Unsteady state contaminants transport in sandy mediums using CFD model

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Abstract. This study was conducted to provide a CFD simulation model to simulate the transfer of pollutants through sandy soils. A physical model and simulation model were designed and implemented with the help of CFD programs using COMSOL 5.4 software to study the process of transporting pollutants within the porous medium. To study the pollutant transmission in the porous media, a sand size of less than 0.36 mm diameters was used as porous media. For an analysis of the problem, several groups of factors were considered and assumed. The first group concerned with the physical properties of the media likes coefficient of adsorption Kd. The second group represented the hydraulic factor of flow likes velocity. The results of the physical and CFD models showed there is a clear effect of soil physical properties due to the coefficient of adsorption Kd action. The velocity has a significant effect on the concentrations of pollutants and the time of transmission where the lower velocities produce lower concentrations and delayed transport of pollutants in the soil. The CFD simulated model showed that the change in the Kd-value has a significant impact on the results. The study also showed a good agreement between the results of the laboratory work provided by the physical model and that of the CFD model depending on several statistical indexes. This indicates that the CFD models could be considered as an efficient tool to simulate the complex problems of contaminates transport through a porous medium.

Keywords: Transfer of soil pollutants; porous media; Contaminant Numerical modeling, CFD

1. Introduction

The transportation of pollutants through porous media is a major problem for the disposal of waste in the soil. Recent field studies by [1] showed that when pollutants travel at speeds similar to the soil flow value, pollutants can absorb and move as a vector. Besides, the troubles of transporting pollutants out of subsurface blueprints have become one of the main investigative goals in earth sciences, hydrology and environmental sciences. The problems of adapting and evaluating soil technologies and aquifers need to be studied and solutions are required [2]. In order to know the effect of transporting pollutants through different types of soil, many researchers carry out experimental investigations through laboratory and practical studies. Also, many of them rely on mathematical and analytical studies to simulate the movement of pollutants in the soil, soil depths and groundwater. Especially with the advent of advanced high-power computers, numerical modelling has gained wide popularity and is, in fact, of very special importance in this field. References in the investigation shall be made regarding both unsaturated and saturated media that are porous [3]. There are two main methods of studying the transport of pollutants with respect to reactions in porous media. These are called random and deterministic methods [4], [5]. Stochastic methods or methods deal with reaction coefficients and are considered as "static processes" [4], [7] or can be verified by the random hydraulic conduction field [4], [8] [31] at the site with appropriate quantities of their own. To simulate the transport of pollutants, the models are very expensive and unreasonable to use in many practical cases [4]. Studies usually assume
a constant source of inlet boundary conditions for solute transport. Boundary conditions (BC) and reaction processes complicate the stimulation of pollutant transport in soil. According to [4], no study has yet been conducted that looked at the phenomenon of pollutant transport and provided a solution to it with the above three factors combined. [9], the researchers' studies have been taken in which to form and find analytical solutions. However, adsorption and dispersion were modelled separately in the heat dispersion equation (CDE). In practice; Absorption and degradation can be simultaneous transport of pollutants into the soil. Mathematical modelling is an accepted scientific and mathematical process that provides a mechanism for comprehensively integrating basic processes and describing a system of human subjective judgments. However, the modelling of different types of pollutants has been studied by many researchers, [10], [11], recently, numerical models have shown to be very good tools for solving the difficulty and complex boundary conditions of subsurface problems. [12] Use the particle force exchange Method to propose a two-dimensional digital sample to simulate the problem of negative pollutant [13] transmission. Surface dimensions of dissolved pollutants. The general arrangement of the finite difference method of binary dispersion equations was examined by [14], to provide a solution to the pollutant transport problem. Three-dimensional transport of pollutants underground was simulated by [15], using the LaGrange-Oilerian finite element method. [16]. He introduced a new class of algorithms to solve the contaminant problem by solving 1dimension, 2 dimension trans-dispersion models, and formulating a statistical model for repeat laboratory flow pole trail for grainy materials with double Porosity. The results of the questionnaires and laboratory tests were accompanied by a good pact for all cases. [17], O'Lerian's method of limited differences was consumed to design a two-dimensional model of pollutants moving through porous media. They have shown that a 2D model can be used to simulate a problem with good accuracy [18], and have proposed a 3D limited item method to solve a broad range of soil pollution problems based on the residual weighted Galerkin index of the 3D shape. Based on a residual statement from Galerkin, [18] he suggested the 3D determinant item method to solve soil pollution problems providing good results. The numerical model was designed by [19], to solve the troubles of Convection - dispersion - adsorption. The model simulates the problem well. [20] and studied the problem of pollutant transport through experimental and digital research. [21] Select digital model and laboratory work using conservative tracking devices. The results indicated that a better experimental assortment and a numerical evaluation method had been established. [22], He used a multi-laboratory experiments on a large scale and pore-scale to simulate and design various homogeneous porous media. It was found that, for a variety of leakage velocities, the determination of the complex nonlinear parameters of the transverse hydrodynamic dispersion is necessary to capture the detected lateral displacement. [23] Use the Soil Column Experiment to report laboratory research on the transport of pollutants through saturated soils, as the problem has also been digitally simulated by the system providing good results. Through an experimental study, the dissolved transport in fractured soil was investigated by [24], and it was found that as the absorption value increases, the concentration will decrease accordingly. Whereas, the higher the diffusion value, the lower the concentration. With respect to both saturated and saturated porous media, [3] he reviewed a wide range of research work of experimental investigations or using an analytical solution and numerical method to solve and simulate the contaminant problem. [25], Kd's logic identified a method for the Permo-Triassic sandstones - a type of aquifer common throughout the world - and advised a better position to determine binding to mineral ions. [26], the absorption properties of atrazine were evaluated using linear and nonlinear balanced formulas with results for absorption data from the laboratory formula. The results indicated that adsorption coffins and organic matter have linear behaviour in soil. The simulation of pollutant transport under hydraulic structures was studied using a physics simulation model and CFD [27]. It was found that the rate of generation and backwardness is that adsorption causes a major role in this problem. The two models provided very good contact results in most cases. The aim of this paper is to uncover a CFD simulation of pollutant transport through sandy porous media taking into consideration the effect of hydraulic parameters and properties of porous media on the concentration and distribution of pollutants through media that have not been taken into account through all the previous work and research that were summarized above. This problem has not been taken into account by all previous
work and research. It is also important to note that all results and solutions obtained in this research were performed under the premise of saturation of the pore water.

2. Laboratory model
The physical model is designed to study the transfer and adsorption of copper considered as the contaminating through two different porous mediums of its constituent materials, which therefore mimics the adsorption of copper and takes an idea of its effect on agricultural lands and lands that contain gravel and sand and a statement of its adsorption capacity. The physical model consists on one tube made of polyethylene with a length of 3 meters and 0.04 m in diameter. The pipe was fixed on a stand of iron with a height of 150 cm. At each distance of 50 cm from the tube contains an opening reached by a polyethylene tube of 4 cm in length and 12 mm in diameter to take samples influent and to measure the pressure using a pressure gauge of the mercury-sensitive type. The system was supplied with polluted water provided from a 250-liter tank using a pump of a maximum capacity of 30 l/m connected between the tank and the pipes. From the outside, the pipe was provided by a filter to prevent penetration of the porous medium to the collected tank capacity of 250 litres, see figure 1, for physical model and figure 2, a plate of the working model.

![Figure 1: The layout of physical modalities.](image1)

![Figure 2: The plate of the Physical model.](image2)

2.1. Porous media
The porous medium represents the land on which the pollutant travels before it reaches the depths of the groundwater. The movement and transmission of pollutants depend on the properties of the porous medium being conducted in. Among the most characteristics that affect the transition process are the porosity, hydraulic conductivity, distribution and size of the minutes. In this study, the used porous media was tested of different sand gradations size consisted of sandy soil sifted of less than 0.36 mm diameters mesh sieve, see figure 3. The media were collected from the site of sandy soil, and it was washed with the prescribed water to rid it of the impurities and salts. Then, it was air-dried and a sieve analysis was done, see figure 4. Table 1 indicates some important tests conducted to show the most important properties.

![Figure 3. Sieving analysis.](image3)

![Figure 4. Sand porous media.](image4)
Table 1. Properties of porous media.

| Properties of the media | Value       |
|-------------------------|-------------|
| porosity                | 0.28        |
| Bulk Density (kg/m3)    | 1562        |
| Effective size d10 (mm) | 0.17        |
| Mean grain size d50 (mm)| 0.38        |
| Coefficient of hydraulic Conductivity (m/s) | 0.0013 |
| Surface area m2/g       | 4.0335      |
| Coefficient of Adsorption l/gm | 0.001409 |

2.2. Contaminated water Prepare
At 250 litres of contaminated water containing blue aqueous copper nitrate Cu(NO3)2.3H2O was prepared by dissolving an amount equal to 26.6 g of copper nitrate obtained from local laboratories in a tank containing 250 litres of tap water with a pH equal to 6 and temperature equal 9°C to obtain a contaminant concentration of 25 mg/l and the pollutant particles were mixed with the tank water well before starting the process of passing the pollutant on the models used in the study.

2.3. Working methods
The media were collected from sandy soil, washed with distilled water and then dried in the oven for an hour at a temperature of 300 degrees Celsius, after which the sieve was done figure 4. The pipe was made from transparent polyethylene with a length of 3 m and filled with sandy soil sample used for the study as shown in the previous paragraphs. The entrance to each pipe was connected by a plastic plug with the inside of the filter and connected to a plastic tube to the pump that connected to the tank in which the contaminated water prepared to provide to the system. However, the water contaminated with aqueous copper nitrate was pumped to the pipe by the pump with a continuous and constant discharge equals to 0.06 l/min. After passing the polluted water through the pipe at the same time, samples of fluent were drawn from the five designed water intake points (1 to 5) at different times throughout the experimental period and collected in small labelled containers. After that, the concentration of the copper nitrate in the labelled containers was measured by an atomic spectrometer in the laboratories of the Iraqi Ministry of Science. The coefficient of adsorption Kd was estimated experimentally in the laboratory by taking a weight of 0.1g of sandy soils for every two samples and dissolved in 40 ml of tap water with a pH equal to 6. At the same time, a standard solution of the pollutant was prepared by dissolving 3.8 g of copper nitrate blue in a glass bottle and completed. The volume reached 1000 litres, where 1 mg/l was prepared and then different concentrations of the standard solution were prepared at the amount of (10,20,30,40,50) mg/l and mixed with the soil in glass test tubes and placed on the vibrator for 300 cycles per minute. The models were then filtered by watt man 40 filter paper and saved in a tube. The remaining copper concentrations $q_e$ found by using an atomic spectrometer, and the adsorption percentage of the element was found by means of equation (1). The Coefficient of adsorption Kd was calculated by finding the slope of the best line drawn for the $q_e$ verse $C_e$ as will be shown in Figures 6 and Figure 7.

\[
q_e = \frac{c_i - c_e}{w} v
\]

Whereas:
$q_e$ is concentration Equilibrium value in (Mg-copper per G-soil)
$c_i$: Primary concentration of a copper ion in the tank (mg/l)
$c_e$: final concentration of copper ion in effluent (mg/l)
$Kd$: Coefficient of adsorption (l/g or m³/Kg)
$V$: The volume of copper ion solution (ml)
$w$: Soil weight (g)
3. Computational fluid dynamic simulation model

In this paper, the CFD model was used to study, understand and predict the water flow process in the closed and open type systems. In this study, simulations will be used to simulate and study the transport of pollutants in sandy porous media (sandy soils). A 2D CFD model was designed to match the dimensions used in the experimental work. Two types of physics were considered in the CFD model. The first one is the Brinkman Equation (br) to simulate the flow in the porous media while the second one is the Transport of Diluted Species in porous media (tds) to simulate the contaminates transport through the porous media. In real work, there are two types of flux:

3.1. In the porous subdomain.

In this type of flow, Brinkmann’s equations are used in Forchheimer’s equation after correction and are according to the equations shown (2), (3), (4) [28].

\[
\frac{\mu}{k} \cdot u = \nabla \left[ -pl + \frac{4}{3} \left( (\nabla u + (\nabla u)^T) \right) \right] - \frac{\rho n C_f}{\sqrt{k}} u |u|
\]  
(2)

\[
\nabla \cdot u = 0
\]  
(3)

\[
C_f = \frac{1.75}{\sqrt{350} \pi^2}
\]  
(4)

3.2. Type flow through porous media (sedimented and diffuse transport).

A contaminant is introduced into the groundwater by surface flow caused by groundwater flow; The dispersion is due to mechanical mixing and molecular diffusion, and the remainder resulting from the adsorption process of pollutants. The mathematical touch between these operations as in equation (5)

\[
R \frac{\partial c}{\partial t} + \frac{\partial}{\partial x} (uc) + \frac{\partial}{\partial y} (vc) = D_x \frac{\partial^2 c}{\partial x^2} + D_y \frac{\partial^2 c}{\partial y^2} + r + s
\]  
(5)

\[
R = n + \rho K_d
\]  
(6)

Where:
- \(c\): Concentration of contaminants
- \(u\): Velocity field in the x-direction
- \(v\): Velocity field in the y-direction
- \(D_x\): Coefficient of Dispersion in the x-direction (m2/s)
- \(D_y\): Coefficient of dispersion in the y-direction (m2/s)
- \(r\): rate of generation, the task of \(C\)
- \(s\): Rate of external source, a function of \(c\)
- \(R\): retardation which is caused her by adsorption
- \(n\): Porosity
- \(K_d\): Adsorption isotherm (m3/kg)
- \(\rho\): the density kg/m3

Also, it was considered that \(r = f(c)\) and \(s = g(c) = 0\). The rate of generation \((r)\) is considered to represent the effect of the chemical properties between copper and the soil. While the rate of an external source \((s)\) is assumed to consider the effect of the sedimentation of the copper in the soil where the soil will play a filter’s role against the contaminates transport. However, function \(g\) was assumed to be zero since there is no external source. While, the function \(f\) is estimated to be \(r = -0.06 c^2\). This assumed several trial forms for them in the simulated model to gain the optimum results that provide the minimum differences between the actual results and the results of the CFD model. The issue now is how to solve these partial differential equations, Equation (2) to the equation (6), in order to provide the solution and results. In this study, the solution was provided depends on CFD technics. From many software and programming available today for these purposes, COMSOL multiphasic version 5.4 was decided to be considered here. Because the predefined multiphasic interface species and porous media flow make it easy to set up and solve such a complex coupled flow regime.

3.3. Initial limits and boundary conditions

The boundary and initial state were satisfied with the following points, see Figure 5
1. At entrains, \( u = V_0 \) and \( C = C_0 \)
2. At Outlet, \( P = 0 \) \( (\nabla u + (\nabla u)^T) = 0 \), pressure, no Viscous stress
3. For all wall no skid \( U = 0 \)
4. First value \( (t = 0) \), \( U = (u, v) = 0 \), \( C(x, y) = 0 \) at time \( t = 0 \)

The walls of the pipe were set as no-slip wall boundary conditions. The CFD model has a physical control mesh of extremely coarse triangular element size type with a number Item of 3162 and 2375 vertices as shown in Figure 6.

4. Plan study
   Through the experimental work of the physical model and the results obtained and entered as data into the CFD simulation model, the process of studying the factors and components that affect the concentration of pollutants through their transmission of porous media was implemented. The first factor is the physical properties of the soil used as a coefficient of adsorption \( k_d \). The second factor represents the hydraulic factor of the flow velocity. It is very important to demonstrate that it is not easy to do all the required experiments in a laboratory. Therefore, the research plan was based on conducting some of these laboratory tests and then comparing the results with the results of the CFD simulated model to verify the model's results. After reaching the required reliability and confidence in the CFD simulated model, it is subsequently relied upon to obtain the required results for other experiments without the need to conduct them in the laboratory in order to reduce effort, time and costs, which is considered one of the most important goals of CFD simulated models.

5. Results and discussion
   A number of experiments were carried out using the physical model for the transport of the pollutant in the medium to perform this study. The results of these experiments were simulated by the Comsol program 5.4 later. Results of laboratory work will be presented and discussed in the following sections.

5.1. \( k_d \) test
   Figure 7 refers to the result of adsorption coefficient values of \( 0.00149 \text{ l/g} \) for the sample. The value of \( k_d \) was evaluated at a temperature of \( (300) \text{ K} \) employing a by using different amounts of concentrations as described above, [29]. From the results, it is clear that the sample has adsorption because the media has precise diameters of less than 0.36 mm due to the negative relationship between minute sizes and surface adsorption capacity [30].
5.2. Simulation of experimental test and model verification

In this part, the results of the laboratory work on transporting pollutants will be presented and compared with the results of the CFD model after applying the soil characteristics used and the contaminated water characteristics in the program. The results of pollutant transport were simulated through the sanding porous medium used in the study. To compare the results of the experimental tests provided for the physical model with that of the CFD simulation model using the Comsol program, the CFD model was designed to be typical of the physical model. Copper nitrate was used as a contaminant with a concentration of 0.3845 mol/m$^3$ with other properties listed in Table 2.

| Name   | Description | Value          |
|--------|-------------|----------------|
| z1     | inlet part  | 0.01 m         |
| z2     | Catalyst part | 3 m          |
| z3     | outlet part  | 0.01 m         |
| eps_p2 | porosity    | 0.28           |
| v0     | inlet velocity (m/s) | 9.82E-04 |
| kappa2 | Permeability | 1.3292E-10 m$^2$ |
| Kd     | Coefficient of adsorption | 0.001409 m$^3$/kg |
| rof    | fluid density | 1000 kg/m$^3$ |
| ros    | Soil density | 1562 kg/m$^3$ |
| Ct     | Ce at tank mol/m$^3$ | 0.3845 |

Figure 8 shows the results of pollutant transfer through the simulated model using a CFD program. Figure 9 shows the compaction of the laboratory and corresponding CFD results of the pollutant transport depends on the five specified points along the tube. The results indicated a good match as it relied on COMSOL 5.4 in analysing the results. Moreover, verification was also tested according to several standard statistical indexes as shown in table 4, and equations (7 To 8). Based on the results of the statistical tests listed in Table 4. CFD Simulation model can be a very good tool to simulate the problem without the physical model needed to reduce cost, time and effort. Therefore, the model is now ready to analyse and study many varied cases of a wide range of values of variables and factors.
Verification of the CFD simulated model results.

\[ \text{RMSE} = \sqrt{\frac{1}{n} \sum_{i=1}^{N} (c_m - c_s)^2} \]  \hspace{1cm} (7)
\[ \text{MSE} = \frac{1}{n} \sum_{i=1}^{N} (c_m - c_s)^2 \]  \hspace{1cm} (8)
\[ \text{MAE} = \frac{1}{n} \sum_{i=1}^{N} |c_m - c_s| \]  \hspace{1cm} (9)
\[ \text{RSE} = \frac{\sum_{i=1}^{N} (c_m - c_s)^2}{\sum_{i=1}^{N} (c_m - \bar{c_m})^2} \]  \hspace{1cm} (10)

**Table 3.** Statistical analysis verifications tests

| Point | RMSE  | MSE   | MAE   | RSE  |
|-------|-------|-------|-------|------|
| A1    | 0.22402 | 0.05018 | 0.19599 | 0.07113 |
| A2    | 0.19039 | 0.03625 | 0.16230 | 0.16238 |
| A3    | 0.18967 | 0.03597 | 0.14954 | 0.32715 |
| A4    | 0.13400 | 0.01796 | 0.10570 | 0.44913 |
| A5    | 0.04619 | 0.00213 | 0.03611 | 0.07914 |

The results of the statistical analysis verification tests proved that the CFD simulated model is able to simulate the experimental results of the transport of pollutants in porous media at an acceptable degree. Thus, it can be relied upon in studying this complex phenomenon without the need for physical...
models and laboratory experiments in order to reduce costs and effort which is the great target by using models. Therefore, this gives legitimacy to study the effect of several factors and variables on this complex phenomenon and to obtain the required results, depending on the CFD model with the least effort, cost and time. Thus, the effect of flow velocity and adsorption coefficient $k_d$ of the porous media was studied as will be shown below.

5.2.1. Velocity consideration. The velocity of flow in porous media is a very important factor in the phenomenon of the spread of pollutants and their concentration in the porous media. In this step, the effect of a velocity change in the results was studied by imposing variable values of velocity between (-20% to 20%) of the laboratory value (0.00098 m/s) from the physical model. Figures 10 and figure 11 showed that the effect of velocity on the phenomenon of the spread of pollutants and their concentration where the lower velocity leads to the slower the spread and the less concentration in porous media. This is because the low speed leads to an increase in the detention time in the media, which leads to an increase in the adsorption of pollutants by the porous medium and vice versa where the high speed leads to a high speed of spread and a high value of the concentrations with short time, due to the lack of adsorption due to reduction in the detention time in the media.

![Figure 10](image1.png) Simulated results for a velocity of +20% $v_0$.  
![Figure 11](image2.png) Simulated results for sample A at $v$ of -20% $v_0$.

5.2.2. $k_d$ Consideration. The adsorption coefficient is the ratio between the concentrations of the primary pollutant when it is put into the soil and its percentage in the soil after moving to a certain distance or interacting with the soil for a certain period of time, that is, the extent to which the pollutant is distributed in the soil,[31]. In this part, the transport of pollutants was simulated by assuming an increase and decrease in the adsorption coefficient to half its initial value, where the laboratory value after conducting the measurement experiment was equal to (0.00149 m$^3$/kg). If we compare the same time required to reach the highest concentration value, we will notice that when the adsorption coefficient increased, the time required to reach the highest concentration value increased compared to the initial model from (22 to 35 minutes approximately), see figure 12. Also, the relationship of time with the increase in the adsorption coefficient is inverse, because when the adsorption coefficient is increased, it means that the pollutant will not come out early with high concentrations from the points of withdrawal. When reducing the $k_d$ value in half, it is noticed an increase in the concentration coming out of the points of withdrawal, as well as a decrease in time to reach a high value of concentration, as shown in Figure 13.

![Figure 12](image3.png) Simulation of $K_d$ effect, $k_d = +50\%$.  
![Figure 13](image4.png) Simulation of $K_d$ effect, $k_d = -50\%$. 


6. Conclusions
From the discussions and analyses presented in this paper, the following knowledge can be inferred. The numerical results provided by the simulated CFD mathematical model give a good agreement with the laboratory work of all the cases imposed for the study. Thus, The CFD technique able to notice the problem it has been studied in the research, taking into account the acceptable error rate. With the increase in the length of the tube, the concentrations in the porous medium redaction due to the adsorption of the pollutant by the soil particles. The physical properties of the porous media represented by kd value have a clear impact on the concentration of pollutants. The rate of the adsorption has a great influence on the concentration. The concentration decreases at slow speeds and the time wanted to link the highest point value is relatively reduced. Adsorption deficiency plays the main role in reducing the concentration and transfer of pollutants. The increase in the value of the adsorption coefficient by 50% led to an increase in the adsorption of pollutants by soil particles, and thus a decrease in the concentrations calculated from the control points. Decreasing the adsorption coefficient leads to an increase in the calculated concentrations from the withdrawal points, as previously shown due to the decrease in the ability of the soil to adsorb pollutants significantly. Increasing the flow velocity leads to an increase in the concentrations from the entry points because the pollutants go through a specific time that is not allowed to fully interact with the medium and allow them to be adsorbed or ion exchange. Based on several statistical standard indexes, the CFD simulated model using Comsol 5.4 provides a good agreement matching with the results of the physical model for the case of pollutant transport processes in porous mediums.

Notations
\( c \) = contaminants Concentration
\( C_f \) = friction Coefficient
\( \bar{c}_m \) = measured concentration
\( c_s \) = simulated concentration
\( D, D_x, D_y \) = Diffusion coefficient
\( e \) = Error
\( H \) = above stream water head
\( K \) = permeability
\( Kd \) = Adsorption, isotherm
\( MAE \) = mean absolute error
\( MSE \) = mean squared error
\( n \) = Porosity
\( r \) = Rate of growth
\( R \) = Retardation which is caused her by adsorption
\( RSE \) = relative squared error
\( RMSE \) = root mean squared error
\( s \) = Rate of outer source, function of c
\( u = V \) - field in the x- axis
\( v = V \) - field in the y- axis
\( \rho \) = Density
\( \mu \) = viscosity Dynamic
\( P \) = Pressure

Reference
[1] Penrose W, Polzer R W L, Essington E., Nelson H D and Orlandini K A 1990 Mobility of plutonium and americium through a shallow aquifer in a semiarid region. EnvironSci. Technol., 24(1): 228-34. https://doi.org/10.1021/es00072a 012
[2] Mark B L. 1994 Transport of reactive contaminants in heterogeneous porous media Anagu journal. 32(3):285-313. https://doi.org/10.1029/94RG00624
[3] Patil S B and Chore H S 2014 Contaminant transport through porous media: An overview of experimental and numerical studies. Advances in environmental research, 3(1):45-69. http://dx.doi.org/10.12989/aer.2014.3.1.045

[4] Gao G, Fu B, Zhan H and Ma Y 2013 Contaminant transport in soil with depth-dependent reaction coefficients and time-dependent boundary conditions. Water research, 47(7):2507-22.

[5] Kia SF. 1991. Subsurface multiphase flow of organic contaminants: Model development and validation. Water Research. 25(10):1225-36. https://doi.org/10.1016/0043-1354(91)90061-T

[6] Chrysikopoulos C V, Kitanidis P K and Roberts P V 1990 Analysis of one-dimensional solute transport through porous media with spatially variable retardation factor. Water Resources Research, 26(3), pp.437-46. https://doi.org/10.1029/WR026i003p00437

[7] Dos Santos D R, Cambier P, Mallmann F J K, Labanowski J, Lamy I, Tessier D and van Oort F 2013 Prospective modeling with Hydrus-2D of 50 years Zn and Pb movements in low and moderately metal-contaminated agricultural soils. Journal of contaminant hydrology, 145, pp.54-66. https://doi.org/10.1016/j.jconhyd.2012.12.001

[8] Miralles-Wilhelm F and Gelhar L W 1996 Stochastic analysis of sorption macrokinetics in heterogeneous aquifers. Water resources research, 32(6):1541-9. https://doi.org/10.1029/96WR00791

[9] Flury M, Wu Q J, Wu L and Xu L 1998 Analytical solution for solute transport with depth-dependent transformation or sorption coefficients. Water resources research, 34(11):2931-7. https://doi.org/10.1029/1998WR902299

[10] Alemi M H, Goldhamer D A and Nielsen D R 1988 Selenate Transport in Steady-State, Water-Saturated Soil Columns 17 (4):608-13 https://doi.org/10.2134/jeq1988.0047242501700040015x.

[11] Alemi, M.H., Goldhamer, D.A. and Nielsen, D.R., 1991. Modeling selenium transport in steady-state, unsaturated soil columns. 20(1):89-95. https://doi.org/10.2134/jeq1991.0047242500200010014x.

[12] Zimmermann, S., Kounoutsakos, P. and Kinzelbach, W., 2001. Simulation of pollutant transport using a particle method. Journal of Computational Physics, 173(1):322-47. https://doi.org/10.1006/jcph.2001.6879.

[13] Chao, W.A.N.G., pei-fang, W. and Yong, L.I., 2003. Composite modeling approach and experimental study for subsurface transport of contaminants from land-disposal sites. Journal of Hydrodynamics Series B-English Edition-, 15(4):1-9.

[14] Ataie-Ashtiani B and Hosseini S A 2005 Numerical errors of explicit finite difference approximation for two-dimensional solute transport equation with linear sorption. Environmental Modelling & Software, 20(7):817-26. https://doi.org/10.1016/j.ecosy.2004.04.010

[15] Li M H, Cheng H P and Yeh G T 2005 An adaptive multigrid approach for the simulation of contaminant transport in the 3D subsurface. Computers & geosciences, 31(8):1028-41. https://doi.org/10.1016/j.cageo.2005.03.010

[16] Rao P and Medina Jr M A 2006. A multiple domain algorithm for modeling two dimensional contaminant transport flows. Applied mathematics and computation, 174(1):117-33. https://doi.org/10.1016/j.amc.2005.03.021

[17] Craig J R and Rabideau A J 2006. Finite difference modeling of contaminant e1087 https://doi.org/10.1016/j.advwatres.2005.08.010

[18] El-Zein, A., Carter, J.P. and W. Airey, D., 2006. Three-dimensional finite elements for the analysis of soil contamination using a multiple-porosity approach. International Journal for Numerical and Analytical Methods in Geomechanics, 30(7):577-97. https://doi.org/10.1002/nag.491

[19] Remešková M 2007 Numerical solution of two-dimensional convection–diffusion–adsorption problems using an operator splitting scheme. Applied mathematics and computation, 184(1):116-30. https://doi.org/10.1016/j.amc.2005.06.018
[20] Fox P J, Lee J and Lenhart J J 2011 Coupled consolidation and contaminant transport in compressible porous media. *International Journal of Geomechanics*, 11(2):113-23. https://doi.org/10.1061/(ASCE)GM.1943-5622.0000035

[21] Ballarini E, Bauer S, Eberhardt C and Beyer C 2012 Evaluation of transverse dispersion effects in tank experiments by numerical modeling Parameter estimation, sensitivity analysis and revision of experimental design, *J. Contam. Hydrol.*, 134(6):22-36. https://doi.org/10.1016/j.jconhyd.2012.04.001.

[22] Rolle M, Hochstetler D, Chiogna G, Kitanidis P K and Grathwohl P 2012 Experimental investigation and pore-scale modeling interpretation of compound-specific transverse dispersion in porous media. *Transport in porous media*, 93(3):347-62. https://doi.org/10.1007/s11242-012-9953-8

[23] Sharma P K and Dixit U 2014. Contaminant transport through fractured-porous media: An experimental study. *Journal of Hydro-environment Research*, 8(3):223-33. https://doi.org/10.1016/j.jher.2013.08.003

[24] Sharma, P.K., Sawant, V.A., Shukla, S.K. and Khan, Z., 2014. Experimental and numerical simulation of contaminant transport through layered soil. *International Journal of Geotechnical Engineering*, 8(4):345-51. https://doi.org/10.1179/1939787913Y.0000000014.

[25] Batty M, 2012, Managing complexity, reworking prediction. *Environment and Planning B: Planning and Design* 39 607–8. doi:10.1068/b3904ed.

[26] Satpute S S, Parkale S and Kashid L M 2015. Study of Sorption behavior of Atrazine toward soil. *Int. Jour. of Environmental Science*, 6(3):0976 – 4402. http://10.0.23.200/ijes.6001.

[27] Muhsun S S, Saleh M S and Qassim A R 2020. Physical and CFD Simulated Models to Analyze the Contaminant Transport through Porous Media under Hydraulic Structures. *KSCE Journal of Civil Engineering*, 24(12):3674-91. https://doi.org/10.1007/s12205-020-1767-6

[28] Amiri A and Vafai K 1998 Transient analysis of incompressible flow through a packed bed. *International Journal of Heat and Mass Transfer*, 41(24):4259-79. https://doi.org/10.1016/S0017-9310(98)00120-3.

[29] Morillo, E., UndaeyJia, T., Maqueda, C. and Ramos, A., 2000. Glyphosate adsorption on soils of different characteristics: Influence of copper addition. *Chemosphere*, 40(1):103-7. https://doi.org/10.1016/S0045-6535(99)00255-6.

[30] Awan M A, Qazi I A and Khalid I 2008 removal of heavy metals through desorption using sand, *Jolunalo f Envioronmental sciences*, Vol. 15(3):413-6.

[31] Lee J H and Doolittle J J 2004 Determination of soil phosphorus and zinc interactions using desorption quantity-intensity relationships. *Korean Journal of Soil Science and Fertilizer*, 37(2):59-65.

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