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Heavy Metals Transport in Soil With Exponential Decay Source

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Abstract Heavy metal pollution is a global environmental concern due to its extreme hazards and complicated challenges in removing it from soil. The behavior of heavy metal migration in soil can be aptly depicted using a mathematical model, specifically the advection-diffusion equation (ADE). This research considers the scenario where a pollutant is injected in an exponentially decaying manner within a fixed time interval $0 < t \leq t_0$, and ceases at $t > t_0$. The solutions are obtained by taking Laplace transform, and the propagation behavior of the pollutant for various exponential decay coefficients are studied. The results show that for $0 < t \leq t_0$, heavy metal concentrations experience an initial rapid rise during injection, peaking at the boundary, followed by dispersion to surrounding areas. Upon injection cessation, a minor concentration rebound occurs due to residual effects, followed by gradual attenuation. The results provide insight for environmental management and pollution control strategies.

Keywords Heavy metal; two-dimensional; exponential decay; analytical solution; Laplace transform.

Mathematics Subject Classification 76R50, 76S05, 60J26, 74N25, 92E20.

1 Introduction

Heavy metal pollution has been confirmed as a type of contamination that is harmful to human health and is difficult to remove and remediate in soil [1–4]. For decades, environmental researchers [5–7] have mainly focused on how to eradicate its persistence in the soil layer, but have had limited success. Subsequently, some researches discovered that studying its transport behavior in the soil layer has aided environmental scholars in more efficiently removing it. Initially, one-dimensional analytical and numerical solutions have demonstrated their capabilities in this regard [8–13]. For example, Kumar et al. [8] and Jaiswal et al. [9] presented a one-dimensional analytical solution with Laplace transform by considering Dirichlet and Neumann boundary conditions, which mainly discussed spatially and temporally dependent coefficients respectively, both without adsorption. The Laplace transform in solving one-dimensional solute transport was also presented in Yadav et al. [13], which considered continuous periodic point source injected through the left boundary. From [14–17], two-dimensional should be more feasible to interpret the behavior of heavy metal transport in soil. For instance, Massabo et al. [15] solved the 2-D analytical solution with Bessel function based on the different initial and boundary conditions which is a chemical decay or adsorption-like reaction, while Tsedendorj et al. [16] tackled the two-dimensional problem of advective diffusion in an infinite domain by considering Neumann boundary condition. Zhou-Hu et al. [17] presented a 2-D analytical computational method for analyzing pollutant mixing zones and iso-concentration lines in wide straight rivers under the constant continuous point source condition where a continuous point source is usually a simplified model of the actual situation. In a real environment, the release of many substances is not completely continuous and there may be fluctuations or erratic releases over a period of time [18]. Batu et al. [19, 20] used Laplace transform to solve the multiple source problem in a two-dimensional model when boundaries are Dirichlet and Cauchy conditions, respectively.

In this research, the boundary condition is a very important factor to describe the transport behavior of heavy metal in soil. Effective boundary conditions accurately describe both the mathematical model and the real-world significance of pollution scenarios. Additionally, they enable better prediction of contaminant migration behavior in soil, Ideally, this should represent the real situation occurring at the source of pollution. Unfortunately, most researches used as constant [21,22]. In reality, pollutants can be introduced into the soil through various pathways, which include industrial discharges, agricultural practices, accidental spills, and more, where these introductions are not always constant but can vary over time.

Using an exponential decay function as a boundary condition to describe the transport behavior of heavy metal has been shown as an effective approach [23, 24]. This method is particularly useful when studying the transport of pollutants in soil. The exponential decay function can effectively represent the gradual decrease of pollutant concentration in soil over time.

Therefore, this research primarily focuses on investigating the migration behavior of two-dimensional heavy metal in soil. The study explores the scenario of exponential decay injection as the boundary condition, simulating a realistic pollution source. To tackle this problem, the Laplace method is employed to derive an analytical solution, offering valuable insights into the dispersion and distribution patterns of heavy metal in the soil environment. The obtained results not only enhance our understanding of the transport mechanisms but also contribute to the development of effective strategies for mitigating heavy metal contamination in soil systems, hence providing valuable scientific knowledge and practical implications for environmental management and remediation efforts.

2 Governing equation

The governing equation in this research is the equation that governs solute transport in soil, which considers the porous medium to be saturated, homogeneous, and isotropic, and the domain of study is a semi-infinite porous medium with two-dimensional convection of pollutants. Extensive experiments and on-site inspections indicate that the adsorption term of the soil particles includes not only adsorption but also desorption. The adsorption term is linear nonequilibrium adsorption, with desorption effects primarily occurring along the $x-$axis [25, 26]. They are assumed to disperse at different rates in both longitudinal and transverse directions. The two-dimensional ADE describing the heavy metal transport in porous media domain, subjected to adsorption and desorption can be written as

$$R\frac{\partial C}{\partial t} = D_x\frac{\partial^2 C}{\partial x^2} + D_y\frac{\partial^2 C}{\partial y^2} - (u - k_x)\frac{\partial C}{\partial x} - v\frac{\partial C}{\partial y} - kC, \tag{1}$$

where R is the retardation factor, C $[ML^{-3}]$ is the concentration of heavy metal ions in seepage, u $[LT^{-1}]$ is the uniform seepage velocity along x or longitudinal direction, v $[LT^{-1}]$ is the uniform seepage velocity along y or transverse direction, t $[T]$ is time, x, y $[L]$ are the migration distance of heavy metal particles, k $[T^{-1}]$ is adsorption coefficient and k_x $[T^{-1}]$ is the desorption coefficients, while D_x $[L^2T^{-1}]$ and D_y $[L^2T^{-1}]$ are dispersion coefficient along longitudinal or transverse direction, respectively.

Furthermore, the diffusion coefficient is considered to be geometrically proportional to the seepage velocity [22, 27, 28], written as

$$D_x = a(u - k_x) \quad \text{and} \quad D_y = bv, \tag{2}$$

where a $[L]$ and b $[L]$ are the coefficients that depend upon pore geometry and average pore size diameter of the porous media.

Initially, there is C_i concentration in the domain. While at the source point, heavy metal contaminants are given in the form of exponential decay until a specific time period t_0, and the injection is terminated when $t > t_0$. Therefore, the initial and boundary conditions can be written as

$$C(x, y, 0) = C_i; \quad 0 \le x < +\infty, \quad 0 \le y < +\infty, \tag{3}$$

$$C(0, 0, t) = \begin{cases} C_0 e^{-\alpha t}, \ 0 < t \le t_0 \\ 0, \ t > t_0 \end{cases} \tag{4}$$

and

$$\frac{\partial C}{\partial x} = 0, \quad \frac{\partial C}{\partial y} = 0, t \ge 0 \quad x \to \infty, y \to \infty, \tag{5}$$

where α is the attenuation coefficient of injection concentration and C_i is the initial concentration of injected heavy metal contaminants. Boundary condition Equation (5) implies that there is no solute flux at the far ends of the medium in both directions. In order to solve Equation (1), introduce a new space variable

$$z = x + y\sqrt{\frac{D_y}{D_x}}. \tag{6}$$

Substituting Equation (2) and Equation (6) into Equation (1) yields

$$R\frac{\partial C}{\partial t} = D\frac{\partial^2 C}{\partial z^2} - U\frac{\partial C}{\partial z} - kC, \tag{7}$$

where,

$$D = D_x(1 + \frac{D_y^2}{D_x^2}), \quad \text{and} \quad U = (u - k_x) + v\sqrt{\frac{bv}{a(u - k_x)}}. \tag{8}$$

By using the same new space variable in Equation (1), the corresponding initial and boundary conditions now become

$$C(z,0) = C_i; 0 \leq z < +\infty, \tag{9}$$

$$C(0,t) = \begin{cases} C_0 e^{-\alpha t}, \ 0 < t \leq t_0 \\ 0, \ t > t_0 \end{cases} \tag{10}$$

and

$$\frac{\partial C(\infty,t)}{\partial z} = 0, \quad z \to \infty. \tag{11}$$

Taking Laplace transform to Equation (7), the general solution of this equation is given as

$$\bar{C}(z,t) = C_1 \exp(\frac{Uz}{2D} + \sqrt{\frac{U^2}{4D^2} + \frac{k+Rs}{D}}) + C_2 \exp(\frac{Uz}{2D} - \sqrt{\frac{U^2}{4D^2} + \frac{k+Rs}{D}}) + \frac{RC_i}{k+Rs}, \tag{12}$$

where C_1 and C_2 are arbitrary constants. By making use of the boundary conditions in Equations (10) and (11), it can be shown that $C_1 = 0$, $C_2 = \frac{C_0}{s+\alpha}\big(1 - \exp(-(s+\alpha)t_0)\big) - \frac{RC_i}{k+Rs}$. Therefore, the solution can be written in the form of

$$\bar{C} = I_1 + I_2 + I_3 + I_4, \tag{13}$$

where

$$I_1 = \frac{C_0 \exp(\frac{Uz}{2D})}{\alpha + s} \exp\left(-z\sqrt{\frac{s - (-\frac{k}{R} - \frac{U^2}{4DR})}{D/R}} \right), \tag{14}$$

$$I_2 = -\frac{C_0 \exp(\frac{Uz}{2D})}{\alpha + s} \exp(-(\alpha+s)t_0) \exp\left(-z\sqrt{\frac{s - (-\frac{k}{R} - \frac{U^2}{4DR})}{D/R}} \right), \tag{15}$$

$$I_3 = -\frac{RC_i \exp(\frac{Uz}{2D})}{k + Rs} \exp\left(-z\sqrt{\frac{s - (-\frac{k}{R} - \frac{U^2}{4DR})}{D/R}} \right) \tag{16}$$

and

$$I_4 = \frac{RC_i}{k+Rs}. \tag{17}$$

Taking inverse Laplace transform to I_1,I_2,I_3 and I_4, respectively, gives

$$\begin{aligned} L^{-1}(I_1) = \frac{C_0}{2} \exp(\frac{Uz}{2D} - \alpha t) \Big\{ &\exp\left(-z\sqrt{\frac{\frac{k}{R} + \frac{U^2}{4DR} - \alpha}{D/R}} \right) \mathrm{erfc}\big(\frac{z}{2\sqrt{Dt/R}} - \sqrt{(\frac{k}{R} + \frac{U^2}{4DR} - \alpha)t} \big) \\ &+ \exp\left(z\sqrt{\frac{\frac{k}{R} + \frac{U^2}{4DR} - \alpha}{D/R}} \right) \mathrm{erfc}\big(\frac{z}{2\sqrt{Dt/R}} + \sqrt{(\frac{k}{R} + \frac{U^2}{4DR} - \alpha)t} \big) \Big\}. \end{aligned} \tag{18}$$

Based on $L^{-1}(I_1)$ and $L^{-1}(I_2) = -e^{-\alpha t_0} L^{-1}(I_1(t-t_0))u(t-t_0)$,

$$L^{-1}(I_2) = -\frac{C_0}{2}\exp(\frac{Uz}{2D} - \alpha(t-t_0))\Big\{\exp\Big(-z\sqrt{\frac{\frac{k}{R}+\frac{U^2}{4DR}-\alpha}{D/R}}\Big) \mathrm{erfc}(\frac{z}{2\sqrt{D(t-t_0)/R}} - \sqrt{(\frac{k}{R}+\frac{U^2}{4DR}-\alpha)(t-t_0)}) + \exp\Big(z\sqrt{\frac{\frac{k}{R}+\frac{U^2}{4DR}-\alpha}{D/R}}\Big) \mathrm{erfc}(\frac{z}{2\sqrt{D(t-t_0)/R}} + \sqrt{(\frac{k}{R}+\frac{U^2}{4DR}-\alpha)(t-t_0)})\Big\}H(t-t_0) \tag{19}$$

where

$$H(t) = \begin{cases} 0, \ t<0 \\ \frac{1}{2}, \ t=0 \\ 1, \ t>0 \end{cases}, \tag{20}$$

$$L^{-1}(I_3) = -\frac{C_i}{2}\exp\big(\frac{Uz}{2D} - (\frac{kt}{R})\big)\Big\{\exp\big(-z\sqrt{\frac{U^2}{4D^2}}\big) \mathrm{erfc}(\frac{z}{2\sqrt{\frac{Dt}{R}}} - \sqrt{\frac{U^2t}{4DR}}) + \exp\big(z\sqrt{\frac{U^2}{4D^2}}\big)\mathrm{erfc}(\frac{z}{2\sqrt{\frac{Dt}{R}}} + \sqrt{\frac{U^2t}{4DR}})\Big\} \tag{21}$$

and

$$L^{-1}(I_4) = C_i \exp(-\frac{kt}{R}). \tag{22}$$

Finally, the desired analytical solution is

$$\begin{aligned} C(z,t) = {} & \frac{C_0}{2}\exp(\frac{Uz}{2D} - \alpha t)\Big\{\exp\Big(-z\sqrt{\frac{\frac{k}{R}+\frac{U^2}{4DR}-\alpha}{D/R}}\Big)\mathrm{erfc}(\frac{z}{2\sqrt{Dt/R}} - \sqrt{(\frac{k}{R}+\frac{U^2}{4DR}-\alpha)t}) \\ & + \exp\Big(z\sqrt{\frac{\frac{k}{R}+\frac{U^2}{4DR}-\alpha}{D/R}}\Big)\mathrm{erfc}(\frac{z}{2\sqrt{Dt/R}} + \sqrt{(\frac{k}{R}+\frac{U^2}{4DR}-\alpha)t})\Big\} - \frac{C_0}{2}\exp(\frac{Uz}{2D} - \alpha(t-t_0)) \\ & \Big\{\exp\Big(-z\sqrt{\frac{\frac{k}{R}+\frac{U^2}{4DR}-\alpha}{D/R}}\Big)\mathrm{erfc}(\frac{z}{2\sqrt{D(t-t_0)/R}} - \sqrt{(\frac{k}{R}+\frac{U^2}{4DR}-\alpha)(t-t_0)}) \\ & + \exp\Big(z\sqrt{\frac{\frac{k}{R}+\frac{U^2}{4DR}-\alpha}{D/R}}\Big)\mathrm{erfc}(\frac{z}{2\sqrt{D(t-t_0)/R}} + \sqrt{(\frac{k}{R}+\frac{U^2}{4DR}-\alpha)(t-t_0)})\Big\}H(t-t_0) \\ & - \frac{C_i}{2}\exp\big(\frac{Uz}{2D} - (\frac{kt}{R})\big)\Big\{\exp\big(-z\sqrt{\frac{U^2}{4D^2}}\big) \\ & \mathrm{erfc}(\frac{z}{2\sqrt{\frac{Dt}{R}}} - \sqrt{\frac{U^2t}{4DR}}) + \exp\big(z\sqrt{\frac{U^2}{4D^2}}\big)\mathrm{erfc}(\frac{z}{2\sqrt{\frac{Dt}{R}}} + \sqrt{\frac{U^2t}{4DR}})\Big\} + C_i\exp(-\frac{kt}{R}). \end{aligned} \tag{23}$$

3 Results and discussion

To visualize the concentration distribution of the derived analytical solution Equation (23) in a two-dimensional heavy metal migration in soil, we present a selected example with assigned numerical values for various variables. Specifically, we set $u = 0.36$ (m/d), $v = 0.036$ (m/d), $k = 0.01, k_x = 0.02$, $a = 0.1, b = 0.2, C_i = 0.05, C_0 = 1$, $D_x = 1.25$ (m^2/d), and $D_y = 0.125$ (m^2/d) [21, 22]. The lateral velocity dispersion component is considered as one-tenth of the longitudinal component [22]. However, due to the important role of velocity in predicting the temporal behavior of the heavy metal, the effects of different v are also investigated. The ratio of longitudinal to lateral dispersity in an aquifer is also an important factor influencing the contaminant's behavior [21].

Figure 1 compares the changes in heavy metal concentrations under the same attenuation factor at three time periods $t < t_0, t = t_0$, and $t > t_0$. For $t < t_0$ and $t = t_0$, the peak concentration of pollutants is observed close to the source due to the immediate influence of the release. However, as the injection is halted at $t > t_0$, a shift in the concentration distribution dynamics becomes evident. The cessation of injection marks the transition from a exponential decay dominated behavior to a diffusive-dominated regime. During this phase, no concentration is introduced at the source ($x = 0, y = 0$), causing the peak concentration at the source to diminish, while heavy metal currently in motion continue to disperse, resulting in a gradual accumulation of concentration in the surrounding areas located some distance away from the point source.

Figure 2 depicts the concentration variation under the same x-axis velocity of 0.36 (m/d), as in Figure 1, but at different y-axis velocities of 0.36 (m/d), 0.72 (m/d), and 1.05 (m/d) for two time domains: $t < t_0$ and $t > t_0$. Generally, the observed behavior in Figure 2 closely resembles that of Figure 1. Additionally, as the velocity increases, the movement of heavy metal particles becomes more rapid and a larger area receives the heavy metal. This relationship implies a positive correlation between velocity and heavy metal transport.

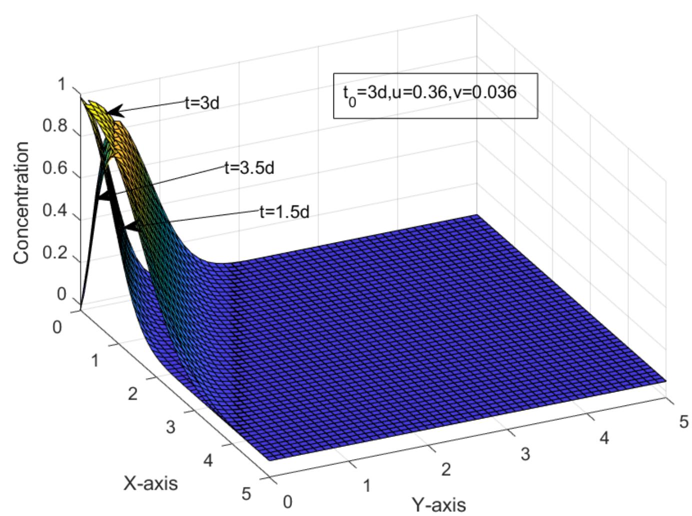
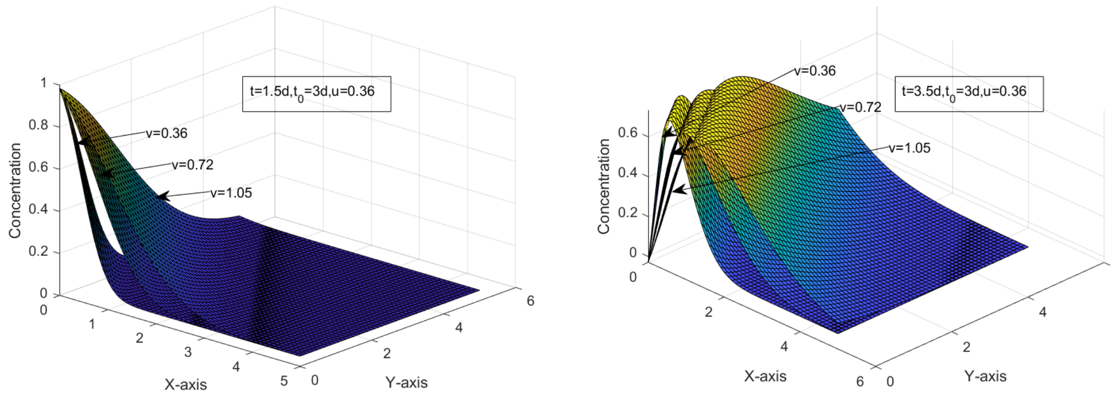


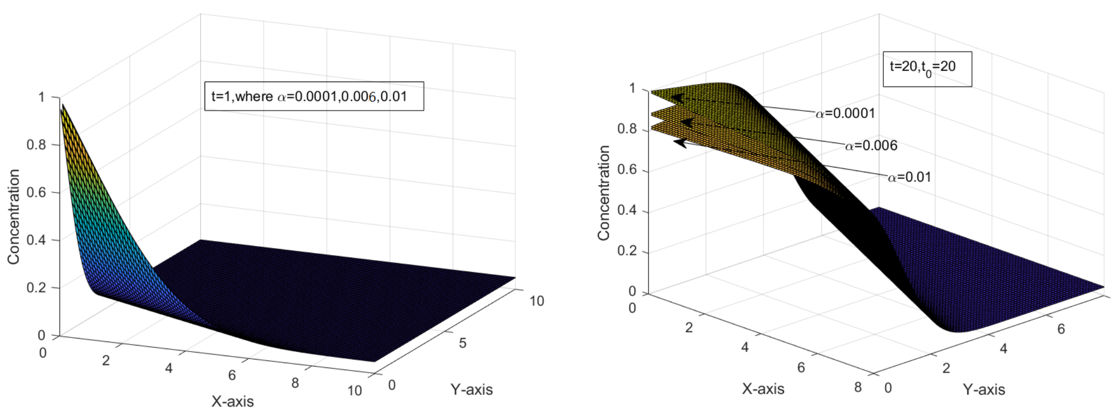
Figure 1: Concentration profiles of heavy metal at different times for fixed α=0.01 and t_0=3 d



$t = 1.5$ d, $t_0 = 3$ d $t = 3.5$ d, $t_0 = 3$ d

Figure 2: The effect of y-axis velocity on concentration for fixed α=0.01 and t_0=3 d, while t=1.5, 3.5 d

The concentration distribution behaviors are depicted in Figure 3 for different values of attenuation coefficient α, namely 0.0001, 0.006, 0.01 at time $t = t_0$, while α controls the decay rate in the exponential decay boundary condition. In Figure **??**, the peak is close to the source, but not much difference can be seen between different decays. Since t is small (t=1), although the value of α increased, the overall impact due to the exponential term is minimal, resulting in the curves to appear relatively very close to each other. Therefore, to contrast Figure **??**, the time length was increased to observe the concentration changes in Figure **??**. Changing the value of α shows a more significant effect on the curve.



$t = 1$ d, $t_0 = 1$ d $t = 20$ d, $t_0 = 20$ d

Figure 3: Comparison with different α values at different time

From Figure 4, it can be observed that as the adsorption coefficient k increases, the variation in peak concentration becomes very apparent, with values decreasing from 0.6644, 0.5439 and 0.0864. This clearly demonstrates the significant impact of adsorption on concentration.

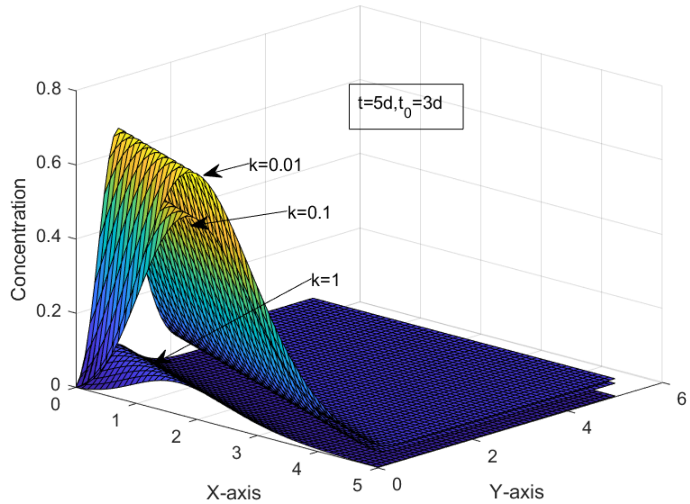


Figure 4: Concentration profiles of heavy metal at different k for fixed α=0.01 and t_0=3 d

4 Conclusion

The analytical solution for two-dimensional advection diffusion equation of heavy metal with exponential decay boundary conditions have been developed and analyzed. During the injection period ($t < t_0$), the peak concentration occurred at source point due to direct contact with the newly injected pollutants. This leads to a rapid increase in concentration, followed by attenuation in the more distant regions. Once the injection of heavy metal ceases, new pollutants are no longer introduced into the system. However, due to the lingering effects of the earlier injections, there is a minor resurgence in the peak concentration. Subsequently, the concentration starts to decline again as the pollutants disperse further into the system. The figures presented in understanding the impact of exponential decay injection boundary conditions on the variation of pollutant concentrations. Thus, the results provide a deeper insight into how heavy metal spread in the environment, where studying the propagation behavior of pollutants for various exponential decay coefficients can inform decision-makers about the most critical times and locations to focus their efforts. Lastly, the findings contribute to the development of policies that regulate the introduction of pollutants into the soil, aiming to minimize their impact on the environment.

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