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ORIGINAL PAPER

Numerical simulation of groundwater contaminant transport in porous media

S. M. A. Banaei[1] · A. H. Javid[1] · A. H. Hassani[1]

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Abstract

Groundwater has been considered as a major pathway for contamination migration which results in both subsurface pollution and soil contamination. This investigation makes an attempt to set up a two-dimensional numerical model to simulate groundwater flow and pollutant transport through porous media. The numerical model is used to simulate both groundwater flow and contaminant migration in porous media; besides, it is capable of considering the effects of sorption, retardation, and volatilization on the contaminant. Jajrud rural district located near Tehran City in Iran is a potentially contaminated site; furthermore, it is regarded as a potential peril for that zone. Groundwater flow and contaminant transport in Jajrud rural been investigated. This model is based on the finite-difference method which has enough ability to predict the pollution migration, and it is validated by several analytical and experimental test cases. The result revealed that the advection could possibly have been regarded as the main process on the contaminant transport in both reactive and non-reactive form of pollutant, as a result of high velocity in this region; furthermore, the reactive pollutant concentration mitigates 1.33 times more that non-reactive one as a result of high dispersion coefficient and contaminant decay term.

Keywords Groundwater · Contaminant transport · Numerical model · Jajrud rural district · Advection

Introduction

Contamination transport through porous media brings about a large number of environmental issues, such as deteriorating freshwater resources and declining quality of drinking water. Both freshwater and the quality of which are imperative parameters affecting the surrounding environment, especially aquifer's quality. Pollutant generally includes high concentrations of compounds such as heavy metal and toxic hazards which jeopardize the water resources (Rahman et al. 2012). The contaminants commonly are outcomes of chemical processes which are derived from an industrial area into the subsurface and transported by groundwater flow and spread into the ecosystem. The complex process of contaminant transport does not stop even after pollutant source has ceased, and it has a long-lasting effect for the environmental. Groundwater flow and pollution transport through porous media have been studied independently, and the effects of those on pollution are considered individually; the combination model of groundwater flow and contaminant transport have not concerned enough. The coupled model of groundwater flow and contaminant transport can be solved the issues of the latest model which are used to simulated either groundwater model or transport models, such as problem about boundary conditions, and compatibility of the geometry. The mathematical relationship which introduces the groundwater through an aquifer considers groundwater flow equation. The steady-state condition of flow is called Laplace equation. Advection-Dispersion-Reaction (ADR) equation is one the most widely cited equation which is used by the environmental engineering to describe the fate of the pollutant (Harbaugh 2005).

There have been reported some preeminent endeavor to understand the mechanism of the groundwater flow and solute transport in porous media in the recent decades (Neretnieks 1980; Wang and Narasimhan 1985; Derradji et al. 2011). Moreover, there has been quite more research addressing the impact of the ground on contaminant transport. Swain and Wexler (1992) linked the surface flow model

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✉ A. H. Javid
a.javid@srbiau.ac.ir

[1] Department of Natural Resources and Environment, Science and Research Branch, Islamic Azad University, Tehran, Iran

with a three-dimensional finite-difference groundwater flow model.

Nowadays, Groundwater Modeling System has significantly been improved and brings about several specialized computer software packages using to predict contaminant transport plume. The numerical model can be based on the finite-difference approach (MODFLOW), the particle-tracking model (MODPATH), the modular three-dimensional transport model (MT3DMS), the finite element approach (SPEED2D), and the multi-phase flow transport model (UTCHEM). There are great numbers of numerical techniques to simulate the groundwater flow and contaminant transport through porous media. Important numerical techniques include finite-difference methods (FDM), finite element methods (FEM), and finite volume methods (FVM). The finite element method is used by Zhao and Valliappan (1994) to simulate the transient contaminant migration problems in infinite porous media. Dehghan (2004) simulated the one-dimensional advection–diffusion equation by using a weighted finite-difference technique. The results of this method have better precision and accuracy in contrast to the classical approach. Karahan (2006) employed an implicit finite-difference method to solve the advection–diffusion equation. The implicit method guarantees the stability of the method and growing the convergence speed by increasing time steps. The finite element method for simulating the fractional advection-dispersion equation is used by Huang et al. (2008). A simple, accurate, and requires no meshing method is introduced by Ciftci et al. (2012); in this technique, a meshless method is used to simulate the contaminant migration. Kaya and Gharehbaghi (2014) used various numerical methods to solve the advection–diffusion equation. They concluded that the results show DQM is a better method than other numerical approach and after that the results of FVM and FOFDM are more reliable. Ahmed et al. (2019) used a 3D simulation model, combining the modular finite-difference flow model and the modular three-dimensional transport model to find a safe groundwater withdrawal away from the pollution sources. They predicted the distribution of heavy metal concentration with both time and distance and determined the safe location for water extraction from this aquifer. The result of their investigation was well located at a minimum of 113 m away from the leachate collection lake to be safe from all studied pollutants. Gharehbaghi (2017) employed a third- and fifth-order of accuracy with finite volume schemes to solve the advection–diffusion equation. The results indicate all both methods prepare acceptable and accurate results for an extremely long distance; however, the third order of accuracy method makes a more reliable prediction of contaminant transport.

Lalehzari et al. (2013) studied nitrate transport and wastewater seepage in the groundwater flow system using a three-dimensional solute transport model and geographical information system. The results show that the developed model is successfully used to simulate flow path and nitrate transport in saturated porous media. Sharma et al. (2014) investigated contaminant transport through fractured porous media. They carried on an experiment to study contaminant transport. The pollutants of the simulation are sodium chloride as a conservative chemical and sodium fluoride as a reactive one. The concentration profiles of the experiments revealed that there is substantial diffusion and sorption in the fractured porous matrix. Faisal et al. (2014) carried out an experiment to investigate the Trichloroethylene migration thorough saturated sandy soil in three dimensional; moreover, COMSOL is used to simulate the contaminant concentration. The average difference between experimental and numerical results which was 5% indicates a favorable agreement. Nazir et al. (2014) used a new method to solve the transport equation called the cubic trigonometric B-splines approach. This method is based on the operator splitting method helping to obtain accurate results. In this technique, the operators are considered separately for physical compatibility. Sarraute et al. (2019) investigated the effect of the diffusivity on the transport and fate of pesticides. They studied diffusion coefficients of six common pesticides and represent new diffusion coefficients for those pesticides which are more acceptable in regard to the latest coefficients.

The main purpose of this study is to make a numerical investigation of the contaminant transport through saturated porous media by imputing some initial data about the hydraulic properties of the aquifer and soil properties of the porous media. This paper proposed an integrated model for simulating the underground water flow and contaminant transport in aquifer systems. This model is applied to the Jajrud rural district, which receives both significant groundwater inflow and potential sources of contamination; consequently, some site information such as geological data, hydraulics head, and concentration of the contamination is obtained. Pollution migration in porous media should be regarded as a preeminent task in environmental engineering, and its consequences should be managed and controlled to avoid a negative impact on the environment.

Methodology

Numerical methods are regarded as an effective way to solve complicated mathematical problems. In this research, it is used to solve both groundwater flow and contaminant transport equations. These equations are introduced below:

Groundwater flow equation

The partial differential equations, describing the groundwater flow, can be expressed as follows (Harbaugh 2005):

$$\frac{\partial}{\partial x}\left(K_x(\psi)\frac{\partial\psi}{\partial x}\right)+\frac{\partial}{\partial y}\left(K_y(\psi)\frac{\partial\psi}{\partial y}\right)+\frac{\partial}{\partial z}\left(K_z(\psi)\frac{\partial\psi}{\partial z}\right)=\left[\frac{\theta}{n}S_s+S_m(\psi)\right]\frac{\partial\psi}{\partial t}+S \tag{1}$$

where ψ is Pressure head, K is hydraulic conductivity, θ is the moisture content, n is porosity, S_s is specific storage, S_m is the specific moisture capacity and S is source or sink term.

Transport equation

The contaminant transport equation is made of three terms: advection, diffusion, and reaction (Harbaugh 2005).

$$D_x\theta\frac{\partial^2 C}{\partial x^2}+D_y\theta\frac{\partial^2 C}{\partial y^2}+D_z\theta\frac{\partial^2 C}{\partial z^2}-u\frac{\partial C}{\partial x}-v\frac{\partial C}{\partial y}-w\frac{\partial C}{\partial z}-\lambda\theta R_d C=\theta R_d\frac{\partial C}{\partial t} \tag{2}$$

where C is contaminant concentration, D is the hydrodynamic dispersion coefficient, (u,v,w) are the component of the velocity field in x, y and z directions, θ is the moisture content, R_d is retardation factor and λ is decay factor.

$$R_d=1+\frac{\rho_b}{n}K_d \tag{3}$$

ρ_b is bulk dry density of the porous media, n is the effective porosity of the porous media and K_d is partition coefficient.

The components of the hydrodynamic dispersion coefficients are also calculated by below equation:

$$D_x=\alpha_L\frac{u^2}{|V|}+\alpha_{TH}\frac{v^2}{|V|}+\alpha_{TV}\frac{w^2}{|V|}+D^* \tag{4}$$

$$D_y=\alpha_L\frac{v^2}{|V|}+\alpha_{TH}\frac{u^2}{|V|}+\alpha_{TV}\frac{w^2}{|V|}+D^* \tag{5}$$

$$D_z=\alpha_L\frac{w^2}{|V|}+\alpha_{TH}\frac{u^2}{|V|}+\alpha_{TV}\frac{v^2}{|V|}+D^* \tag{6}$$

where α_L is the longitudinal dispersivity, α_{TH} is the horizontal transverse dispersivity, α_{TV} is the vertical transverse dispersivity, D^* is molecular diffusion coefficient and $|V|$ is the velocity average.

Numerical approach

The numerical technique which is used in this article is the finite-difference method. This method is used to discretize both underground flow and contaminant transport equations.

Groundwater flow equation

Discretizing Eq. (1) results in:

$$\left[\frac{\theta}{n}S_s+S_m(\psi)\right]\frac{\psi^{n+1}_{i\cdot j}-\psi^n_{i\cdot j}}{\Delta t}=K_x\left(\frac{\psi^n_{i+1\cdot j}-2\psi^n_{i\cdot j}+\psi^n_{i-1\cdot j}}{\Delta x^2}\right)+K_z\left(\frac{\psi^n_{i\cdot j+1}-2\psi^n_{i\cdot j}+\psi^n_{i\cdot j-1}}{\Delta z^2}\right) \tag{7}$$

Contaminant transport equation

The transport equation consists of three terms, advection, dispersion, and reaction terms.

The one-dimensional advection equation is discretized by third order of accuracy method.

$$\frac{\partial C}{\partial t}=\frac{\partial(uc)}{\partial x} \tag{8}$$

$$C_i^{n+1}=\left(\frac{1}{6}\left|\varepsilon^3\right|-\frac{1}{6}|\varepsilon|\right)C^n_{i-2}+\left(-\frac{1}{2}\left|\varepsilon^3\right|+\frac{1}{2}\varepsilon^2+|\varepsilon|\right)C^n_{i-1}+\left(\frac{1}{2}\left|\varepsilon^3\right|-\varepsilon^2-\frac{1}{2}|\varepsilon|+1\right)C^n_i+\left(-\frac{1}{6}\left|\varepsilon^3\right|+\frac{1}{2}\varepsilon^2-\frac{1}{3}|\varepsilon|\right)C^n_{i+1} \tag{9}$$

The one-dimensional diffusion equation can be discretized as follow:

$$\frac{\partial C}{\partial t}=\frac{\partial\left(D_x C\right)}{\partial x} \tag{10}$$

$$C^{n+1}_{i\cdot j}=\frac{D_x\Delta t}{\Delta x^2}\left(C^n_{i+1\cdot j}+C^n_{i-1\cdot j}\right)+\left(1-\frac{2D_x\Delta t}{\Delta x^2}\right)C^n_{i\cdot j} \tag{11}$$

The reaction term is discretized as follow:

$$\frac{\partial C}{\partial t}=\lambda C \tag{12}$$

$$C^{n+1}_{i\cdot j}=\frac{C^n_{i\cdot j}}{1-\lambda\Delta t} \tag{13}$$

The stability conditions for the equation are:

$$0<\varepsilon=\frac{u\Delta t}{\Delta x}<1 \tag{14}$$

$$0<\frac{D_x\Delta t}{\Delta x^2}<0.5 \tag{15}$$

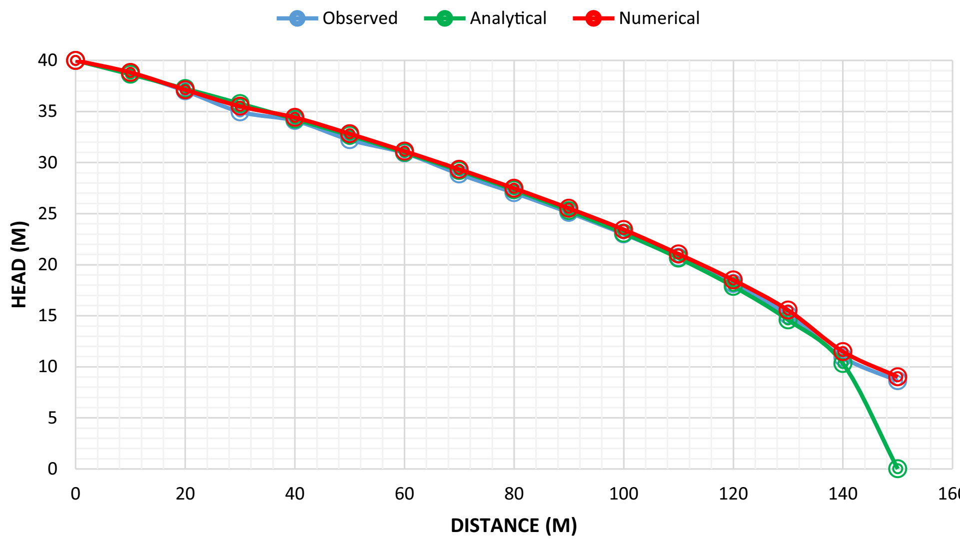


Fig. 1 Comparison of the numerical results and experimental of the flow model

Boundary condition

A couple of boundary conditions can be considered in the simulation practice, first, which the parameter is constant and its value is known (Dirichlet B.C.), second, the other when the flow rate is known. Every of the mentioned stages are prepared for the acceptable definition of the boundary conditions.

Verification

The performance of the presented numerical model has been verified by a couple of test cases to ensure its capabilities and accuracy. The performance of the numerical model is assessed with statistical parameters. Following parameters that is mean error (ME) and root mean square error (RMSE).

Verification of the groundwater flow model

To validate the flow model, the results of the test carried out by Afzali et al. (2009) are used. They conducted an experiment to simulate the water flow in the porous media. The boundary conditions at the upstream and downstream heads are fixed and equal to 40 and 0 m, respectively.

The results are plotted against the measured hydraulics head showing in Fig. 1. The comparison indicates that the results of the numerical model and the experimental data have a good agreement; however, an analytical approach cannot prepare a proper prediction.

$$\mathrm{ME} = \frac{1}{n}\sum_{i=1}^{n}\left(H_{\mathrm{sim}} - H_{\mathrm{obs}}\right) \tag{16}$$

$$\mathrm{RMSE} = \left[\frac{1}{n}\sum_{i=1}^{n}\left(H_{\mathrm{sim}} - H_{\mathrm{obs}}\right)^2\right]^{0.5} \tag{17}$$

H_{sim} is the simulated head and H_{obs} is observation head.

ME parameter is 0.12 m and RMSE is 0.134 m. The parameters magnitudes prove the acceptable accuracy of the numerical model.

Validation of contaminant transport model

In order to validate the contaminant transport model and verify the capability, accuracy, and efficiency of which, an analytical approach is used. This analytical solution is proposed by Van Genuchten and Alves (1982). The initial and boundary conditions are expressed as:

$$0 < x < \infty \quad t = 0 \quad C(x = 0) = 0 \tag{18}$$

$$t > 0 \quad x = 0 \quad C(0 \cdot t) = C_0 \tag{19}$$

$$t \geq 0 \quad x = \infty \quad \frac{\partial C(\infty \cdot t)}{\partial x} = 0 \tag{20}$$

The analytical solution is presented:

$$C(x \cdot t) = \frac{C_0}{2}\left[\exp\left(\frac{x}{2D_x}(U - V)\right)\mathrm{erfc}\left(\frac{x - \frac{vt}{R_d}}{2\sqrt{\frac{D_x t}{R_d}}}\right) + \exp\left(\frac{x}{2D_x}(U - V)\right)\mathrm{erfc}\left(\frac{x + \frac{vt}{R_d}}{2\sqrt{\frac{D_x t}{R_d}}}\right)\right. \tag{21}$$

where

$$V = \sqrt{U^2 + 4\lambda D_x R_d}$$

and erfc is error function.

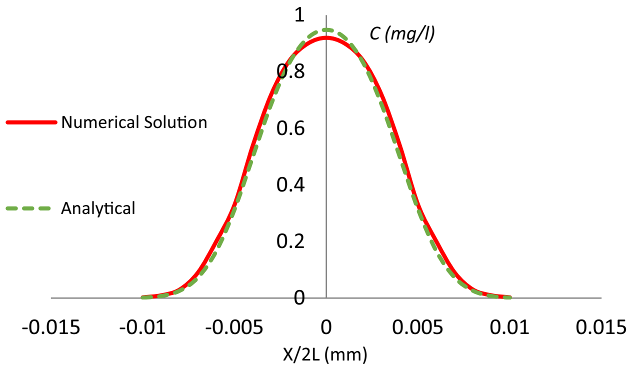


Fig. 2 Comparison of the numerical results and analytical solution of the transport model

The dimensions of the experiment are $200 \times 4000 \times 10$ mm^3. The less thickness of the model causes the model can be regarded as two dimensional. The contaminant concentration is calculated in several points with the same height; consequently, the concentration is plotted through the length in the fixed height.

The results of the analytical and numerical result have been shown in Fig. 2.

$$\mathrm{ME} = \frac{1}{n}\sum_{i=1}^{n}\left(C_{\mathrm{sim}} - C_{\mathrm{anl}}\right) \tag{22}$$

$$\mathrm{RMSE} = \left[\frac{1}{n}\sum_{i=1}^{n}\left(C_{\mathrm{sim}} - C_{\mathrm{anl}}\right)^2\right]^{0.5} \tag{23}$$

C_{sim} is the simulated concentration and C_{anl} is analytical head.

ME parameter is 0.27 mg/l and RMSE is 0.324 mg/l. These statistics parameters prove the acceptable accuracy of the numerical model.

The contaminant transport model has been successfully verified. Therefore, the coupled model is attested by the experimental and analytical solution. The intergraded model is a robust and accurate model to simulate the groundwater flow and contaminant transport.

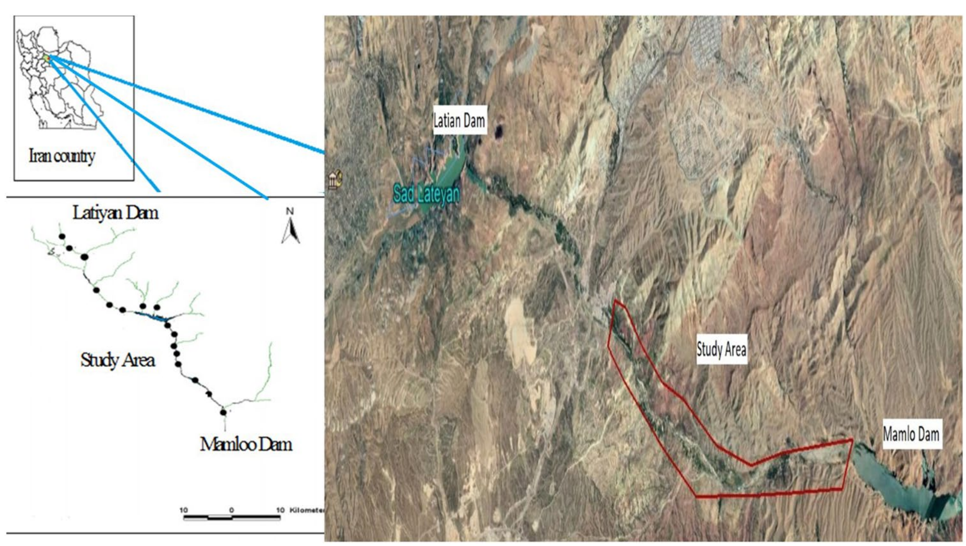
Information on the study site in situ

Description of the study site

The study site, Jajrud rural district, is a rural district in Pardis County, Tehran Province, Iran. The area is about 1750 km^2 and is located upstream of the Mamloo basin dam, (Fig. 3). The topography in this part of the Jajrud rural district is generally flat lying. The study area ranges in elevation from 1650 to 1750 m above sea level and the mean slope is about 15 m/km. The slope conture has been shown in Fig. 4.

The study is lies between the longitudes N 35° 42′ 36″ and N 35° 40′ 12″ and latitude E 51° 40′ 12″ and E 51° 47′ 24″, and it is occupied a total area of 10,548 m^2. The mean value of precipitation in this area is 25,054.4 mm/year, and the value of the evaporation is 1852 mm/year. It extends from northeast to southeast Tehran province, Iran. The maximum and minimum elevations are 3000 and 867 m, respectively. Land covers were rangeland, badland, sand borrow, agriculture land, and urban regions. Climate according to the weather station is sub-humid, semi-arid, and arid in the north, central, and south regions, respectively. The majority of rain and snow falls from November to April.

Fig. 3 Location of study area



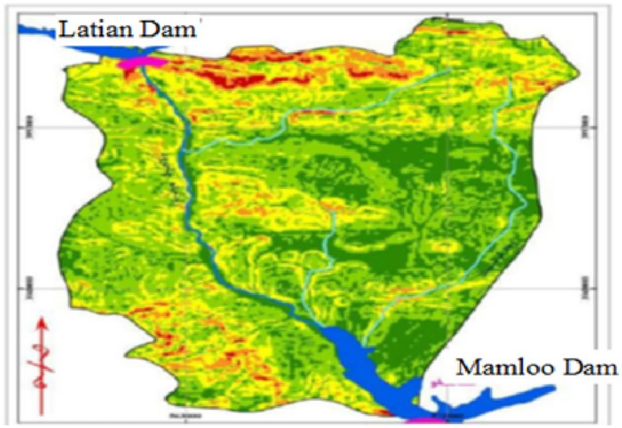


Fig. 4 The slope counters in the study area

Geological and hydrological characteristics

The bedrock of the area shows that the study area and varies in elevation from 1650 to 1750 m above sea level. In some special portions of the study area, gravel overlies the clay.

Twelve boreholes with a thickness of about 3.8 m are used to collect initial and input data. The boreholes are three rows and four columns (Fig. 5). The soil profile is determined with some major hydraulics, and geological data are obtained. The general soil structure is silty clay, and the hydraulic conductivity is 5.5 cm/h. The mean hydraulic head of all boreholes indicated 0.03 hydraulic gradients.

The boundary conditions of both upstream and downstream mainly derived from data of the in situ boreholes monthly measured in 2015. The soil of the study area was assumed to be isotropic, and the mean hydraulic conductivity of area was taken from in situ and laboratory hydraulic test as shown in Table 1. Finally, the different parameters of the contaminant source were obtained from a laboratory sampling test which was carried out in December 2015.

The soil layers are defined in Fig. 6; moreover, the mesh of the study area is shown.

Fig. 5 Arrangement of the boreholes

Discussion

Prediction of the pollutant plume in the jajrud rural district needs the information on the geological parameter, topography, monthly rainfalls, the soil profile, pollutant concentrations, and the hydraulic head taken from in situ boreholes.

In order to make an accurate numerical simulation of the groundwater flow and contaminant transport processes, proper description of both geological and hydraulics conditions is essential. The geometry and boundaries of the study area are arising from the topographic survey data.

Table 1 Model parameter

Parameter	Value	Unit
Porosity	0.33	–
Top layer conductivity	1.2	m/h
Second layer conductivity	0.34	m/h
Deepest layer conductivity	0.0061	m/h
Upstream boundary condition	40	m
Downstream boundary condition	20	m

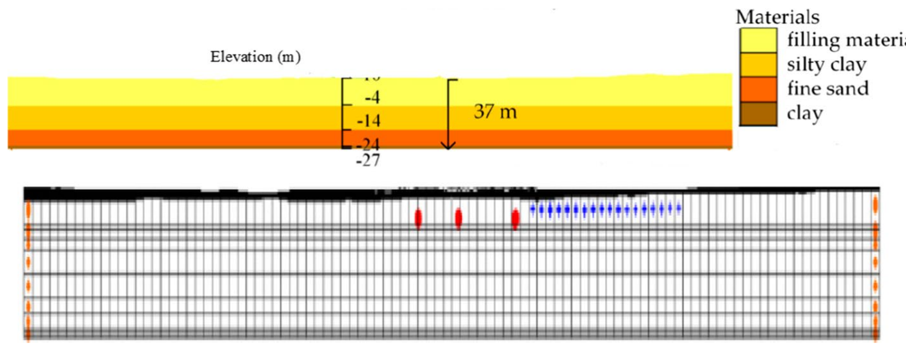


Fig. 6 Calculation domain and mesh of study area

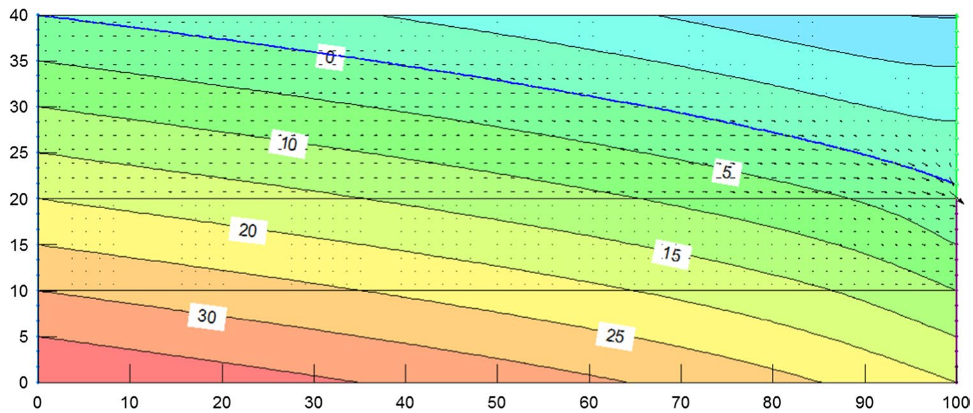


Fig. 7 Simulated pressure head

The first step for simulation is to collect some hydraulic in situ data. These parameters should be either measure or calculated. After collecting both geological and hydraulics parameters simulation is started.

After collecting a great deal of the data, the numerical models are used. First, the flow model is used to extract the velocity field after that transport model is used to simulate and predict the pollution plume.

Flow model

The developed model is used to simulate the underground water flow. The model has 135 columns, 110 rows and 4 layers with different hydraulic properties. The hydraulic conductivity of which is presented at Table 1.

The impermeable bedrock was set as a no-flow boundary beneath the model layers. The upper and lower boundary condition is obtained by the experiments.

The simulation results from the flow model provided the pressure head distribution in the aquifer. By the distribution of which the velocity field is obtained (Fig. 7).

The results of the computed pressure heads were verified against the field measurements and SEEP/W results (Fig. 8). The results indicate the acceptable agreement among the results which utterly verify the numerical model performances in the prediction of groundwater flow through porous media.

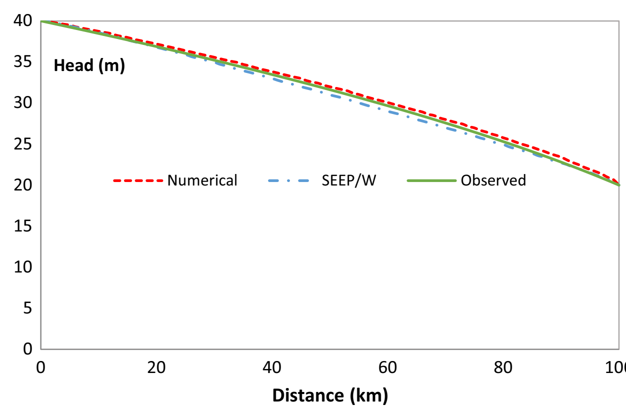


Fig. 8 Phreatic line of the study area

The results of the groundwater table clarify the bound of the saturated and unsaturated zones which is a conspicuous parameter for simulation of contaminant transport. In addition, Fig. 8 reveals that approximately great area of the porous media can be regarded as a saturated zone since the groundwater table is nearly close to surface and the vadose zone is not considerable; furthermore, in this configuration of soil layers, the top layer which has more hydraulic conductivity in comparison with the other layers has the least drawdown and more velocity. In fact, the permeable layer conveys groundwater flow with less energy loss in contrast

Table 2 Transport model input

Parameter	Value	Unit
Reactive pollutant molecular diffusion coefficient	0.00005	m^2/year
Non-reactive pollutant molecular diffusion coefficient	0.000036	m^2/year
Decay factor	0.00001	S^{-1}
Hydrodynamics dispersion coefficient	0.01	m^2/year
Longtidual despersivity	12.3	m
Transverse dispersivity	1.23	m
Retardation factor	1	–
Concentration of source point	100	mg/l

to less permeable layers. The less permeable layer is, the more pressure head decreases. By increasing the width of the permeable layer, pressure head and hydraulic head has less reduction.

Transport model

The flow model results include the velocity field which gives this opportunity to use the contaminant transport model. The aquifer was assumed homogeneous, and it is contaminated by source point pollution. The longitudinal and transverse dispersivity are shown in Table 2.

The experiment has been done with both kinds of reactive and non-reactive pollutants.

The reactive pollutant is dried milk powder and the acid sulfuric used as a tracer of which and the Fluorescein sodium is utilized as a non-reactive pollutant. Molecular Formula of which is $C_{20}H_{10}Na_2O_5$.

Fluorescein sodium concentration cannot be measured directly. The wavelength of which can be measured by spectrophotometer and the relation of the wavelength, and the concentration was used to calculate the contaminant concentration. The set model is DR6000 which made by the HACH company (Fig. 9).

- Reactive pollutant

In order to follow the reactive pollutant plume, the dried milk is injected at the farthest borehole, and the pollutant concentration is measured in the different wells at the various time intervals. The simulation by the proposed model is presented in Fig. 10.

To get a deeper understanding of the contaminant migration, the pollution plume is simulated by the proposed

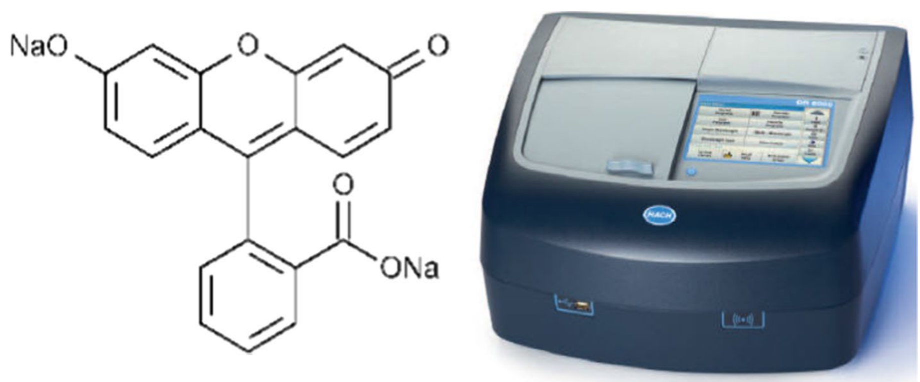


Fig. 9 Fluorescein sodium structure and spectrophotometer tool to determine the concentration of Fluorescein sodium

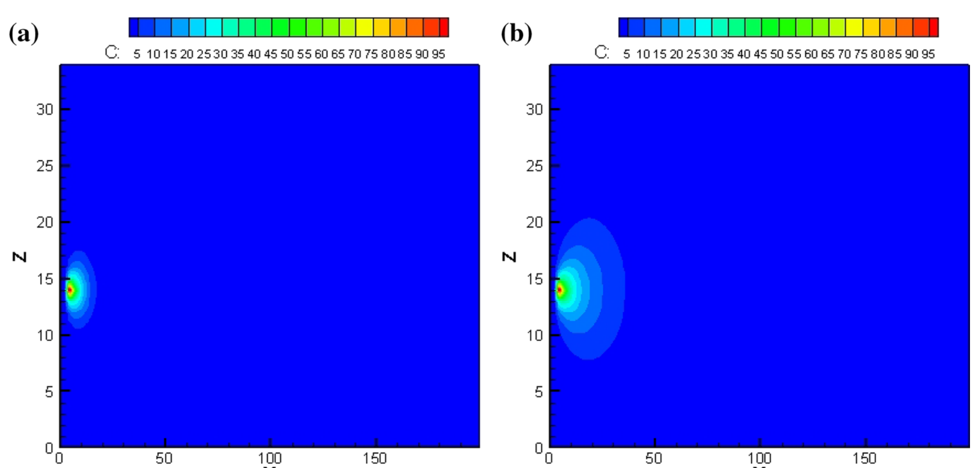


Fig. 10 Pollution plume of reactive pollutant after 36 and 72 h

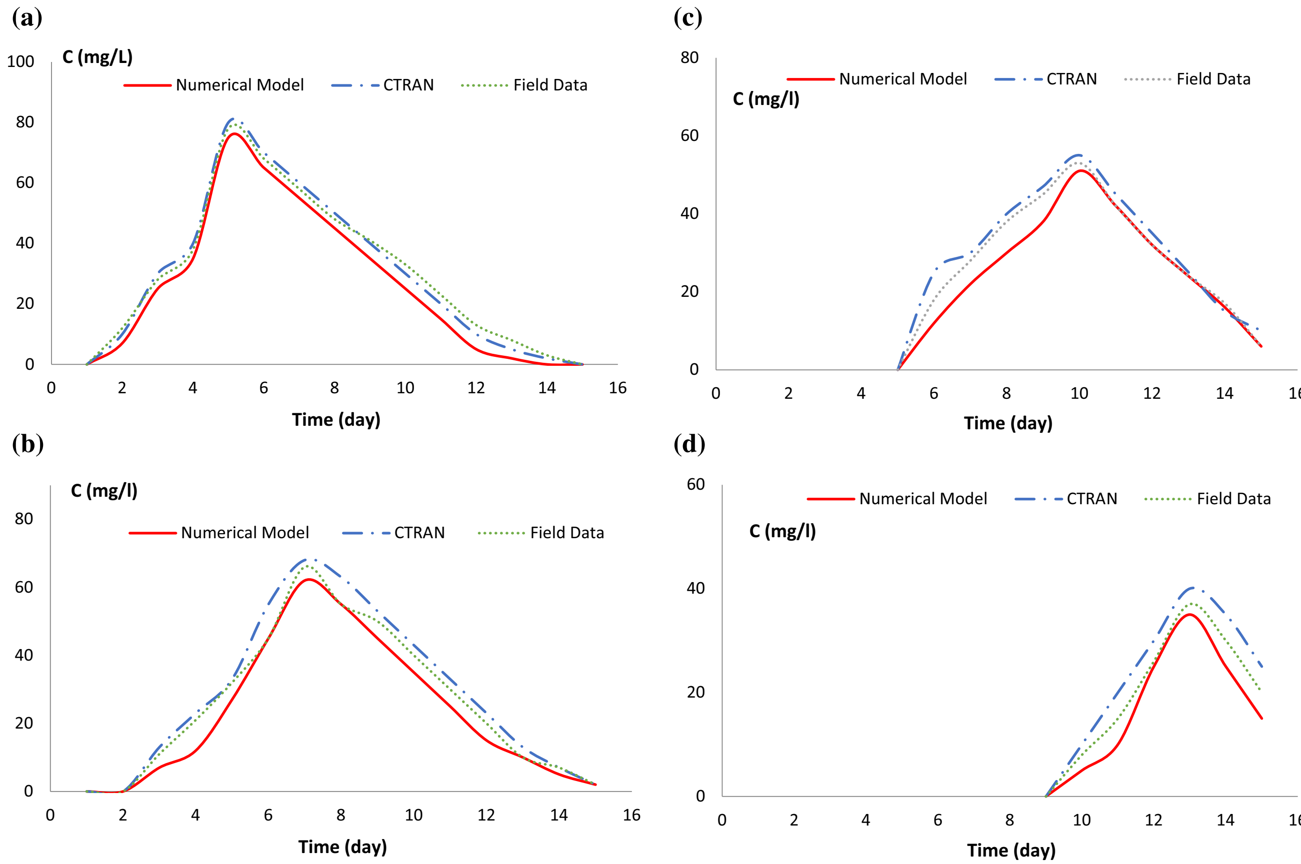


Fig. 11 Pollution plume of the reactive pollutant in the different boreholes. **a** first borehole **b** second borehole **c** third borehole **d** last borehole

model and CTRAN (commercial model) at the point of boreholes. Figure 11 shows the comparison of the contaminant migration in the porous media different methods.

Figure 11 indicates that the numerical model has enough capability of determining contaminant transport since the results of the numerical model are in great acceptance with both CTRAN results and field data. Besides, the results show by time passing, the peak of contaminant concentration in the boreholes decreases as a result of dispersion, diffusion, and some reactions in the porous media. All of which results in the reduction in concentration during a time period. 14 days is a period during which a reactive contaminant migrates the distance between first and last boreholes, and the ratio of contaminant concentration at the initial time to the final time nearly equal 0.4.

- Non-reactive pollutant

The same procedure is done for the non-reactive pollutant (Fig. 12). The comparison among the different results of the pollution plume has been shown in Fig. 13.

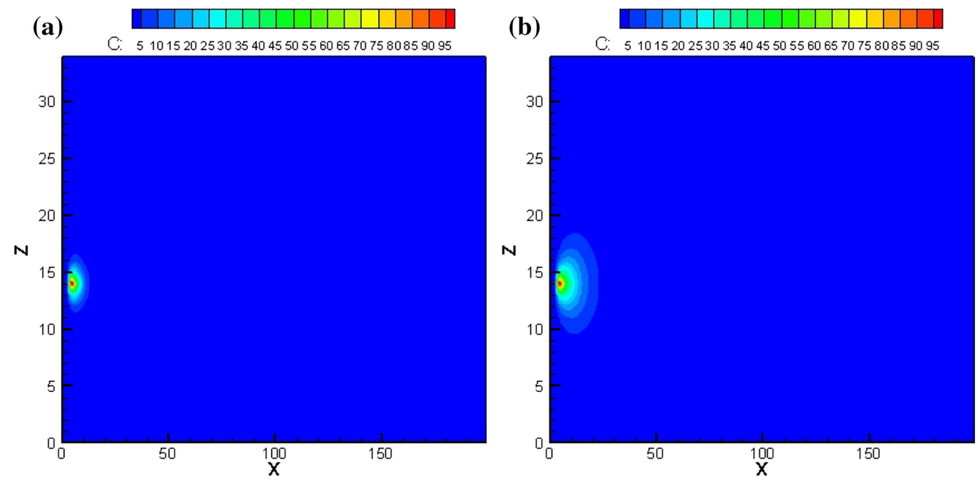
To get an acute insight into the performance of the numerical model in predicting contaminant transport through porous media, CTRAN and field data have been compared with the outcome of numerical simulation.

The comparison of the numerical model outcome and the commercial model results and field data represents great accordance between the results which validate the accuracy of the numerical model to determine pollution plume. Similar to the last case, the concentration of contaminant dwindles over a time period; nevertheless, the reduction in the concentration is less than the last case since the contaminant is not reactive as was the last case; thus, the contaminant does not have reaction and reduction in concentration. The ratio of contaminant concentration at the initial time to the final time closely equals 0.55.

The comparison between the reactive and non-reactive contaminant concentration and the taken time to reach the last borehole have been presented in Table 3.

By comparing the results of contaminant transport in both cases (non-reactive and reactive contaminants) the following outcomes have been drawn. As it is shown in Figs. 10, 11, 12, and 13 advection rate in both conditions is the same, and it prevailed other terms in the contaminant transport process because both cases have the same hydraulic condition and similar velocity field. The results clearly indicate the advection rate is the dominant phenomenon in the contaminant migration. As a result of the same velocity field and identical configuration for porous media, longitudinal and horizontal

Fig. 12 Pollution plume of non-reactive pollutant after 36 and 72 h



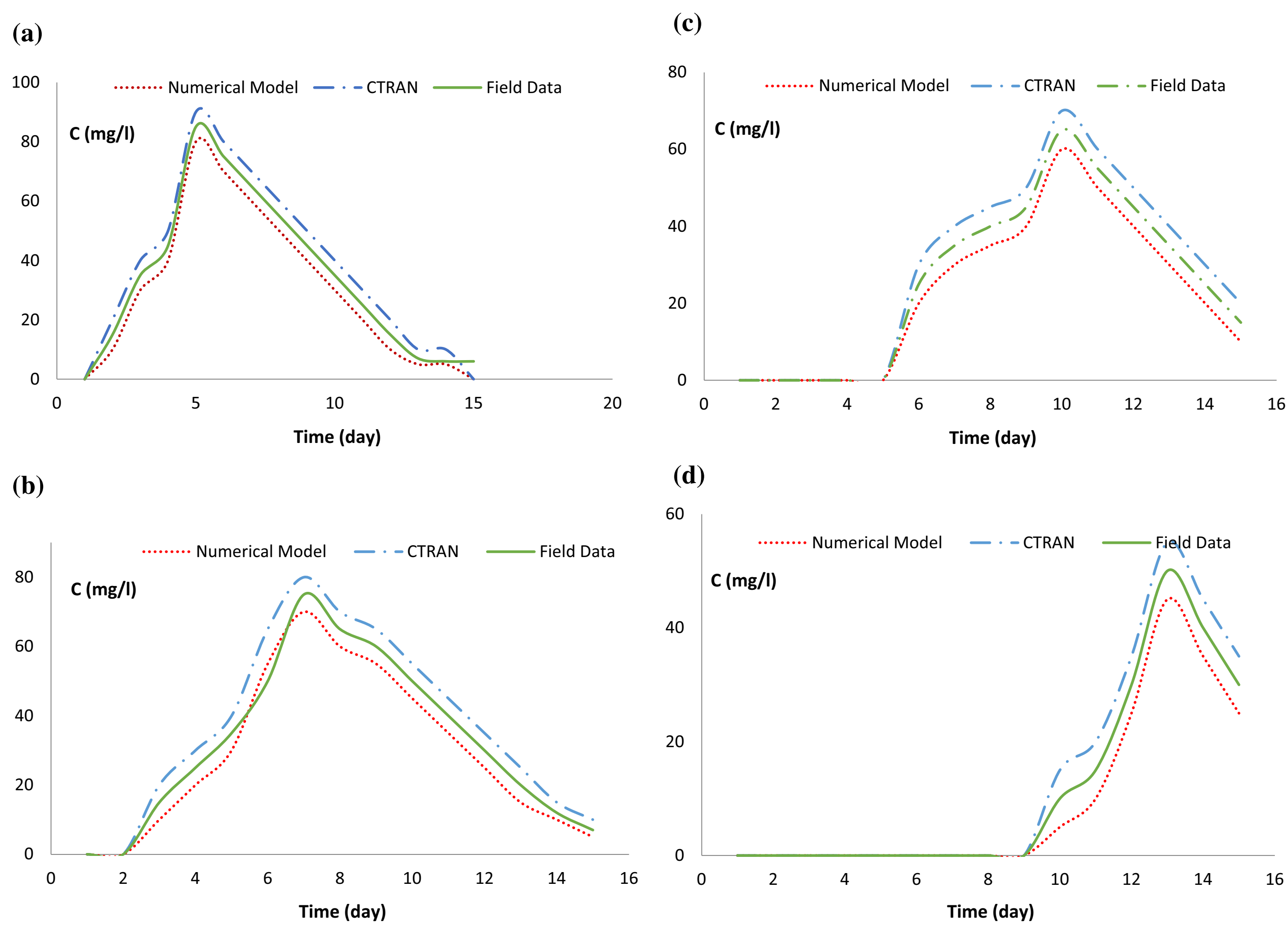


Fig. 13 Pollution plume of the non-reactive pollutant in the different boreholes. **a** First borehole **b** second borehole **c** third borehole **d** last borehole

dispersitivity is the same in both conditions; however, the diffusion rate is not the same since the coefficient of the molecular diffusion in both conditions differ. Decay term is the main difference of the cases which causes the concentration of the contaminant reduces. Decay term in the reactive pollutant makes concentration diminish. The reactive pollutant has less contaminant concentration as a result of more diffusion rate and reactions which triggers the concentration of the contaminant dwindles in every step. Furthermore, the result indicates the advection rate is much more than the dispersion and decay terms in both conditions, which means the advection is the predominant process at the contaminant transport in the

Table 3 Comparison of reactive and non-reactive contaminant migration

Contaminant	Concentration (mg/l)	Taken time (days)
Reactive pollutant	54	14
Non-reactive pollutant	37	14

aquifers, and it does not depend on contaminant properties. The comparison of the concentration of reactive and non-reactive pollutant revealed that in the non-reactive pollutant case the concentration of the contaminant is roughly 15% more the concentration of reactive pollutant which means reactions of the pollutant with porous media decline approximately 10% of the contaminant concentration and advection and dispersion is the main reason of the reduction in the contaminant concentration through porous media.

The recent investigation shows the advection term has much more importance in contaminant transport and the same results have been drawn for both reactive and non-reactive contaminant transport. Furthermore, similar to the previous research results indicated that the portion of the reaction in the reduction in the contaminant throughout migration in porous media is not as significant as the other terms.

Scenarios

In this section, different states have been considered to investigate the contaminant migration through porous media. The description of each of the scenarios has been defined in Table 4. The reactive contaminant has been selected for the investigation of contaminant simulation. The scenarios aim to investigate the effect of the injection point distance and the initial concentration of the contaminant.

Groundwater flow and contaminant concentration have been simulated for all the above-mentioned scenarios and Fig. 14 shows the results of those.

Figure 14 shows the concentration of the reactive contaminant in the different scenarios. As it is shown in Fig. 14, increase in injection point distance is accompanied by dwindling of pollution concentration in the porous media; because by the increase in the injection point, contaminant dispersed more through porous media; thus, the concentration of the contaminant decline greater. As the dispersion is not the dominant phenomenon in the contaminant transport process the impact of elevating the injection point distance does not play a vital role in the decline of the reduction in the contaminant concentration. The results show by the increase of 100 m to the injection point the contaminant concentration just decrease by almost 10%. Another impact of the increasing distance of the injection point is that it brings about the contaminant takes more time to reach downstream which is an important parameter to control

Table 4 Scenarios description

Scenario	Injection point distance (m)	Initial concentration (mg/l)
1	100	100
2	100	200
3	200	100
4	200	200
5	300	100
6	300	200
7	400	100
8	400	200

the pollution. The difference between the contaminant taken time to reach downstream by the change of the distance of the injection point has been shown in Table 5.

On the other hand, the raise of the concentration of the initial condition brings about the growth of contaminant concentration through the porous media due to the fact that contaminant distribution will be a negligible part of the total concentration reduction. It should be mentioned that the concentration peak will not increase as much as the growth of the initial condition.

The effect of the initial contaminant concentration on the pollution concentration through porous media is more significant than the distance of the injection point.

Conclusion

In this paper, groundwater flow and contaminant transport were numerically and experimentally investigated. A coupled model was presented to predict the groundwater flow and pollution migration. The groundwater flow model simulates groundwater through both saturated and unsaturated zone, and the contaminant transport model uses special techniques, which are illustrated in the numerical

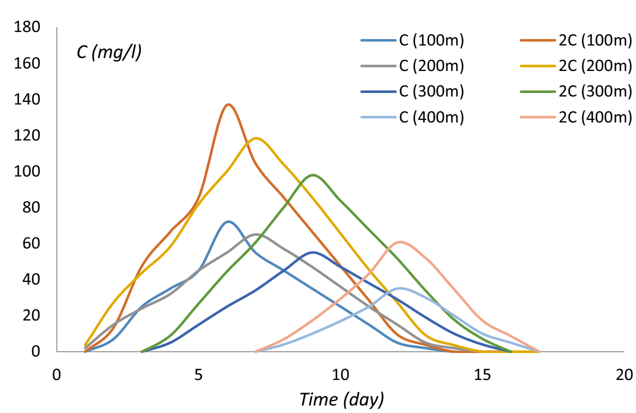


Fig. 14 Contaminant concentration of the reactive pollutant in the different scenarios

Table 5 Comparison of contaminant migration by the change of distance of the injection point

Distance (m)	Concentration (mg/l)	Taken time (days)
100	72.3	6
200	65.8	7
300	55.1	9
400	35.5	12

approach section, to predict both reactive and non-reactive pollutants. Besides, some experimental was carried out to find the migration of reactive and non-reactive pollutants fate in porous media. The numerical model results and experimental data are compared with each other to validate the numerical model and get an acute insight into contaminant transport through porous media.

The results indicate that the proposed numerical model is capable of simulation of groundwater flow and contaminant transport even in the complex geometry which using analytical calculations are impossible.

This research investigates a couple of pollutants with different properties. The first one decays and having more dispersion which triggers the more contaminant concentration reduction. The reduction effect because of the mentioned terms is about 33 percent in comparison with the non-reactive pollutant.

The increase in injection distance could possibly have mitigated the pollution through greater contaminant distribution; furthermore, the growth of initial concentration leads to a greater peak concentration.

When contaminant spread out in groundwater aquifers, the contaminant convects fast; consequently, the advection is the dominant process in the contaminant transport through saturated porous media. In order to stop the contamination risks and the ecosystem damage, it is highly recommended that take some actions to stop or decrease the velocity filed which brings about less advection and less pollution. Dispersion has played an important role in decreasing the contaminant concentration and distribution of pollution plume. To reduce the pollutant concentration more the distribution should be increased.

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References

Afzali SH, Abedini MJ, Monadjemi P (2009) Simulation of flow in porous media using coupled pressurized-free surface interconnected conduit network. Iran Water Resour Res 5(2):27–29

Ahmed AT, Alluqmani AE, Shafiquzzaman M (2019) Impacts of landfill leachate on groundwater quality in desert climate regions. Int J Environ Sci Technol 16:6753–6762

Ciftci E, Avci CB, Borekci OS, Sahin AU (2012) Assessment of advective-dispersive contaminant transport in heterogeneous aquifers using a meshless method. Environ Earth Sci 67:2399–2409

Dehghan M (2004) Weighted finite difference techniques for the one-dimensional advection-diffusion equation. Appl Math Comput 147:307–319

Derradji EF, Benmeziane F, Maoui A, Bousnoubra H (2011) Evaluation of salinity, organic and metal pollution in groundwater of the Mafragh watershed, NE Algeria. Arab J Sci Eng 36:573–580

Faisal AH, Kubba F, Madhloom H (2014) Modeling of trichloroethylene migration in three-dimensional saturated sandy soil. Arab J Sci Eng 39:7763–7769

Gharehbaghi A (2017) Third- and fifth-order finite volume schemes for advection–diffusion equation with variable coefficients in semi-infinite domain. Water Environ J 31(2):184–193

Harbaugh AW (2005) Modflow the U.S. geological survey modular ground-water model of the ground-water flow process. U.S. Department of the Interior, U.S. Geological Survey, Reston, VA, USA

Huang Q, Huang G, Zhan H (2008) A finite element solution for the fractional advection-dispersion equation. Adv Water Resour 31:1578–1589

Karahan H (2006) Implicit finite difference techniques for the advection–diffusion equation using spreadsheets. Adv Eng Softw 37:601–608

Kaya B, Gharehbaghi A (2014) Implicit solutions of advection diffusion equation by various numerical methods. Aust J Basic Appl Sci 8(1):381–391

Lalehzari R, Tabatabaei SH, Kholghi M (2013) Simulation of nitrate transport and wastewater seepage in groundwater flow system. Int J Environ Sci Technol 10:1367–1376

Nazir T, Abbas M, Ismail AIM, Majid AA, Rashid A (2014) The numerical solution of advection–diffusion problems using new cubic trigonometric B-splines approach. Appl Math Modell 40(7–8):4586–4611

Neretnieks I (1980) Diffusion in the rock matrix: an important factor in radionuclide retardation. J Geophys Res 85:4379–4399

Rahman SH, Khanam D, Adyel TM, Islam MS, Ahsan MA, Akbor MA (2012) Assessment of heavy metal contamination of agricultural soil around Dhaka export processing zone (DEPZ), Bangladesh: implication of seasonal variation and indices. Appl Sci 2(3):584–601

Sarraute S, Husson P, Gomes MC (2019) Effect of the diffusivity on the transport and fate of pesticides in water. Int J Environ Sci Technol 16:1857–1872

Sharma PK, Sawant VA, Shukla SK, Khan Z (2014) Experimental and numerical simulation of contaminant transport through layered soil. Int J Geotech Eng 8(4):345–351

Swain ED, Wexler EJ (1992) A coupled surface-water and ground water flow model for simulation of stream—aquifer interaction. U.S. Geological Survey Open-File Report, pp 92–138

van Genuchten MTh, Alves WJ (1982) Analytical solutions of the one-dimensional convective-dispersive solute transport equation. USDA ARS Technical Bulletin Number 1661. U.S. Salinity Laboratory, 4500 Glenwood Drive, Riverside, CA 92501

Wang JSY, Narasimhan TN (1985) Hydrologic mechanisms governing fluid flow in a partially saturated, fractured, porous medium. Water Resour Res 2(12):1861–1874

Zhao C, Valliappan S (1994) Numerical modelling of transient contaminant migration problems in infinite porous fractured media using finite/infinite element technique: theory. Int J Numer Anal Meth Geomech 18:523–541