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RESEARCH ARTICLE

Two-Dimensional Heavy Metal Migration in Soil with Adsorption and Instantaneous Injection

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Abstract This paper studies a two-dimensional transport model to investigate the behavior of heavy metal migration in porous media, specifically considering their transport in soil. The model takes into consideration the combination of adsorption term as well as instantaneous injection at the boundary. Also, the model accounts for both longitudinal and transverse movements, providing a comprehensive understanding of heavy metal transport phenomena. In order to obtain the analytical solution Laplace transform has been implemented. It is found that the peak concentration of heavy metals is found to be greatly affected by the changes in the instantaneous injection value. Additionally, a correlation is observed between retardation factors and heavy metal concentrations, with a decrease in retardation factors resulting in an increase in heavy metal concentration.

Keywords: Advection diffusion equation, Instantaneous injection, Laplace transform, Two-dimensional, Heavy metal.

Introduction

Heavy metal pollution is a serious environmental pollution, and it is difficult to eradicate from the soil, which caused many scholars to study its related behaviour such as its transport ability. Establishing a mathematical model will help environmentalists and relevant personnel understand its characteristics, so as to establish a better method to repair the soil. The Advection Diffusion Equation (ADE) is a common model adopted to describe the heavy metal transport in soil. Many scholars have discussed and studied the dispersion of pollution in soil and porous media through mathematical model, which greatly promoted the progress of understanding pollutant migration in soil. Although some progress has been made, the remediation of heavy metal pollution in soil is still a topic of research interest. For example, adsorption in heavy metal migration in soil has been verified to effect the pollutants transport in soil [1-3]. It is an important factor in pollutant transport in soil, such that it examined the processes governing heavy metal migration.

A lot of analytical solutions have been proposed in one-dimensional ADE [4-12]. For example, Kumar *et al.* [9] solved a one-dimensional advection diffusion equation with variable coefficients under the point source media of uniformity. Then, Kumar *et al.* [10] extend the research that studied for semi-infinite range heterogeneous media. The effects of spatial and temporal dependence on concentration dispersion are studied with the help of the respective parameters. Meanwhile, Yadav and Kumar [11] has studied the analytical solution of one-dimensional solute transport problem in homogeneous porous domain, by considering the seepage velocity is exponentially decreasing, and diffusion parameter and retardation factor that are space dependent. The analytical solution used Laplace transport techniques with uniform input point source condition. Later, Yadav and Roy [12] also studied the analytical solution

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of one-dimensional solute transport in a semi-infinite heterogeneous continuous periodic point source through a localized adsorption porous through a left boundary injection. Both researches used Laplace transform to get the solutions in only one-dimensional equation

Besides one-dimensional ADE research in pollution migration in porous media, two-dimensional development seems to be an inevitable trend. Fedi *et al*. [13] considered a parallel plate geometry and discusses a semi-infinite and laterally bounded domain based on Dirichlet and mixed boundary condition. Chen *et al*. [14] also used the Dirichlet and mixed boundary conditions to study the solution of ADE but for finite domain only. Meanwhile, Chen *et al*. [15] explained the influence of inlet conditions on two-dimensional solute transport in porous media where the inlet concentration is known. In addition, Derya and Yetim [16] focused on the advection-diffusion equation with the Atangana-Baleanu derivative, which is a fractional derivative. Furthermore, Yadav and Kumar [17] found that the concentration patterns and levels are influenced by the varying nature of the input concentration.

For most of the ADE research, the boundary conditions can be divided into some types of injections, such as short-time injection, continuous injection and instantaneous injection. In previous studies, Wang *et al*. [18] have considered the instantaneous injection of a tracer to apply to an experiment, and it is only a linear graphical method for hydro dispersive. Then, Aral and Liao [19] mentioned about instantaneous injection as a boundary for their special case. It is two-dimensional ADE, but it is not about heavy metal migration in soil. Later on, Smedt *et al*. [20] obtained the solution by a tracer of instantaneous injection in river domain, and this study presented an analytical solution for one-dimensional solute transport in rivers, considering transient storage effects. Sushil [21] introduced a simple method and an optimization method for estimating specific dispersity and injected mass from an ideal breakthrough curve resulting from an instantaneous solute injection. However, it is still a one-dimensional solution. Guerrero *et al*. [4] and Huang *et al*. [22] investigated a general pollutant diffusion patterns that concentrate on understanding the behaviour of pollutants in a particular environment.

This study aims to explore the heavy metal transport in soil based on a two-dimensional ADE with adsorption and instantaneous injection. By using Laplace transform technique, the analytical solution for the instantaneous boundary condition will be obtained. This study is expected to improve the understanding of the heavy metal migration in soil, in which it provides the solution and the transport which could be further exploited computationally and experimentally as the potential proof for future new research and environment management. Furthermore, 2D heavy metal migration with instantaneous injection boundary may have a broader scope, focusing on heavy metal migration scenarios and their potential impacts on the environment.

Governing Equation

The two-dimensional ADE describing heavy metal transport in a porous medium is given by

$$R\frac{\partial C}{\partial t} = D_{\mathrm{x}}\frac{\partial^2 \mathrm{C}}{\partial \mathrm{x}^2} + D_{\mathrm{y}}\frac{\partial^2 \mathrm{C}}{\partial \mathrm{y}^2} - u\frac{\partial C}{\partial x} - v\frac{\partial C}{\partial y} - \frac{\rho}{\theta}\frac{\partial S}{\partial t} \tag{1}$$

where the $\frac{\partial S}{\partial t}$ is the adsorption term. R is the retardation factor, C $[ML^{-3}]$ is the concentration of heavy metal ions in seepage. S $[M^3]$ is the adsorption concentration; θ is the porosity of porous media; 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 $[L]$ is the migration distance of heavy metal particles, ρ $[ML^{-3}]$ is the particle density ; D_x and D_y $[L^2T^{-1}]$ are dispersion coefficient along longitudinal or transverse direction respectively. For the adsorption term, the effect of diffusion with the x and y axis is [23, 24]

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

where k_x and k_y are the release coefficients through *x* and *y*. Therefore, equation (1) becomes.

$$R\frac{\partial C}{\partial t} = D_x\frac{\partial^2 C}{\partial x^2} + D_y\frac{\partial^2 C}{\partial y^2} + (k_y - u)\frac{\partial C}{\partial x} - v\frac{\partial C}{\partial y} - k_x C \tag{3}$$

The diffusion equation is considered to be geometrically proportional to the seepage velocity [25], namely

$$D_x = au, \text{ and } D_y = bv \tag{4}$$

where a and b are the coefficients that depends upon pore geometry and average pore size diameter of the porous media.
In many cases, the heavy metal is instantaneously introduced to the porous medium (soil)

typically taken to be a uniform pulse type point source [26, 27] . Also, it is assumed C_0 of heavy metal concentration initially and flux type boundary condition. Hence, the corresponding initial and boundary conditions are

$$C(x,y,0) = c_0; \;\; 0 \le x < +\infty, 0 \le y < +\infty \tag{5}$$

$$C(0,0,t) = \frac{m}{Q}\delta(t), \tag{6}$$

$$\frac{\partial C}{\partial x} = 0, \frac{\partial C}{\partial y} = 0; \;\; x \to \infty, y \to \infty \tag{7}$$

where, m $[M]$ is the mass of implanted heavy metal ion particles, Q is void fraction, δ is the Dirac Delta function. Let's introduce a new space variable

$$z = x + y\sqrt{\frac{D_y}{D_x}} \tag{8}$$

Substituting this into equation (1) and combining with equation (2), yields

$$R\frac{\partial C}{\partial t} = D\frac{\partial^2 C}{\partial z^2} - U\frac{\partial C}{\partial z} - k_x \tag{9}$$

where,

$$D = D_x\left(1 + \frac{D_y^2}{D_x^2}\right), \;\text{ and }\; U = (u - k_y) + v\sqrt{\frac{bv}{a(u-k_y)}} \tag{10}$$

Additionally, the initial and the boundary condition given by above equation (5) - (7) are now become

$$C(z,0) = c_0; \;\; 0 \le z < +\infty \tag{11}$$

$$C(0,t) = \frac{m}{Q}\delta(t), \tag{12}$$

$$\frac{\partial C}{\partial z} = 0; \;\; z \to \infty, \tag{13}$$

In order to solve equation (9), Laplace transformation techniques is applied with respect to t, which transform equation (9) and its initial and boundary conditions (11)-(13) into

$$Rs\bar{C} - Rc_0 = D\frac{\partial^2 \bar{C}}{\partial z^2} - U\frac{\partial \bar{C}}{\partial z} - k_x\bar{C} \tag{14}$$

with $\bar{C}(0,s) = \frac{m}{Q}$, and $\frac{\partial \bar{C}(\infty,s)}{\partial z} = 0.$

Hence, after some vital working, the solution for $\bar{C}$ can be shown to be in the form of

$$\bar{C} = I_1 + I_2 + I_3 \tag{15}$$

where

$$I_1 = \frac{m}{Q}\exp\left(\frac{Uz}{2D}\right)\exp\left(-z\sqrt{\frac{U^2}{4D^2} + \frac{Rs+k_x}{D}}\right) \tag{16}$$

$$I_2 = -\frac{Rc_0}{k_x+Rs}\exp\left(\frac{Uz}{2D}\right)\exp\left(-z\sqrt{\frac{U^2}{4D^2} + \frac{Rs+k_x}{D}}\right) \tag{17}$$

and

$$I_3 = \frac{Rc_0}{k_x+Rs} \tag{18}$$

Then, taking inverse Laplace to each I_1, I_2 and I_3

$$L^{-1}(I_1)=\frac{m\sqrt{R}z}{2Q\sqrt{\pi Dt^3}}\exp[-(\frac{U^2}{4DR}+\frac{k_x}{R})t]\exp(\frac{Uz}{2D})\exp(-\frac{z^2R}{4Dt}) \tag{19}$$

$$L^{-1}(I_2)=-\frac{c_0}{2}\exp[(\frac{Uz}{2D}-\frac{k_xt}{R})]\{\exp(-z\sqrt{\frac{U^2}{4D^2}})\mathrm{erfc}(\frac{z\sqrt{R}}{2\sqrt{Dt}}-\sqrt{\frac{U^2t}{4DR}})$$
$$+(\exp(z\sqrt{\frac{U^2}{4D^2}}))\mathrm{erfc}(\frac{z\sqrt{R}}{2\sqrt{Dt}}+\sqrt{\frac{U^2t}{4DR}})\} \tag{20}$$

and

$$L^{-1}(I_3)=c_0\exp(-\frac{k_xt}{R}) \tag{21}$$

Finally, the desired analytical solution is obtained as

$$C(z,t)=\frac{m\sqrt{R}z}{2Q\sqrt{\pi Dt^3}}\exp[-(\frac{U^2}{4DR}+\frac{k_x}{R})t]\exp(\frac{Uz}{2D})\exp(-\frac{z^2R}{4Dt})-\frac{c_0}{2}\exp[(\frac{Uz}{2D}-\frac{k_xt}{R})]\{\exp(-z\sqrt{\frac{U^2}{4D^2}})\mathrm{erfc}(\frac{z\sqrt{R}}{2\sqrt{Dt}}$$
$$-\sqrt{\frac{U^2t}{4DR}})+\exp(z\sqrt{\frac{U^2}{4D^2}}))\mathrm{erfc}(\frac{z\sqrt{R}}{2\sqrt{Dt}}+\sqrt{\frac{U^2t}{4DR}})\}+c_0\exp(-\frac{k_xt}{R}) \tag{22}$$

For comparison, for a simple case when R=1, U=0 and C_0 =0, the solution (22) is reduced to a solution for ADE

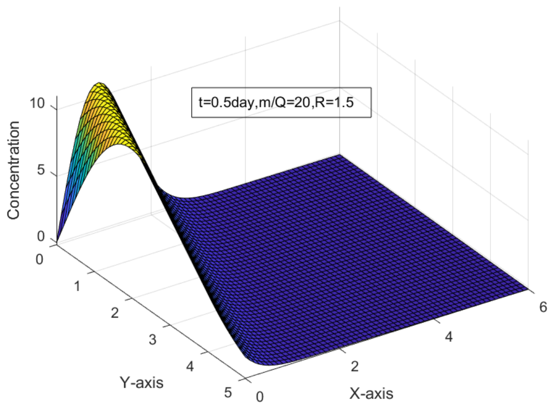
$$C(z,t)=\frac{mz}{2Q\sqrt{\pi Dt^3}}\exp\left[-k_xt-\frac{z^2}{4Dt}\right] \tag{23}$$

which similar to the problem by Mojtabi *et al*. [7] and Wang *et al*. [28].

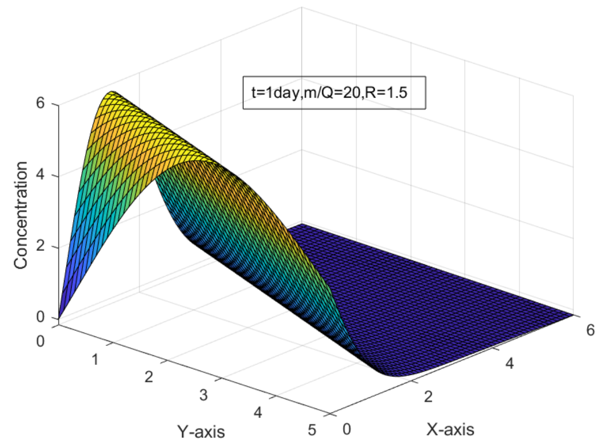
Results and Discussion

Concentration distributions of heavy metal in the soil are evaluated from the analytical solution equation (21). The initial heavy metal concentration is $c_0=0.05$, for the *x* and *y* domain from 0 to 5 respectively. In the general practical field-like case, due to the existence of longitudinal gravity, the diffusion or flow of heavy metal pollutants in the longitudinal direction is faster than that in the transverse direction. Considering the above and previous research results, the lateral velocity and diffusion coefficient are considered to be one-tenth of the longitudinal velocity and diffusion coefficient [25]. Therefore, the longitudinal and transverse seepage velocity and diffusion coefficient are respectively [29, 30], u=0.75 m/day; v=0.075 m/day; D_x=0.95 m^2/day ; D_y=0.095 m^2 /day . Additionally, k_x=0.01 /day, k_y=0.002/day, m/Q=20 and R=1.5.

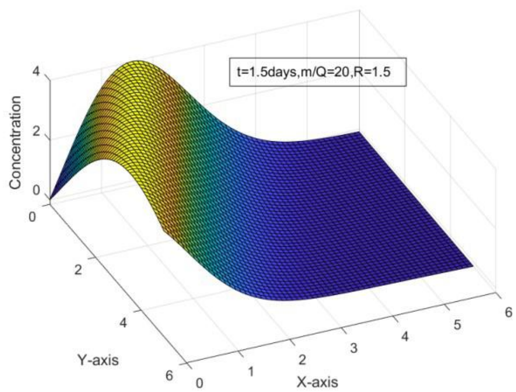
Figure 1 shows the heavy metal concentrations corresponding to 4 different times. As can be seen from Figure 1, the concentration of heavy metals is low at small area close to the point of injection. Then, rapidly rose to the peak followed by a gradual decrease, and finally returned to the plateau. In addition, with the increase of time, the peak concentration decreases. Overall, the heavy metals seem to move from the origin to the surrounding area as the peak can be seen to occur at farther distances as time increases.



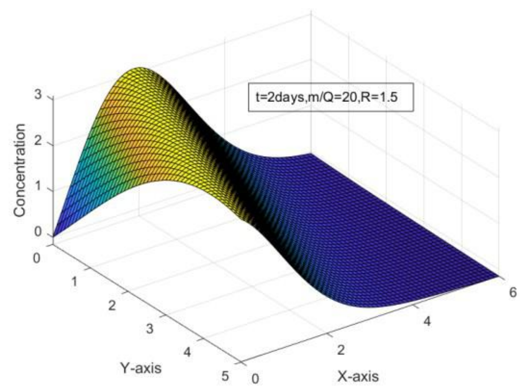
(a) 0.5 day



(b) 1 day



(b) 1.5 days



(d) 2 days

Figure 1. Concentration profiles of heavy metal at different time

Figure 2 investigates the effect of different instantaneous injection values on the migration of heavy metal pollutants in soil by fixing the time at t=2 and R=1.5, where the subplots (a), (b), (c) and (d) show the change in concentration when m/Q equals 1,10,25, and 50, respectively. As expected, similar to Figure 1, they all rise from zero to the peak and then fall back to an equilibrium concentration. Furthermore, the larger the value of instantaneous injection, the larger the value of the concentration at the peak, which is adequately reasonable.

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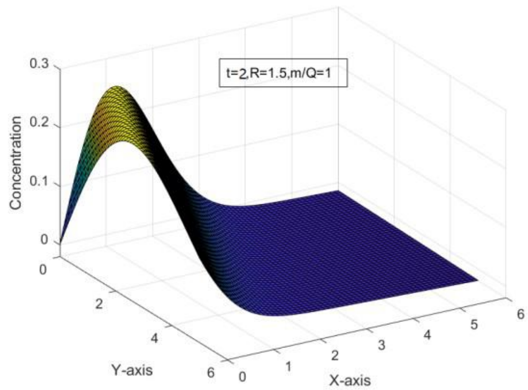
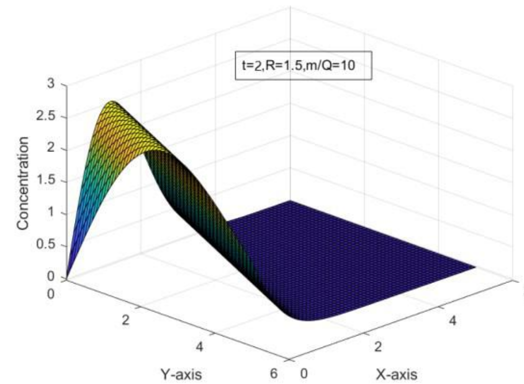
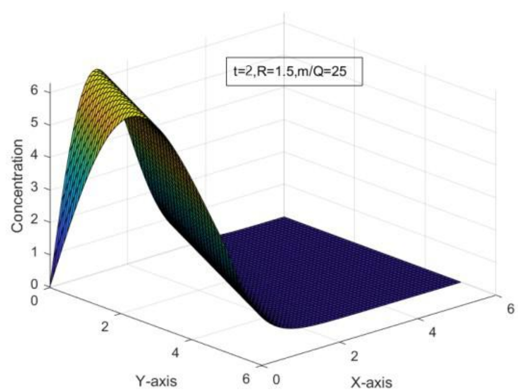


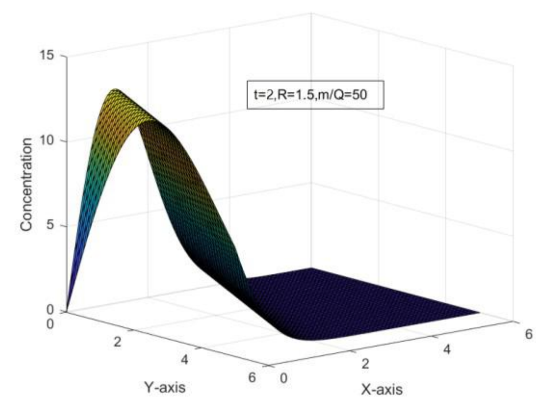
(a) *m/Q*=1



(b) *m/Q*=10



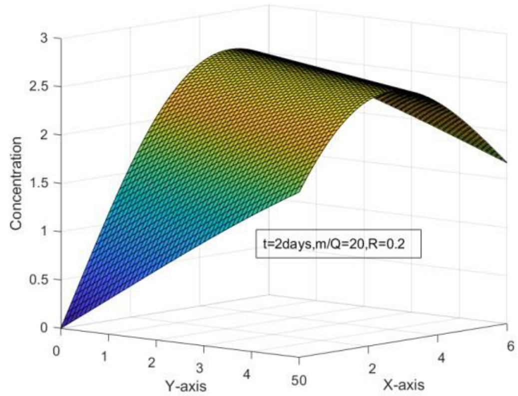
(c) *m/Q*=25



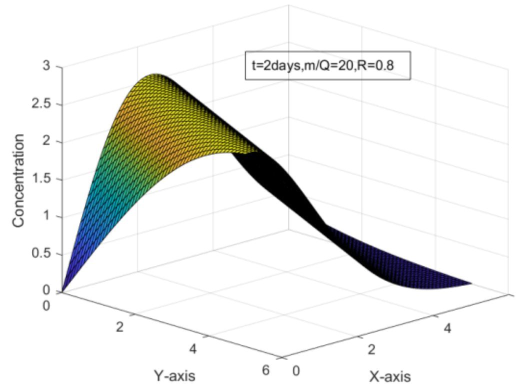
(d) *m/Q*=50

Figure 2. Concentration profiles for different instantaneous injection value

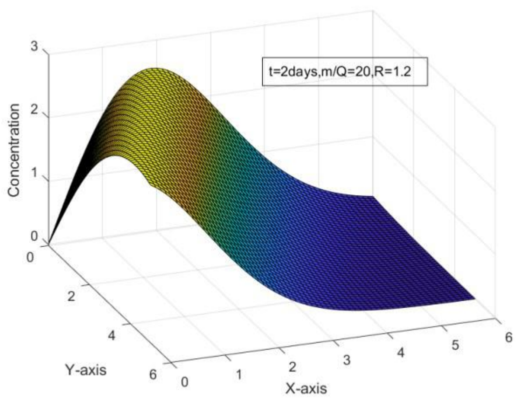
Moreover, Figure 3 shows the migration of heavy metal pollutants in the soil layer at time *t*=2 and *m/Q*=20. The subplots (a), (b), (c) and (d) show the change in concentration when *R* equals 0.2,0.8,1.2, and 2.5, respectively, in order to study the effect of different retardation factors. It is observed that they all rise from zero to the peak and then fall back, and finally fall back to an equilibrium point. That means the concentration of heavy metal is infected by retardation.



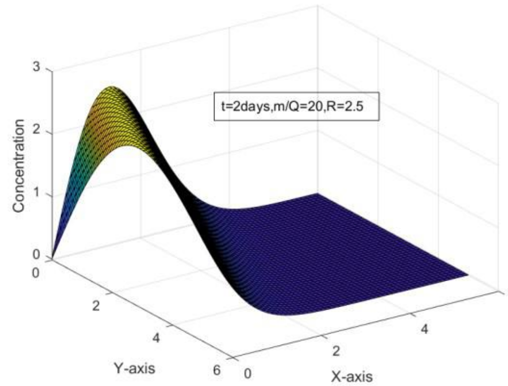
(a) *R*=0.2



(b) *R*=0.8



(c) *R*=1.2



(d) *R*=2.5

Figure 3 Concentration profiles for different retardation factors

Conclusions

In this paper, analytical solution to a two-dimensional transport model of heavy metal ions in porous media is studied such that adsorption is considered in the model, together with instantaneous injection at the boundary. The analytical solution is provenly agreed to the problem by Mojtabi *et al*. [7] and Wang *et al*. [28]. The result is first interpreted for different time. Then the effect of different instantaneous injection value and retardation factor are investigated.

Through the analysis of concentration variations over time, it becomes evident that the concentration of heavy metal is low at a very small area to injection. After that, there is an area where the concentration is the highest followed by an equilibrium concentration for the rest.

Additionally, we observed that the peak concentration of heavy metals is significantly influenced by changes in the instantaneous injection coefficient. Furthermore, the peak concentration of heavy metals was found to be directly proportional to the magnitude of the instantaneous injection coefficient. Higher values of the injection coefficient resulted in higher peak concentrations, indicating a stronger impact of the instantaneous injection on the solute transport and dispersion within the medium.

Moreover, our investigation also revealed the correlation between the retardation factors and heavy metal concentrations. Specifically, when the retardation factors decrease, there is an associated increase in the concentration of heavy metals. This finding underscores the significance of understanding and accounting for retardation processes to accurately predict and manage heavy metal contamination in soil or other similar context such as groundwater system.

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