# Point Source Heavy Metal Migration in Soil with Adsorption and Desorption under Neumann Boundary Condition

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Abstract Heavy metal pollution has always been a serious global environmental issue worldwide, and many scholars have demonstrated the feasibility of advection diffusion equation (ADE) to describe its transport in soil. In previous models, for boundary conditions involving instantaneous release of the source term, Dirichlet boundary condition was often used. This study examines Neumann boundary conditions, focusing on the evolution of concentration gradients, the influence of retardation factors, and the effect of the particle release ratio. Initially, sharp concentration gradients form near the point source, with the peak concentration shifting over time as the contaminant front progresses. Lower retardation factors increase migration speed and broaden the contaminant distribution. Additionally, a higher particle release ratio leads to higher local concentrations, underscoring the significant impact of soil porosity on contaminant transport. These findings provide insights for developing more accurate predictive tools for environmental remediation of heavy metal pollution.

**Keywords** Heavy metal, Advection diffusion equation, Neumann boundary condition, Laplace transform.

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

#### 1 Introduction

Heavy metal pollution is a serious environmental issue over the world that must be addressed to ensure a safe and healthy life. Various strategies have been implemented by authorities to mitigate this problem from multiple perspectives. Notably, mathematics also can be employed to predict the behavior of heavy metals, aiding in the development of effective remediation

strategies. Mathematically, the advection-diffusion equation (ADE) is a very useful model to describe the transport of heavy metal in a medium. For example, ADE has been successfully used by Nriagu [1], Zheng and Bennett [2], Freeze [3], and Anderson et al. [4] to study heavy metal in the groundwater by which leads to repair techniques. In the scope of heavy metal in soil, Liang and Isa [5,6], Aral and Liao [7] have made significant contributions to the field, particularly in studying Dirichlet boundary conditions in two-dimensional (2D) advection-diffusion equations, focusing on time variation, adsorption, retardation factors, and the behavior of instantaneous point source releases of heavy metals in soil.

One-dimensional (1D) ADE is the simplest model to study the behavior of pollutant migration in groundwater or soil systems. Some models have successfully addressed issues such as the prediction of contaminant concentration profiles and understanding of the interplay between advection, diffusion, and others. For example, Bear [8] provided the theoretical basis for understanding the ADE in 1D models which covered the principles of fluid dynamics in porous media. Later on, Fitts [9] outlined the transport of contaminants, making it a key source of understanding 1D ADE applications. Mojtabi et al. [10] presented 1D ADE and solved it analytically by separation of variables and numerically by the finite element method, which compared how was different between these two solutions. Dilip et al. [11] explained 1D ADE analytical solution which diffusion with continuous input point source. However, real-world scenarios often involve more complex geometries and interactions that cannot be adequately captured by 1D models alone. Recognizing the advantages of a two-dimensional (2D) model, some researchers have studied the ADE within a 2D domain. There has been a significant shift towards 2D ADE models, which provided a more comprehensive spreading and anisotropic conditions, offering their evolution over time [12,13]. For instance, Tirabassi et al. [14] got the analytical solution in 2D model which pollutant is on the ground. Lowry and Li [15] obtained the solution in the space-time domain did not discretize the derivative term. In addition, Dirichlet boundary condition is a common used in ADE model during the latest decades, because of its boundary values are known, which makes the definition and solving process of the problem clearer. For some practical problems, such as the fixed emission concentration of the source, the Dirichlet boundary condition can describe the concentration at the boundary. Bazilevs and Hughes [16] compared with weakly and strongly enforced Dirichlet boundary conditions for boundary layer solutions of the ADE which found out the weakly enforced condition is better. However, for some movement system, for example, pollutants migrate outward through groundwater systems, Neumann boundary condition describe that progress is better. Cao et al. [17] used a fourthorder compact finite difference scheme to solve the ADE with Neumann boundary conditions. Also, Dirichlet -to-Neumann boundary conditions are for multiple problems [18].

In all the above, no analytical solution has been developed to solve 2D ADE with adsorption and desorption with Neumann boundary conditions. This study mainly introduce the analytical solution of 2D ADE based on the Neumann boundary condition specifically for point source with instantaneous release. Specially, Neumann boundary conditions can be used to describe dynamic flux changes over time, which is of great significance for the study of heavy metal migration from instantaneous point source releases (such as accidental spills). In this case, the flux may vary with time, and Neumann boundary conditions can flexibly describe these changes. So, the Neumann boundary condition is a good supplement for the heavy metal transport in soil.

## 2 Governing equation

To model the transport of contaminants in 2D porous media, it is essential to consider various factors such as advection, diffusion, adsorption, and source term. The governing equation that encapsulates these dynamics in a 2D framework is given by [5, 19, 20] as

$$R\frac{\partial C}{\partial t} = D_x \frac{\partial^2 C}{\partial x^2} + D_y \frac{\partial^2 C}{\partial y^2} - u \frac{\partial C}{\partial x} - v \frac{\partial C}{\partial y} - \frac{\rho}{\theta} \frac{\partial S}{\partial t} + F, \tag{1}$$

where the  $\frac{\partial S}{\partial t}$  is the adsorption term. R is the retardation factor which is essentially a measure of how much slower a heavy metals moves through soil; C is the concentration of heavy metal ions in seepage,  $[ML^{-3}]$ ; S is the adsorption concentration,  $[M^0]$ ;  $\theta$  is the porosity of porous media;  $[L^2T^{-1}]$ ; u is the uniform velocity along x or longitudinal direction,  $[LT^{-1}]$ ; v is the uniform velocity along v or transverse direction v is source term, and v is time v is the spatial variables, v is the particle density v in v and v is the fundamental units, where v is the presents mass, v is the particle density v in v in v in v in v in v is the fundamental units, where v is the presents length, and v is the presents time.

The effects of diffusion and source terms in 2D space lead to changes in concentration over time, accounting for the rate of concentration with respect to spatial variations. Adsorption condition is considered as [21,22]

$$\frac{\rho}{\theta} \frac{\partial S}{\partial t} = kC(x, y, t) - k_x \frac{\partial C}{\partial x} - k_y \frac{\partial C}{\partial y}.$$
 (2)

The first term on the right-hand side represents the adsorption of the solute in the soil, governed by the adsorption coefficient k, which quantifies the rate at which pollutants transfer from the fluid phase to the solid phase, proportional to the mobile concentration. In contrast, the last two terms describe desorption along the x- and y-axes, characterized by the release coefficients  $k_x$  and  $k_y$ , which measure the extent to which pollutants are released back into the fluid phase due to spatial concentration gradients. This equation captures a dynamic system where pollutants continuously undergo adsorption onto and desorption from soil particles, influenced by local pollutant concentrations and spatial variations. The inclusion of the  $k_x$  and  $k_y$  terms accounts for anisotropy in the soil, reflecting the possibility that desorption occurs more readily in specific directions due to variations in soil properties or flow conditions.

Using Neumann boundary conditions helps to more accurately describe the adsorption and desorption processes of contaminants in soil. Since these processes are closely related to the concentration gradient of the contaminants, Neumann boundary conditions can capture these dynamic changes, thereby improving the accuracy and predictive capability of the model.

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

$$\frac{\partial C(0,0,t)}{\partial x} = 0, \quad \frac{\partial C(0,0,t)}{\partial y} = 0, \tag{4}$$

and

$$C(+\infty, +\infty, t) = 0. (5)$$

Combining the above equations (1) and (2) yields

$$R\frac{\partial C}{\partial t} = D_x \frac{\partial^2 C}{\partial x^2} + D_y \frac{\partial^2 C}{\partial y^2} - (u - k_x) \frac{\partial C}{\partial x} - (v - k_y) \frac{\partial C}{\partial y} - kC + F.$$
 (6)

Considering diffusion is directly proportional to velocity, when pollutants penetrate the soil, and at the same time, adsorption occurs. As heavy metals desorb from the soil, they re-enter the soil and participate in the diffusion process, thereby increasing the migration rate of heavy metals in the soil, namely

$$D_x = a(u - k_x), \quad \text{and} \quad D_y = b(v - k_y), \tag{7}$$

where a and b are constants which depend on the pore geometry and pore average size of the porous medium in the equation.

Introduce a new space variable

$$z = x + y\sqrt{\frac{D_y}{D_x}}. (8)$$

To facilitate derivation, a new spatial variable which is from equation (8) is substituted into the equation (6), then, a 1D second-order constant coefficient partial differential equation as follows

$$R\frac{\partial C}{\partial t} = D\frac{\partial^2 C}{\partial z^2} - U\frac{\partial C}{\partial z} - kC + F,$$
(9)

where

$$D = D_x \left(1 + \frac{D_y^2}{D_x^2}\right), \quad U = (u - k_x) + (v - k_y) \sqrt{\frac{b(v - k_y)}{a(u - k_x)}}.$$
 (10)

The new initial and the boundary conditions of equation (9) are

$$C(z,0) = 0; \quad 0 \le z < +\infty,$$
 (11)

$$\frac{\partial C(0,t)}{\partial z} = 0,\tag{12}$$

and

$$C(+\infty, t) = 0. (13)$$

Taking Laplace transform to equation (9) with respect to t, and rearranging the equation will result

$$D\frac{\partial^2 \bar{C}(z,p)}{\partial z^2} - U\frac{\partial \bar{C}(z,p)}{\partial z} - (k+Rp)\bar{C}(z,p) + \bar{F} = 0.$$
 (14)

Taking Laplace transform with respect to the space variable z, yields

$$D[s^{2}\bar{C}^{z}(s,p) - s\bar{C}(0,p) - \frac{\partial\bar{C}(0,p)}{\partial z}] - U[s\bar{C}^{z}(s,p) - \bar{C}(0,p)] - (k+Rp)\bar{C}^{z}(s,p) + \bar{F}^{z} = 0, (15)$$

and from boundary condition equation 12, applying the Laplace transform yields

$$\frac{\partial \bar{C}(0,p)}{\partial z} = 0. {16}$$

Substituting the equation (16) into (15) and rearranging the equation, then we get the new function as follow

$$\bar{C}^{z}(s,p) = \frac{s\bar{C}(0,p)}{(s-J_{1}+J_{2})(s-J_{1}-J_{2})} - \frac{\frac{U}{D}\bar{C}(0,p)}{(s-J_{1}+J_{2})(s-J_{1}-J_{2})} - \frac{\frac{\bar{F}^{z}}{D}}{(s-J_{1}+J_{2})(s-J_{1}-J_{2})},$$
(17)

where

$$J_1 = \frac{U}{2D}$$
, and  $J_2 = \sqrt{\frac{U^2}{4D^2} + \frac{k + Rp}{D}}$ . (18)

Let

$$\bar{C}^z = I_1 + I_2 + I_3, \tag{19}$$

where

$$I_1 = \frac{s\bar{C}(0,p)}{(s - J_1 + J_2)(s - J_1 - J_2)},\tag{20}$$

$$I_2 = -\frac{\frac{U}{D}\bar{C}(0,p)}{(s - J_1 + J_2)(s - J_1 - J_2)},\tag{21}$$

and

$$I_3 = -\frac{\frac{\bar{F}^z}{\bar{D}}}{(s - J_1 + J_2)(s - J_1 - J_2)}. (22)$$

Taking inverse Laplace to  $I_1$ ,  $I_2$ ,  $I_3$ , respectively

$$L^{-1}(I_1) = \bar{C}(0, p) \frac{(J_2 - J_1) \exp((J_1 - J_2)z) + (J_1 + J_2) \exp((J_1 + J_2)z)}{2J_2},$$
 (23)

$$L^{-1}(I_2) = \frac{U}{D}\bar{C}(0,p)\frac{\exp((J_1 - J_2)z) - \exp((J_1 + J_2)z)}{2J_2},$$
(24)

and

$$L^{-1}(I_3) = \frac{1}{2J_2D} \int_0^z \bar{F}\left[\exp((J_1 - J_2)(z - \tau)) - \exp((J_1 + J_2)(z - \tau))\right] d\tau.$$
 (25)

Combine and rearrange the above equations (23) - (25), provides

$$\bar{C}(z,p) = \bar{C}(0,p) \frac{(J_2 - J_1) \exp((J_1 - J_2)z) + (J_1 + J_2) \exp((J_1 + J_2)z)}{2J_2} 
+ \frac{U}{D} \bar{C}(0,p) \frac{\exp((J_1 - J_2)z) - \exp((J_1 + J_2)z)}{2J_2} 
+ \frac{1}{2J_2D} \int_0^z \bar{F} \left[ \exp((J_1 - J_2)(z - \tau)) - \exp((J_1 + J_2)(z - \tau)) \right] d\tau.$$
(26)

Let z approach infinity in equation (26) as in boundary condition equation (13). It is obtained that

$$\bar{C}(0,p) = \frac{\int_0^\infty \frac{\bar{F}}{D} \exp(-\tau(J_1 + J_2))}{J_2 - J_1} d\tau.$$
 (27)

Substitute the equation (27) into the equation (26), rearranging the equation

$$\bar{C} = \frac{J_1 \int_0^\infty \bar{F} \exp(J_1(z-\tau)) \exp(-J_2(z+\tau)) d\tau}{J_2 D(J_2 - J_1)} + \frac{\int_0^\infty \bar{F} \exp(J_1(z-\tau)) \exp(-J_2(z+\tau)) d\tau}{2DJ_2} + \frac{\int_0^\infty \bar{F} \exp(J_1(z-\tau)) \exp(J_2(z-\tau)) d\tau}{2D(J_2 - J_1)} - \int_0^\infty \frac{J_1 \bar{F} \exp(J_1(z-\tau)) \exp(J_2(z-\tau))}{2DJ_2(J_2 - J_1)} d\tau. + \int_0^z \frac{\bar{F} \exp(J_1(z-\tau)) \exp(-J_2(z-\tau))}{2J_2 D} d\tau - \int_0^z \frac{\bar{F} \exp(J_1(z-\tau)) \exp(J_2(z-\tau))}{2J_2 D} d\tau = I_{t1} + I_{t2} + I_{t3} + I_{t4} + I_{t5} + I_{t6}.$$
(28)

Taking inverse Laplace transform to equation (28) respect to t, then it is obtained

$$L^{-1}(I_{t1}) = \frac{U}{2DR} \int_0^\infty \int_0^t F \exp\left(\frac{-U\tau}{D}\right) \exp\left((-\frac{k}{R})(t-\zeta)\right)$$

$$\operatorname{erfc}\left[\frac{\sqrt{R}(z+\tau)}{2\sqrt{D(t-\zeta)}} - \frac{U\sqrt{t-\zeta}}{2\sqrt{DR}}\right] d\zeta d\tau,$$
(29)

$$L^{-1}(I_{t2}) = \frac{1}{2\sqrt{DR}} \int_0^\infty \int_0^t F \exp\left(\frac{U(z-\tau)}{2D}\right) \exp\left(-\left(\frac{U^2}{4DR} + \frac{k}{R}\right)(t-\zeta)\right)$$

$$\frac{1}{\sqrt{\pi(t-\zeta)}} \exp\left(\frac{-R(z+\tau)^2}{4D(t-\zeta)}\right) d\zeta d\tau,$$
(30)

$$L^{-1}(I_{t3}) = \frac{1}{2\sqrt{DR}} \int_0^\infty \int_0^t F \exp\left(\frac{U(z-\tau)}{2D}\right) \exp\left(-\left(\frac{U^2}{4DR} + \frac{k}{R}\right)(t-\zeta)\right)$$

$$\frac{1}{\sqrt{\pi(t-\zeta)}} \exp\left(\frac{-R(z-\tau)^2}{4D(t-\zeta)}\right) + \int_0^\infty \int_0^t \frac{UF}{4DR} \exp\left(-\frac{k}{R}(t-\zeta)\right)$$

$$\exp\left(\frac{U(z-\tau)}{D}\right) \operatorname{erfc}\left[-\frac{\sqrt{R}(z-\tau)}{2\sqrt{D(t-\zeta)}} - \frac{U\sqrt{t-\zeta}}{2\sqrt{DR}}\right] d\zeta d\tau,$$
(31)

$$L^{-1}(I_{t4}) = -\int_0^\infty \int_0^t \frac{UF}{2DR} \exp(\frac{U(z-\tau)}{D}) \exp\left(-\frac{k}{R}(t-\zeta)\right) \times \operatorname{erfc}\left[-\frac{\sqrt{R}(z-\tau)}{2\sqrt{D(t-\zeta)}} - \frac{U\sqrt{t-\zeta}}{2\sqrt{DR}}\right] d\zeta d\tau,$$
(32)

$$L^{-1}(I_{t5}) = \frac{1}{2\sqrt{DR}} \int_0^z \int_0^t F \exp(\frac{U(z-\tau)}{2D}) \exp(-(\frac{U^2}{4DR} + \frac{k}{R})(t-\zeta))$$

$$\frac{1}{\sqrt{\pi(t-\zeta)}} \exp(-\frac{R(z-\tau)^2}{4D(t-\zeta)}) d\zeta d\tau,$$
(33)

and

$$L^{-1}(I_{t6}) = -\frac{1}{2\sqrt{DR}} \int_0^z \int_0^t F \exp(\frac{U(z-\tau)}{2D}) \exp(-(\frac{U^2}{4DR} + \frac{k}{R})(t-\zeta))$$

$$\frac{1}{\sqrt{\pi(t-\zeta)}} \exp(-\frac{R(z-\tau)^2}{4D(t-\zeta)}) d\zeta d\tau.$$
(34)

Combine equations (29) - (34) and rearranging, we can get a final general solution of equation (1) as follow

$$C(z,t) = \frac{U}{2DR} \int_0^\infty \int_0^t F \exp\left(\frac{-U\tau}{D}\right) \exp\left((-\frac{k}{R})(t-\zeta)\right) \operatorname{erfc}\left[\frac{\sqrt{R}(z+\tau)}{2\sqrt{D(t-\zeta)}} - \frac{U\sqrt{t-\zeta}}{2\sqrt{DR}}\right] d\zeta d\tau$$

$$+ \int_0^\infty \int_0^t \frac{F \exp(\frac{U(z-\tau)}{D})}{2\sqrt{DR\pi(t-\zeta)}} \exp\left(-\left(\frac{U^2}{4DR} + \frac{k}{R}\right)(t-\zeta)\right)$$

$$\times \left[\exp\left(\frac{-R(z+\tau)^2}{4D(t-\zeta)}\right) + \exp\left(\frac{-R(z-\tau)^2}{4D(t-\zeta)}\right)\right] d\zeta d\tau$$
(35)

The point source term is expressed by the following function.

$$F = W(z)G(t), (36)$$

where

$$W(z) = \frac{1}{\theta}\delta(z - z_0), \quad G(t) = M\delta(t - t_0).$$
 (37)

By substituting equations (36) - (37) into the equation (35) and evaluating the integrals, the final solution of equation (35) result in

$$C(z,t) = \frac{UQ}{2DR} \exp\left(\frac{-Uz_0}{D}\right) \exp\left((-\frac{k}{R})(t-t_0)\right) \operatorname{erfc}\left[\frac{\sqrt{R}(z+z_0)}{2\sqrt{D(t-t_0)}} - \frac{U\sqrt{t-t_0}}{2\sqrt{DR}}\right] + \frac{Q \exp\left(\frac{U(z-z_0)}{D}\right)}{2\sqrt{DR\pi(t-t_0)}} \exp\left(-\left(\frac{U^2}{4DR} + \frac{k}{R}\right)(t-t_0)\right) \times \left[\exp\left(\frac{-R(z+\tau)^2}{4D(t-t_0)}\right) + \exp\left(\frac{-R(z-z_0)^2}{4D(t-t_0)}\right)\right],$$
(38)

where  $Q = \frac{M}{\theta}$  reflects the proportion of a substance released into the environment compared to the total amount initially refers to the point source intensity of pollutants at  $z = z_0$ .

### 3 Results and discussion

This section presents some simulations based on the analytical solution (38), derived from the developed governing equation. It is assumed that the heavy metal is released at time  $t_0$  and at one specific point  $z_0$ , which is later transformed into its original spacial coordinates (x, y). Besides, the parameters used in (1), (2), (7) and (37) are as in Table 1.

Parameters	Values
$k_x$ (/day)	0.01
$k_y$ (/day)	0.02
R	1.5
a	0.1
b	0.2
u  (m/day)	0.36
v  (m/day)	0.036
$t_0$	0.08
$z_0$	0.5
Q	1
k	0.1

Table 1: Model parameters for simulations [19, 20]

Figure 1 presents the concentration profiles of heavy metals transport at different earliest times of 0.081 d, 0.095 d and 0.5 d. At the earliest time, the concentration peak is confined at the region close to the source, and move towards the right edge, where advection (flow-driven transport) dominates initially, pushing the plume toward the right edge. As time progresses, the concentration decreases in magnitude. Also, the sharp peak near the release point broadens, and the concentration becomes more evenly distributed as can be seen when t=0.5 d. The peak broadening signifies mechanical dispersion (spreading due to heterogeneous flow paths) and molecular diffusion (solute movement from high to low concentration). Starting from t=1 d, the concentration peak decreases as time progress which can be seen at Figure 2. It can be clearly observed that the concentration gradually spreads outward from the midpoint we set.

The behaviors shown in Figures 1 and Figure 2 are due to the contaminant front moving rapidly, while the trailing part still catching up. As the concentration graDdients become less steep, the advection's relative impact diminishes, and diffusion causes to spread more slowly in all directions. This trend aligns with the expected behavior of heavy metals dispersing and diluting over time.

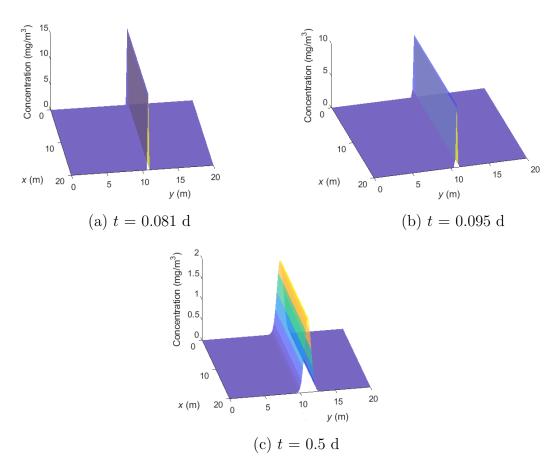


Figure 1: Concentration profiles of heavy metals at different earliest times for fixed Q=1 and R=1.5 with instantaneous release source heavy metals is introduced at (2.5, 2.5)

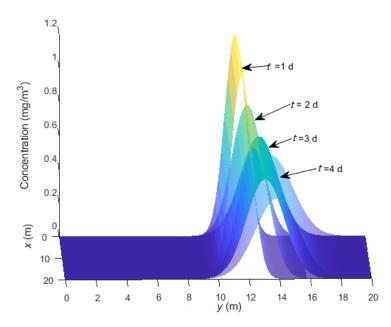


Figure 2: Concentration profiles of heavy metals at different time for fixed Q = 1 and R = 1.5 with instantaneous release source heavy metals is introduced at (2.5, 2.5)

Figure 3 shows the effect of retardation factors on the heavy metals transport in soil. As the retardation factor decreases, the migration speed of the contaminant increases, and the position of the concentration peak gradually moves left ledge from the release point. Meanwhile, the concentration distribution becomes more uniform, and the diffusion range expands. This indicates that the strength of the retardation effect directly influences the migration speed and spatial distribution of the contaminant in the soil.

Figure 4 indicates the variation of the concentration under different Q values on the first day. The increase in the Q value, which represents the ratio of particle release to the porosity of the porous medium, has a significant impact on the peak concentration. When the ratio of particle release to porosity is high, a larger number of particles are released into soil. This can lead to higher local concentrations of contaminants.

Comparison of heavy metal transport in soil with or without adsorption is illustrated in Figure 5. The red line considers both adsorption and desorption showing a gradual decline in concentration over time. The green line only adsorption is considered, leading to a faster decrease in concentration compared to the case with both adsorption and desorption. This suggests that without desorption, the heavy metal particles are retained in the soil more effectively. While the scenario excludes both adsorption and desorption, leading to the slowest rate of concentration reduction over time, indicating minimal interaction with the soil particles.

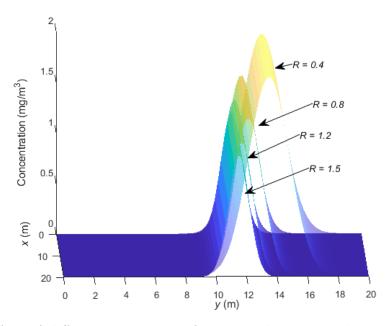


Figure 3: The effect of different retardation factors on heavy metal concentration from point source with instantaneous release plotted at Q=1 and t=1 d

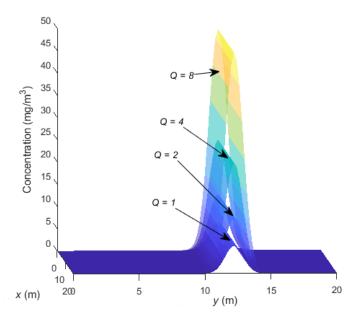


Figure 4: The effect of different particle release amounts and porosity ratios on heavy metal concentration plotted at time  $t=1~\mathrm{d}$ 

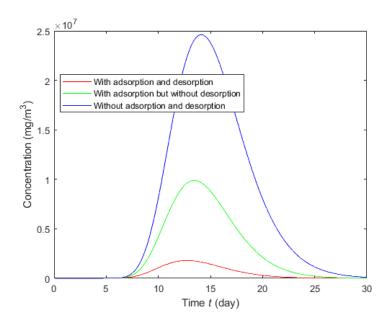


Figure 5: Comparison of heavy metal transport in soil with different conditions of adsorption and desorption plotted for x = 5 and y = 5

### 4 Conclusion

The study explores the transport behavior of heavy metals in soil using the ADE. It investigates how concentration gradients evolve over time, highlighting the initial formation of sharp gradients near the point source and the subsequent shift of peak concentration away from the source as the contaminant front advances. The impact of retardation factors is also analyzed, demonstrating that lower retardation leads to faster contaminant migration and a broader, more uniform distribution. Additionally, the effect of the particle release ratio (Q value) on the concentration is examined, revealing that higher ratios result in elevated local contaminant concentrations due to the increased particle release into the soil. The findings also imply that models incorporating adsorption and desorption dynamics are essential for accurately predicting the transport and retention of heavy metals in soils. For environmental management, this means that remediation efforts should consider both adsorption and desorption.

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