of the medium on the diffusion process.

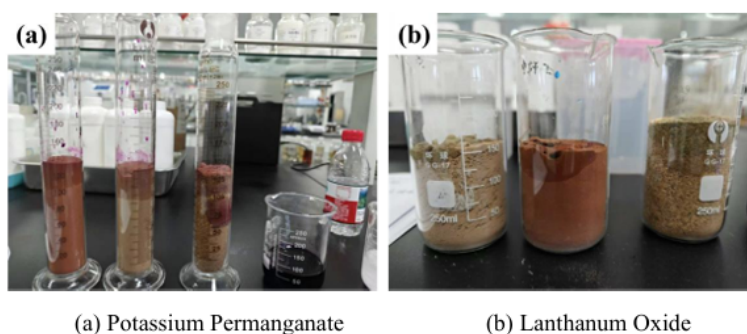


Figure 9. Diffusion experiment of potassium permanganate and lanthanum oxide in different media(sandy soil, loam, and clay)

5. Results and model validation

To further analyze the diffusion behavior of pollutants in different media and validate the derived model, Tables 1 and 2 respectively list the data on pollutant diffusion distances with time and changes in media, as measured in the experiments in Chapter 4.

Table 1. Pollutant diffusion distance-time experiment results

Experiment	Vertical Diffusion Distance				
	1 minute	2 minute	5 minute	10 minute	30 minute
Potassium Permanganate Diffusion Distance-Time Experiment in Sandy Soil	4.28cm	5.17cm	5.62cm	5.82cm	6.15cm
Potassium Permanganate Diffusion Distance-Time Experiment in Loam Soil	2.04cm	2.44cm	2.72cm	2.88cm	3.05cm
Potassium Permanganate Diffusion Distance-Time Experiment in Clay Soil	1.75cm	2.25cm	2.50cm	2.62cm	2.68cm
Potassium Permanganate Diffusion Distance-Time Experiment in Mixed Soil	2.42cm	3.35cm	3.82cm	3.98cm	4.06cm
Lanthanum Oxide Diffusion Distance-Time Experiment in Sandy Soil	4.51cm	5.45cm	5.93cm	6.14cm	6.48cm
Lanthanum Oxide Diffusion Distance-Time Experiment in Loam Soil	2.18cm	2.61cm	2.90cm	3.07cm	3.25cm
Lanthanum Oxide Diffusion Distance-Time Experiment in Clay Soil	1.90cm	2.44cm	2.71cm	2.84cm	2.91cm
Lanthanum Oxide Diffusion Distance-Time Experiment in Mixed Soil	2.78cm	3.51cm	3.84cm	4.01cm	4.13cm

The pollutant diffusion velocity over time was plotted based on the experimental data in the tables, as shown in Figure 10(a) and 10(b). The graph follows an inverse function trend where diffusion velocity of contaminants are highest at first, then gradually slows down as time goes on/as diffusion distance increases, indicating that the diffusion velocity is spatiotemporal. Both potassium

permanganate and lanthanum oxide experiments reveal the same trend curve where velocity's decreasing rate is highest at first, then gradually slowing down in rate of decrease.

By substituting the pollutant diffusion parameters obtained from the experiments in Chapter 4 into the convection-diffusion equation established in this study, numerical solutions were obtained using MATLAB, resulting in the pollutant migration velocity change curve at different times, as shown in Figure 10(c). The results show that the simulated curve is in high agreement with the diffusion velocity trends measured in the experiments, indicating that the derived model can accurately describe the migration behavior of pollutants in different media, providing strong evidence for the model's validity and applicability.

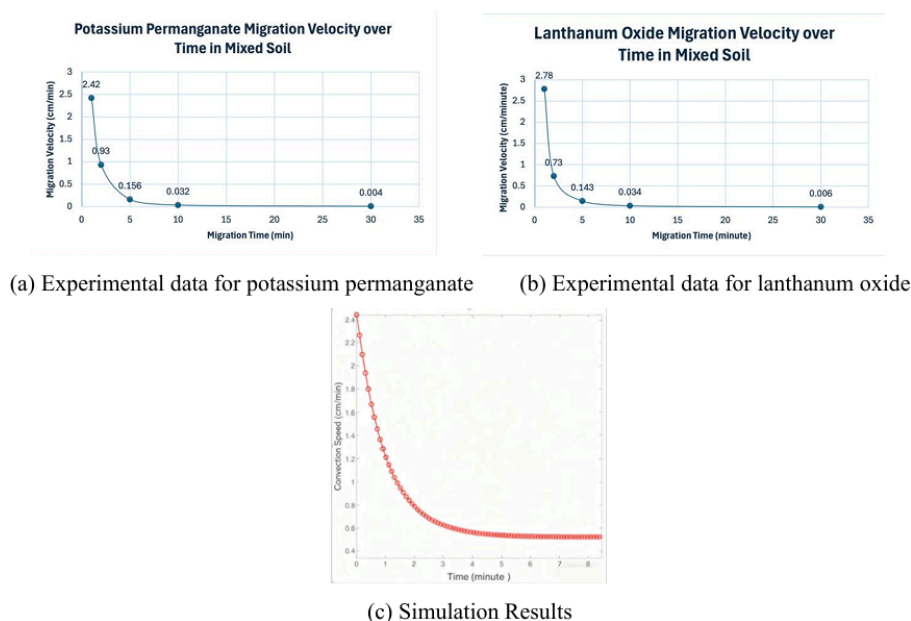


Figure 10. Variation curve of migration velocity with time

Table 2. Pollutant diffusion distance-media experiment results

Experiment	Vertical Diffusion Distance of Contaminants in Sandy Soil	Vertical Diffusion Distance of Contaminants in Loam	Vertical Diffusion Distance of Contaminants in Clay	Diffusion Time
Potassium Permanganate Diffusion Distance-Medium Experiment	4.8cm	2.2cm	2.0cm	1min20s
	5.6cm	2.6cm	2.24cm	3min
	5.8cm	2.8cm	2.6cm	10min
	6.2cm	3.0cm	2.72cm	30min
Lanthanum Oxide Diffusion Distance-Medium Experiment	5.1cm	2.4cm	2.1cm	1min20s
	6.6cm	2.7cm	2.25cm	3min
	6.9cm	2.92cm	2.6cm	10min
	7.1cm	3.2cm	2.71cm	30min

For the soil media used in the experiment, sandy soil, loam, and clay have different pore structures and physical properties, with diffusion coefficients of $10^{-2}\text{cm}^2/\text{s}$, $10^{-3}\text{cm}^2/\text{s}$ and $10^{-5}\text{cm}^2/\text{s}$ respectively. Higher diffusion coefficients results in lower resistance, meaning that acceleration by

gravity will have larger impact. This explains why all solutions moves fastest in sandy soil, slower in loam soil, slowest in clay soil (as shown in Table 2), demonstrating the significant regulatory effect of the medium on the diffusion process.

The experimental results, shown in Figure 11, indicate that the migration velocity of lanthanum oxide is generally higher than that of potassium permanganate, and this difference gradually diminishes as the soil diffusion coefficient decreases. This pattern can be explained by the derived convection-diffusion model: during the vertical migration of pollutants, their resistance is proportional to the migration velocity. Potassium permanganate and lanthanum oxide have different molecular weights, densities, and molecular volumes. Potassium permanganate has a larger molecular volume, which leads to greater resistance under the same soil conditions, and the diffusion velocity of lanthanum oxide is slightly higher than that of potassium permanganate. Therefore, when solving the diffusion process of lanthanum oxide with PINN, the diffusion coefficient was correspondingly adjusted to be higher than that of potassium permanganate.

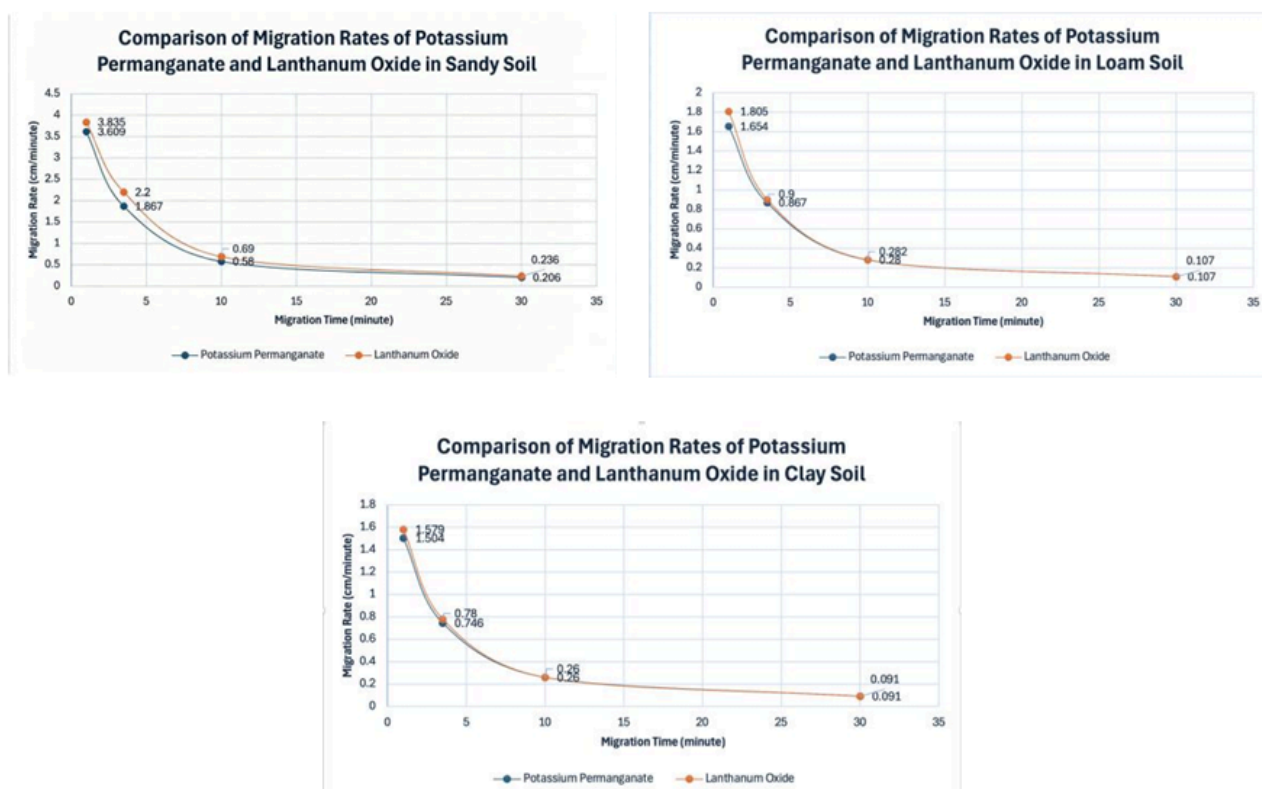
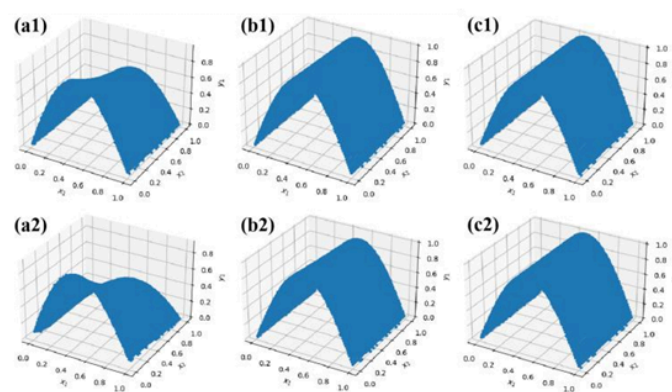


Figure 11. Comparison of migration velocities of potassium permanganate and lanthanum oxide in different media

The diffusion velocities in different soils were numerically solved using the PINN, and the simulation results were compared with experimental data, as shown in Figure 12. The results indicate that, in sandy soil, the migration velocity of lanthanum oxide is significantly higher than that of potassium permanganate; in loam soil and clay soil, the migration velocities of both pollutants are similar. This trend is in strong agreement with the experimental results, effectively validating the reliability of the model and the PINN solution method.



(a1) Potassium Permanganate - Sandy Soil; (a2) Lanthanum Oxide - Sandy Soil;
(b1) Potassium Permanganate - Loam; (b2) Lanthanum Oxide - Loam;
(c1) Potassium Permanganate - Clay; (c2) Lanthanum Oxide - Clay

Figure 12. Simulation results of longitudinal diffusion and migration velocity of potassium permanganate and lanthanum oxide solutions in different soil media with time

Figure 13 illustrates the migration velocity of KMnO_4 , comparing experimental values with PINN simulation results, as well as prediction errors of traditional machine learning methods. The PINN simulation curve is highly consistent with experimental trends.

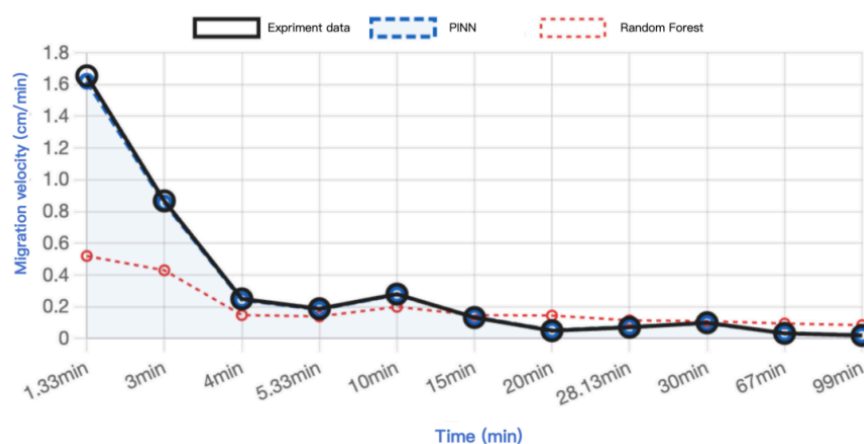


Figure 13. Migration velocity prediction comparison between PINN and traditional machine learning method

Compared with traditional machine-learning methods, PINN demonstrates a stronger ability to capture the dynamic behavior of groundwater pollutants, especially being adept at adapting to complex boundaries and initial conditions.

6. Conclusion

The migration behavior of heavy metal pollutants in groundwater and soil is an important research direction in environmental science. Previous models often used constant convection velocities, which could not accurately describe the spatiotemporal variation of pollutants in different soil media. To address this issue, this study proposes a diffusion-convection-reaction equation and solves

it using PINN to achieve spatiotemporal predictions of pollutant concentrations. The main conclusions are as follows:

1. Model Development and Theoretical Analysis: A one-dimensional diffusion-convection-reaction equation under semi-infinite boundary conditions was derived, considering convection velocity as a time and location-dependent variable function. The model can describe the concentration variation of potassium permanganate and lanthanum oxide in sandy soil, loam, clay, and mixed soil, providing a theoretical foundation for groundwater heavy metal pollution migration modeling.

2. Experimental Design and Validation: A vertical infiltration experimental system was established, using potassium permanganate and lanthanum oxide solutions, combined with sandy soil, loam, clay, and mixed soil for diffusion distance-time and diffusion distance-media experiments. The experimental results show that the diffusion velocity of lanthanum oxide is generally higher than that of potassium permanganate, and as the soil diffusion coefficient decreases, this difference gradually diminishes, validating the model's sensitivity to soil media and diffusion behavior.

3. Method Innovation and Performance: Using PINN for training and solving the diffusion-convection-reaction equation allows for accurate prediction of pollutant concentrations with limited experimental data while maintaining physical consistency. The numerical simulation results are in high agreement with the experimental trends, validating the reliability of the model and demonstrating the advantages of PINN in handling boundary conditions and capturing the dynamic changes of pollutants.

References

- [1] Gorelick, S. M., Evans, B., & Remson, I. (1983). Identifying sources of groundwater pollution: An optimization approach. *Water Resources Research*, 19(3), 779-790.
- [2] Aral, M. M., Guan, J. B., & Maslia, M. L. (2001). Identification of contaminant source location and release history in aquifers. *Journal of Hydrologic Engineering*, 6(3), 225-234.
- [3] Zhang, S. S., Liu, H. H., Qiang, J., Gao, H. Z., Galar, D., & Lin, J. (2019). Optimization of well position and sampling frequency for groundwater monitoring and inverse identification of contamination source conditions using Bayes' theorem. *Computer Modeling in Engineering & Sciences*, 119(2), 373-394.
- [4] Yin, S., & Zhu, X. P. (2015). Intelligent particle filter and its application to fault detection of nonlinear system. *IEEE Transactions on Industrial Electronics*, 62(6), 3852-3861.
- [5] Wang, Z. B., Lu, W. X., Chang, Z. B., & Wang, H. (2022). Simultaneous identification of groundwater contaminant source and simulation model parameters based on an ensemble Kalman filter – Adaptive step length ant colony optimization algorithm. *Journal of Hydrology*, 605.
- [6] He, K. M., Zhang, X. Y., Ren, S. Q., & Sun, J. (2016). Deep residual learning for image recognition. In 2016 IEEE Conference on Computer Vision and Pattern Recognition (CVPR) (pp. 770-778). Seattle, WA.
- [7] Anshuman, A., & Eldho, T. I. (2023). A parallel workflow framework using encoder-decoder LSTMs for uncertainty quantification in contaminant source identification in groundwater. *Journal of Hydrology*, 619.
- [8] Tompson, J., Schlachter, K., Sprechmann, P., & Perlin, K. (2017). Accelerating Eulerian fluid simulation with convolutional networks. International Conference on Learning Representations. In 34th International Conference on Machine Learning. Sydney, Australia.
- [9] Gao, Y. Y., Pu, Q., & Wang, Z. (2025). A review of numerical simulation techniques and applications in groundwater. *Resources, Environment and Engineering*, 39(2), 197-205.
- [10] Raissi, M., Perdikaris, P., & Karniadakis, G. E. (2017). Physics informed deep learning (part I): Data-driven solutions of nonlinear partial differential equations. *arXiv preprint arXiv: 1711.10561*.
- [11] Raissi, M., Perdikaris, P., & Karniadakis, G. E. (2019). Physics-informed neural networks: A deep learning framework for solving forward and inverse problems involving nonlinear partial differential equations. *Journal of Computational Physics*, 378, 686-707.

- [12] Goswami, S., Anitescu, C., Chakraborty, S., & Rabczuk, T. (2020). Transfer learning enhanced physics informed neural network for phase-field modeling of fracture. *Theoretical and Applied Fracture Mechanics*, 106.
- [13] Lauzon, D. (2024). A U-Net architecture as a surrogate model combined with a geostatistical spectral algorithm for transient groundwater flow inverse problems. *Advances in Water Resources*, 189.
- [14] MathWorks. (n.d.). What are Physics-informed neural networks (PINNs)? Retrieved from <https://ww2.mathworks.cn/en/discovery/physics-informed-neural-networks.html>