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Numerical simulation of oil hydrocarbons and heavy metals transport in soil

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Abstract

Extensive entrance of oil hydrocarbons and heavy metals into subsurface soil and groundwater resources and characteristics of their propagation has become an important matter. The aim of this study is investigating the factors affecting the propagation of the contaminants in the soil using a numerical model called CTRAN/W. Hence a soil environment with 20 meters depth and 45 meters length analyzed. Boundary condition, initial condition and material properties in these simulations varied in every section. According to analyses, in coarse soils, the emission pattern is vertical and downward; however in fine soils horizontal distribution pattern is dominant. In other words generally in coarse soil the emission depth of soil pollution is more than emission length and in fine-grained the length of pollution is greater. With an increase in the density of contaminants, it has penetrated further into the aquifer and this makes it less spread on the surface of the aquifer. In both fine and coarse, the mainstream emission is vertical with an increase in transverse dispersion coefficient, the extent of pollution in the horizon increases. With an increase in longitudinal dispersion coefficient in both fine and coarse soil environment, a broader pattern of propagation is reached and other words in both horizontally and vertically, the emissions will increase. It was also observed that by increasing the ion exchange capacity, the arrival time of pollutants in the soil column increases and steep rise in emissions to reach its maximum is reduced. By increasing alkalinity, ion exchange capacity increases and therefore much more polluting soil adsorbs.

Keywords: Oil hydrocarbons, Heavy metals, Contaminants transport, Numerical modeling.

Introduction

Nowadays soil pollution is an important environmental issue that should be taken into consideration. The human in his daily activities enters considerable amounts of various contaminants in water, soil and the air. Soil, water and air are considered major environmental components. The primary origins of the discharge of heavy metals in soil, industrial activities such as mining, metal smelting, electroplating industry, metalworking, fuel consumption, sewage discharge and urban and industrial waste as well as the use of pesticides, fertilizers and sewage sludge in agriculture. Most of the contaminations transfer happens when the contaminants reached the aquifer; it dissolves in water and along with underground water and contaminates the environment. Thus the importance of studying how to move and spread of pollution, as well as recycling and unsaturated zone to reach the aquifer is determined.

Analysis of pollution movement in a permeable soil is of noticeable importance for an extensive spectrum of fields like engineering and bio medical treatments such as pollution removal, fuel uprooting, and destruction of atomic scraps[1]. Recently, the intensive investigations have been handled to completely explain the movement procedure, transportation, and conversion and impacts of pollutants discharge[2]. Numerous numerical models have been generated to consider for pollutants transportation in penetrable soil with various circumstances concerning groundwater migration, with special regard given to the movement process. Javadi et al. developed a mathematical model for analysis of movement of liquid and ventilation and pollutant transportation in unsaturated soils[3]. S. A. Kartha et al. formed a model to examine the impact of stationary content of water in the time of occurrence of the pollutant at the bottom of an unsaturated soil column[4]. Bandilla et al. offered a new developed approach named "Analytic Element Method (AEM)" which is an approach for analysis of macro scale underground pollutant transportation. It mixes the underground water with the Streamline Method, a split-operator, for representing radioactive transportation[5]. Mousavi Nezhad et al. presented improvement and utilization of a mathematical simulation of contaminant transportation regarding their heterogeneity in soil[6]. Feng Pan et al. investigated the contingency investigations for forecasting the flow and pollution transportation in a layered soil. They demonstrated the notable consequences of parameter correspondences on the irritability and uncertainty of unsaturated movement and transport[7].

In recent years, has seen a tremendous growth in interest in the focus on heavy metals movement. Chotpantarat et al. examined the transfer of singular, paired and multi-metal arrangements through soil samples and local advection–dispersion equilibrium model, or two-site unequilibrium model computationally and experimentally[8]. Tamer A. Elbana et al. assessed the pattern and collection of Heavy Metals as an outcome of long-range irrigation with household wastewater.

Plenty of heavy metal concentrations compared to the soil depth indicated that lead (plumbum) reposition was mostly in the top of soil[9].

A number of studies have applied mathematical equations in transport modeling. Bing Bai et al. shown that an exponentially deteriorated contaminant added to the penetrable medium moves progressively to the bottom and width of the permeable soil because of water movement and the diffusion caused by mechanical and molecular movement, with the displacement of the contaminant on the fixed model covering[10]. M.E. Gharamti et al. investigate the one-step-ahead formulation to acquire a new method which includes a level of the position between two successive simulation steps. The simulation shows a correspondence but different than the last which first develops the statue with the simulation then refreshes it with an updated investigation, the suggested design launch by an updated measure, supported a combination step[11]. In recent years, D. Ngo-Cong et al. changed the two dimentional diffusion and advection equation to its one dimentional estimation. The one dimentional simulation helps to instantly determine the horizontal extent of pollutants based on the simulation variables[12]. Shaymaa Mustafa et al. presented an analytic answer for contaminant transportation in river bank filtration which examines the impact of pumping and moving times[13].

Some of researchers considered external condition on contaminant transport. Yong Yin et al. examines the function of temporal and spatial equating of discharge in the calibration of TCE contaminant transportation factors by a flux-based approach for determining corresponding permeability to improve mathematical equilibrium[14]. Zi Wu et al. describe the effects of wetlands vegetation in which the single factor Alfa(α) could bring the longitudinal compression of the pollutant plume and the transformation of the form of the concentration profiles[15]. Marzena Rachwal et al. investigated the utilization of mixed approaches for quantitative and qualitative evaluation of top-soils of forest which is most vulnerable to be destroyed by the industrial emissions[16].

The research is structured as follows: in Section 2, Governing equations and solutions used in the software are presented. Modeling procedure has explained in section 3.Modeling results and software calibration has expressed in section 4.

Methodology

In this section governing equations and solutions has expressed. The general equation for pollution transportation is the one-dimensional advection-dispersion equality. The pollutant transportation equation can be obtained by analyzing the mass flux in an elemental amount of porous substance. The total pure mass flux over the element is:

$$M = \frac{\partial q}{\partial x}\, dx \tag{1}$$

In other word,

$$\frac{\partial M}{\partial t}\, dx = -\frac{\partial q}{\partial x}\, dx \tag{2}$$

If we consider C as the concentration and M as the mass of dissolved contaminants:

$$C = \frac{M}{V_W} \;\; \rightarrow \;\; M = C.V_W \tag{3}$$

and

$$M = C\Theta \tag{4}$$

Replacing M in equation.3 and dividing it by dx direct to:

$$\Theta \frac{\partial C}{\partial t} = -\frac{\partial q}{\partial x} \tag{5}$$

The two main mechanisms in transportantion are:

$$advection = v\Theta C = UC$$
$$dispersion = -\Theta D \frac{\partial C}{\partial x} \tag{6}$$

Where: N = average linear velocity, Θ = water content volumetric, D = hydrodynamic dispersion, coefficient, C = concentration, U = D'Arcy velocity (specific discharge).

By replacing the mentioned two expressions into Eq. (6) drives to the fundamental transport equation:

$$\Theta \frac{\partial C}{\partial t} = -\frac{\partial}{\partial x}\left(-\Theta D \frac{\partial C}{\partial x} + UC\right) = \Theta D \frac{\partial^2 C}{\partial x^2} - U \frac{\partial C}{\partial x} \tag{7}$$

Modeling procedure

CTRAN/W software: This software can model groundwater contaminant transportation queries. It is planned to employ the leekage flow velocities calculated because of water movement in the saturated and unsaturated soils. Simulating the migration of pollutant within the soil is a complicated kind of investigation. Pollutant transportation will be directed by adsorption, water movement, dispersion, diffusion, and radioactive decay.

There are three primary boundary conditions for pollution transportation: i. Detailed dispersive and advective flux (Cauchy). ii. Particularized concentration (Dirichlet); and, iii. Defined dispersive flux (Neumann).

When investigating the groundwater, we usually deal with this doubt by putting the exit line adequately distant from the region. We can use this method in transportation analysis, and the boundary can either be defined as a fixed intensity or fixed mass state.

Model Verification: In this section, we present analytical sample examples that have been used to compare the results of each of these cases and ultimately to determine the correct application and verification of the numerical model used in this research.

First validation example: This example was first presented by Bond and Wierenga in 1990, consists of a soil column with an 88.2 meters height. The experiments were carried out utilizing the 2 mm sample of covering soil. The composition of the exterior soil was 93% sand, 4% clay, and 3% silt. This soil stuff were completely mixed, wetted by the proper initial dilution to content of water equals to 0.034 kg/kg and bound in samples to an average dry bulk density of 1.73mg. m-3. The columns were moulded from clear acrylic sections, having an internal diameter of 20 mm and lengths varying from 5 to 25 mm. These columns allowed both breakthrough curves and resident concentration patterns to be marked[19].

The numerical model made by the Geo Studio software also has the boundary specifications and conditions described above. For example, the length of the dispersion coefficient is 0.2 m and the dispersion coefficient is perpendicular to the flow direction of 0.1 m. The results of solving this problem using two methods mentioned above and the results are compared with each other. It should be noted that the results shown in this figure are related to the relative concentration of the end point of the pathway of the pillars of the earth as compared to the initial concentration of pollution, which has been modified over time.

As it is known, after about two days of contamination, the path has reached the end of the path, and little has increased concentration at this end point. In general, there is good coordination between the outputs of the two methods as it has been showed in Figure-1.

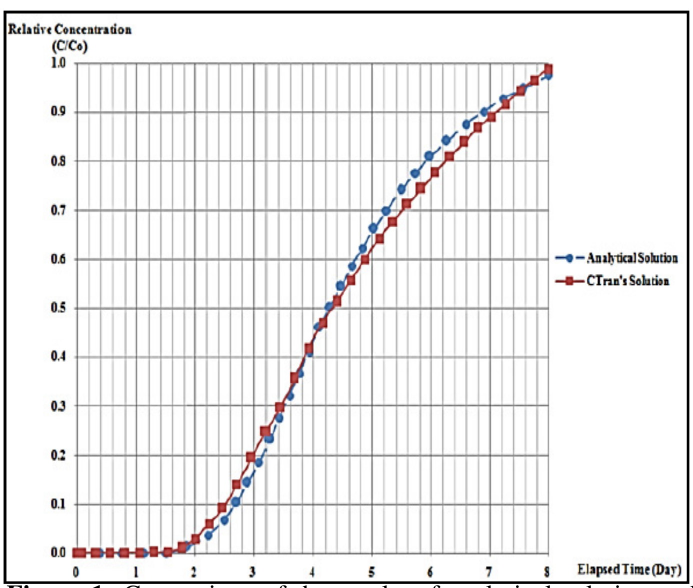


Figure-1: Comparison of the results of analytical solution and software solution CTRAN/W.

The second validation example: A layout of the experimental container used for D-NAPL movement experiments is represented in Figure-2. The container had a depth of 15 cm, width of 150 cm, and height of 82.5 cm. The container constructed of a main permeable material that was full of sands.. The chambers were joined with the main permeable material through a stainless steel web that blocked migration of sands and allowed for pore fluid effluent and two boxes placed at both sides of the main permeable material[20].

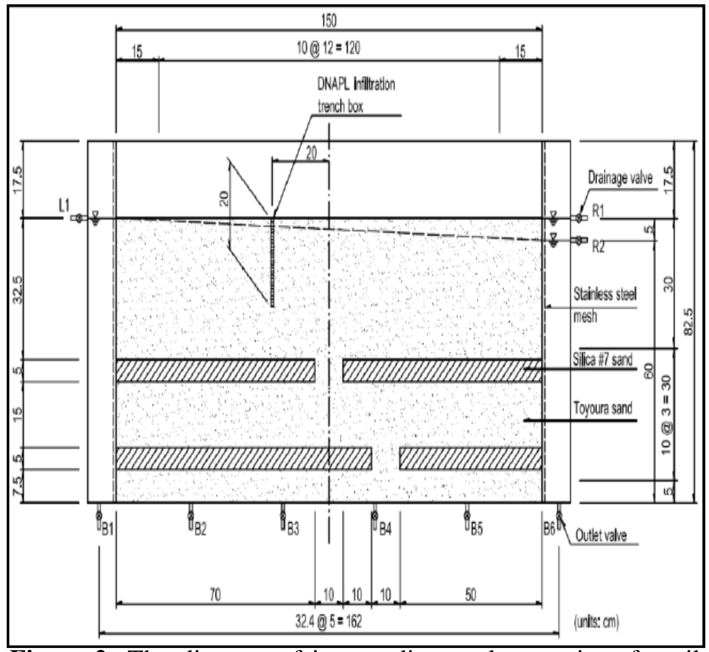


Figure-2: The diagram of intermediate-scale container for oil movement tests[20].

Viewed measurement outcomes of oil movement tests without underground water flow are presented in Figure-3. This figure shows photographs were captured 1, 4, and 7 h after injection. The contaminants moved from the injection point at the bottom of the trench box, as shown in Figure-3a. The migration pattern is shown below and it is like a water drop which moves to spread as if a balloon is being inflated.

For proving the validity of the empirical outcomes and confirm the availability of mathematical investigation as a means for foretelling two-phase current in permeable soil, mathematical studies conducted utilizing the 2D finite difference code. This mathematical code is suitable to examine multi-phase current with a sequence equating.

For the mathematical investigation, only the lower elevation portion of the bottom of the hollow case is regarded as the scientific field, as shown in Figure-4. The base edge of the container was impermeable to the liquid phase. The water pressure heads of both surfaces and the top were determined CONSIDERING the initial circumstances, therewith allowing water flow through the sides.

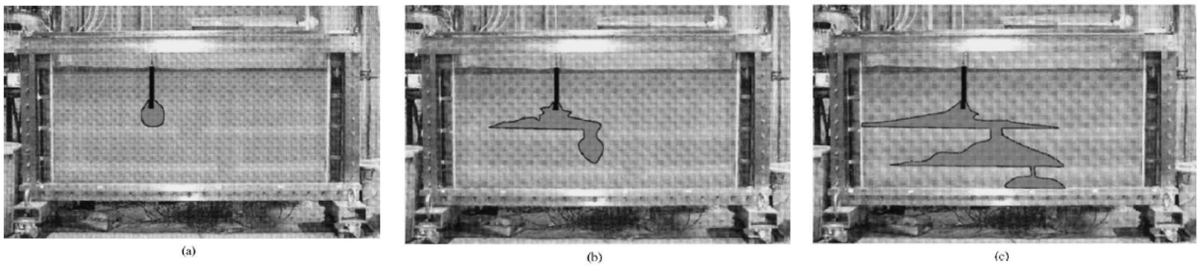


Figure-3: Contaminanrs transport outcomes without groundwater flow, i = 0.000: (a)after 1 hour; (b)after 4 hours; and (c)after 7 hours[20].

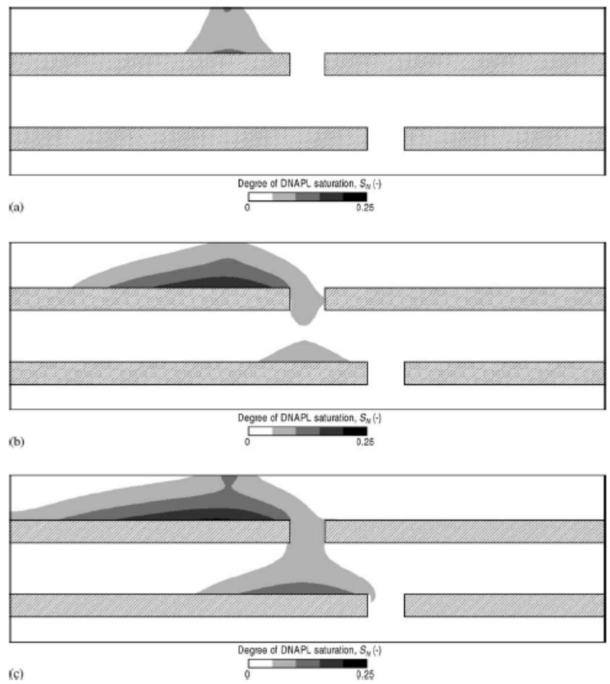


Figure-4: The results of computational analysis[20].

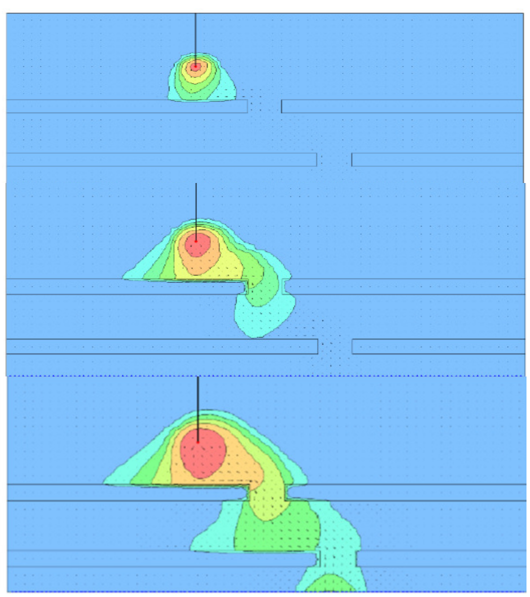


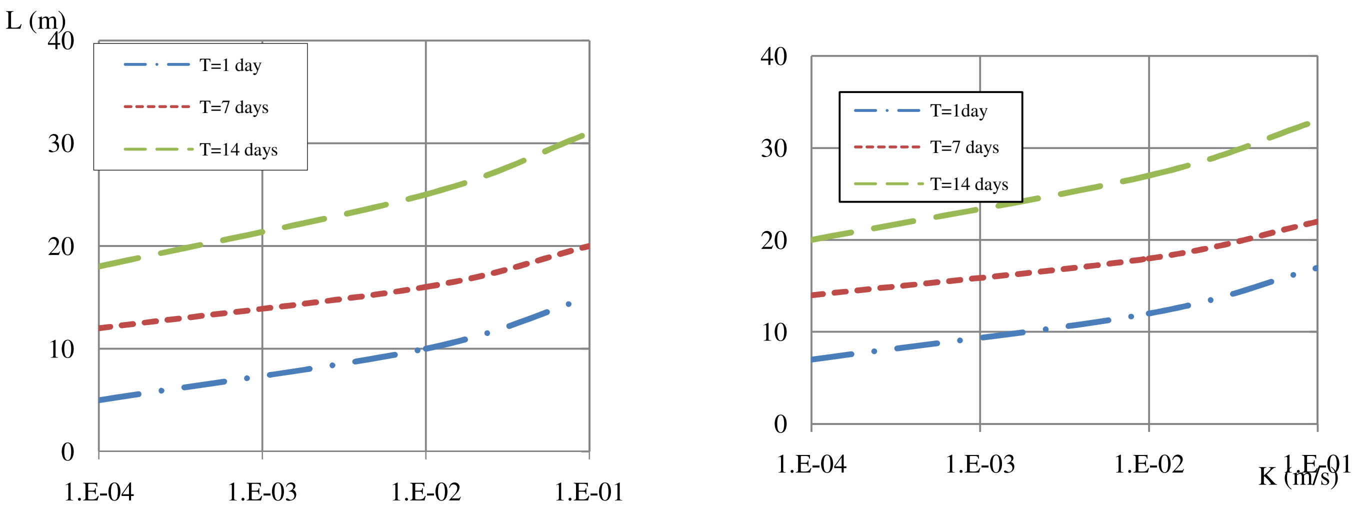
Figure-5: The results of Numerical simulation by CTRAN/W.

Modeling results

Here the effects of various parameters on the behavior and propagation pattern of pollution are discussed. In general, effects of different variables the permeability of the soil and the inflow discharge of pollutants in the soil site study to a depth of 20 meters and 45 meters length were analyzed. It is noteworthy that two parameters D and L, respectively are depth and length of pollution emission and measured subject to the point where contamination has spread to about 0.05 to 0.1 of initial concentration.

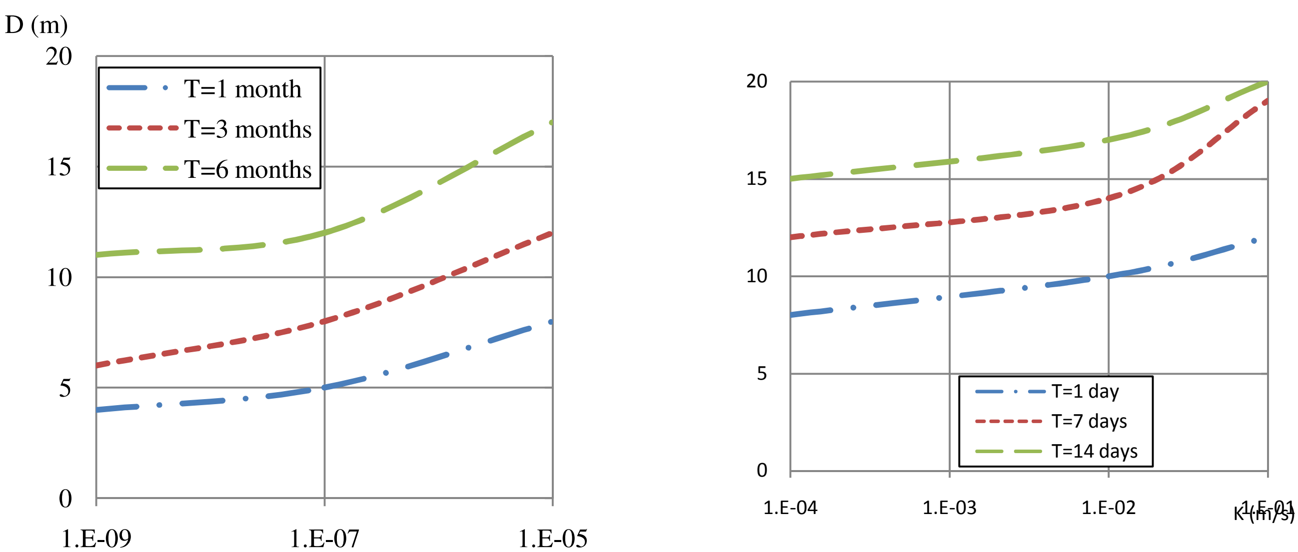
The effect of soil permeability on contaminant transport: For this analysis, two types of coarse and fine grained soil that contains different amounts of permeability of 10^{-1} meters per second to 10^{-9} meters per second is considered.

The sensitivity analysis for a variety of pollutants inflow, coarse-grained soil at 1, 7 and 14 days and fine grained soils at 1, 3 and 6 months considered. The relative density is equal to 1.2 for all models and underground water table assumed 5 meters.



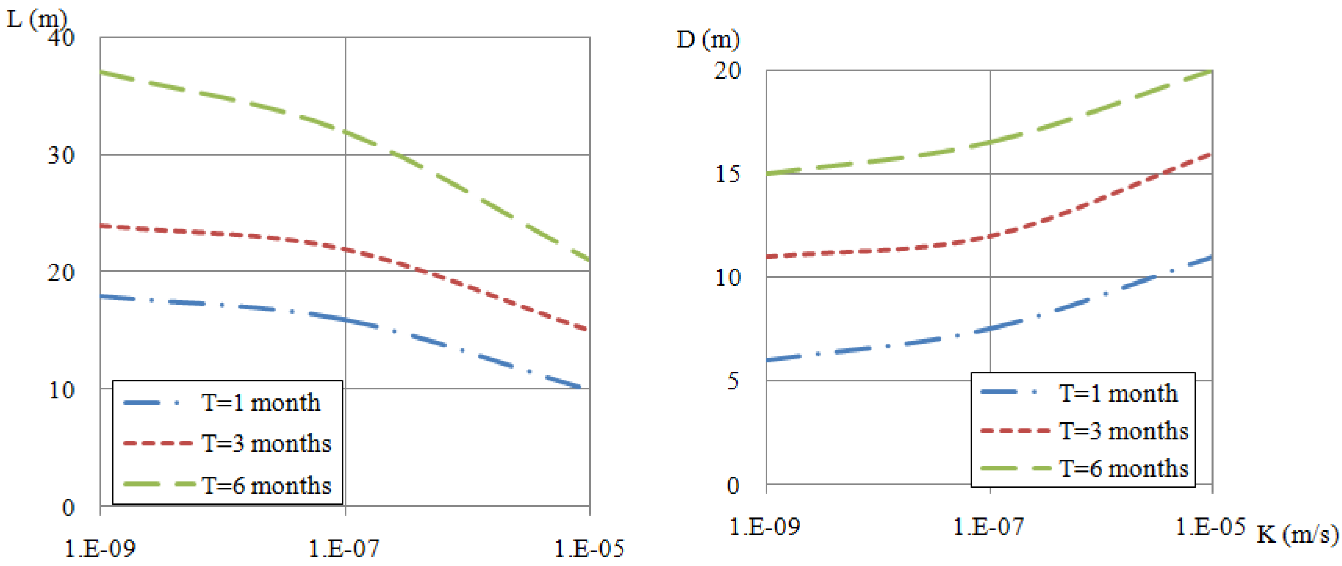
(a)Q=1E-6(m^3/s) (b) Q=1E-5(m^3/s)

Figure-6: Length variations of contamination in coarse soils according to changes in the permeability of the soil.



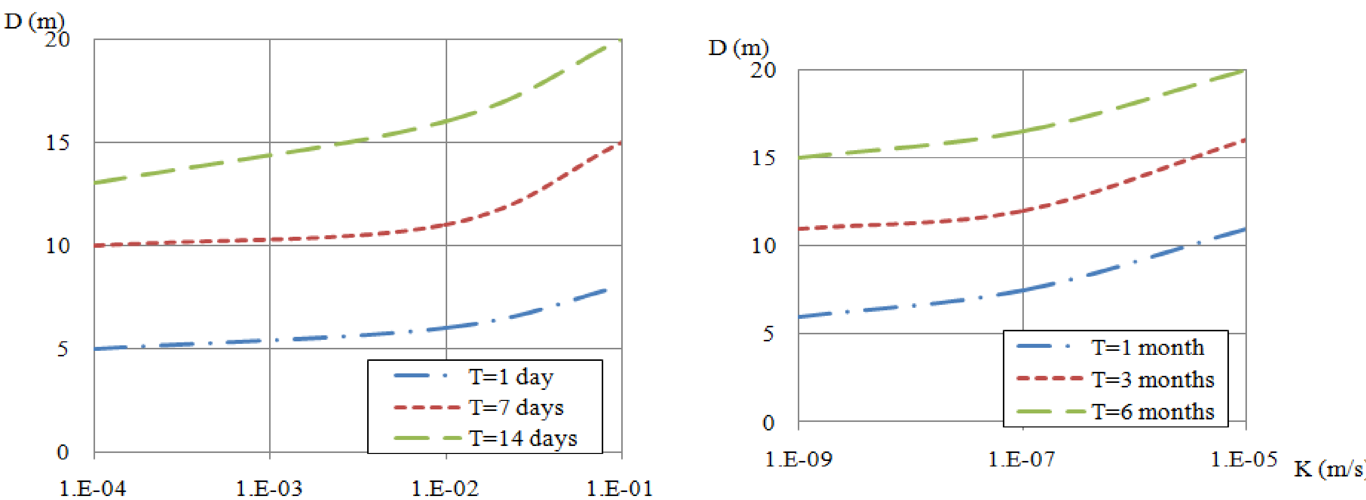
(a)Q=1E-6(m^3/s) (b) Q=1E-5(m^3/s)

Figure-7: Depth variations of contamination in coarse soils according to changes in the permeability of the soil.



(a)Q=1E-6(m^3/s) (b) Q=1E-5(m^3/s)

Figure-8: Length variations of contamination in fine soils according to changes in the permeability of the soil.



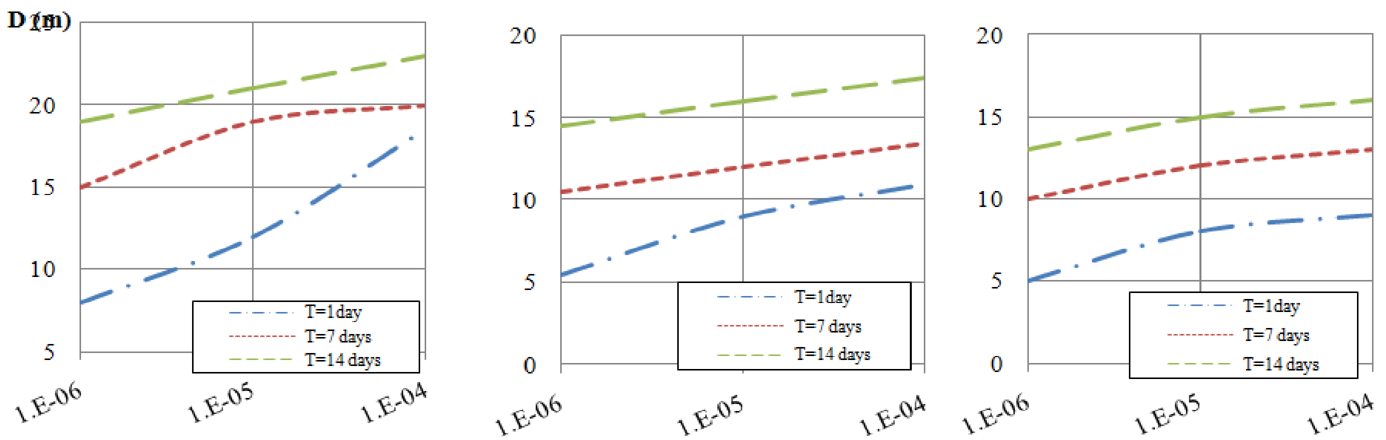
(a)Q=1E-6(m^3/s) (b) Q=1E-5(m^3/s)

Figure-9: Depth variations of contamination in fine soils according to changes in the permeability of the soil.

According to presenting figures, in coarse aggregate soils for a considered time and specific pollutants discharge, the relationship between increasing pollution emission and increasing the permeability is relatively linear. But depth of contamination with increased permeability initially has a linear relationship and gradually increased and by approaching to permeability limit of sandy soil, the gravity has a greater impact than depth and the relationship between increase the depth of pollution by increasing the permeability of the soil become linear.

The effect of inflow discharge on the movement of contaminants: Here for the coarse soil, three permeability of 10^{-1}, 10^{-3} and 10^{-4} meters per second, and for the fine soil, three permeability of 10^{-5}, 10^{-7} and 10^{-9} meters per second were considered.

For the coarse and fine grained soils, different contaminants discharges of 10^{-6} cubic meters per second to 10^{-4} cubic meters per second is considered.



(a) k=1E-1(m/s) (b) k=1E-3(m/s) (c) k=1E-4(m/s)

Figure-10: Length variations of contamination in fine soils according to changes in the inflow discharge of the contaminant in coarse soils with different permeability.

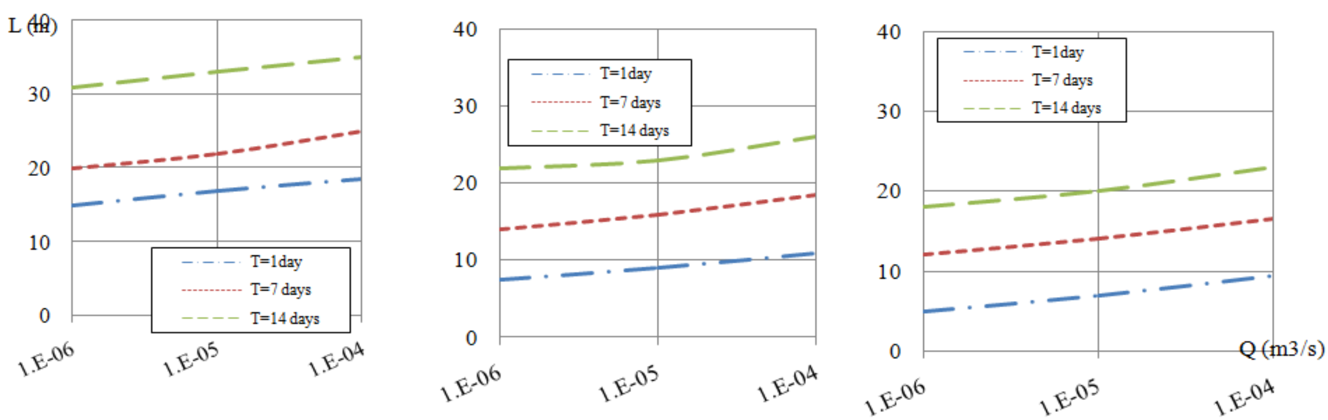
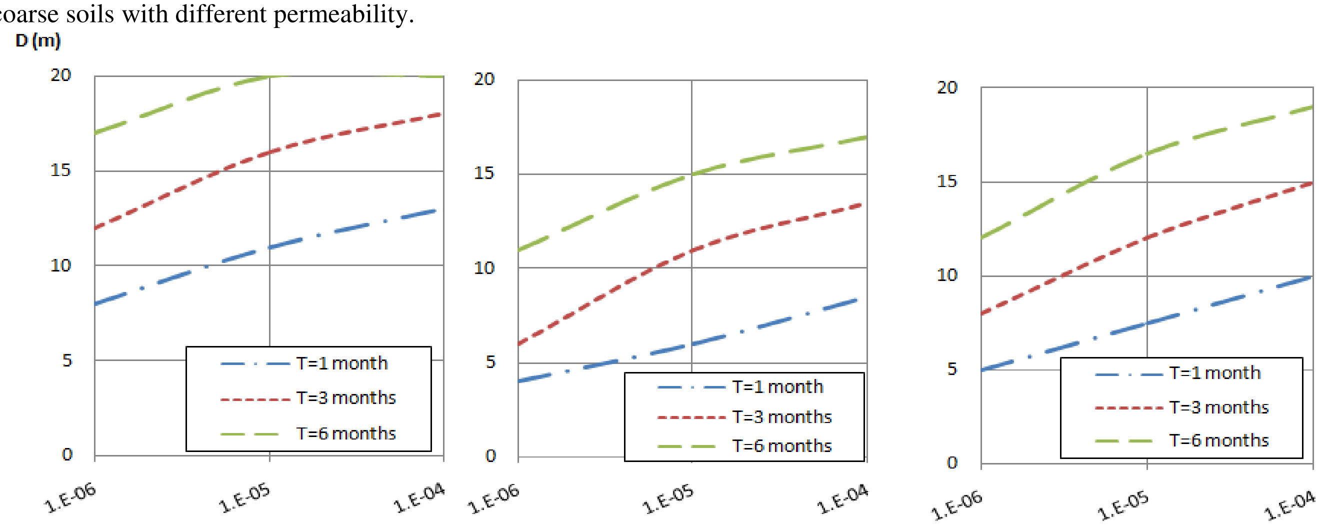


Figure-11: Depth variations of contamination in fine soils according to changes in the inflow discharge of the contaminant in coarse soils with different permeability.



(a) k=1E-5(m/s) (b) k=1E-7(m/s) (c) k=1E-9(m/s)

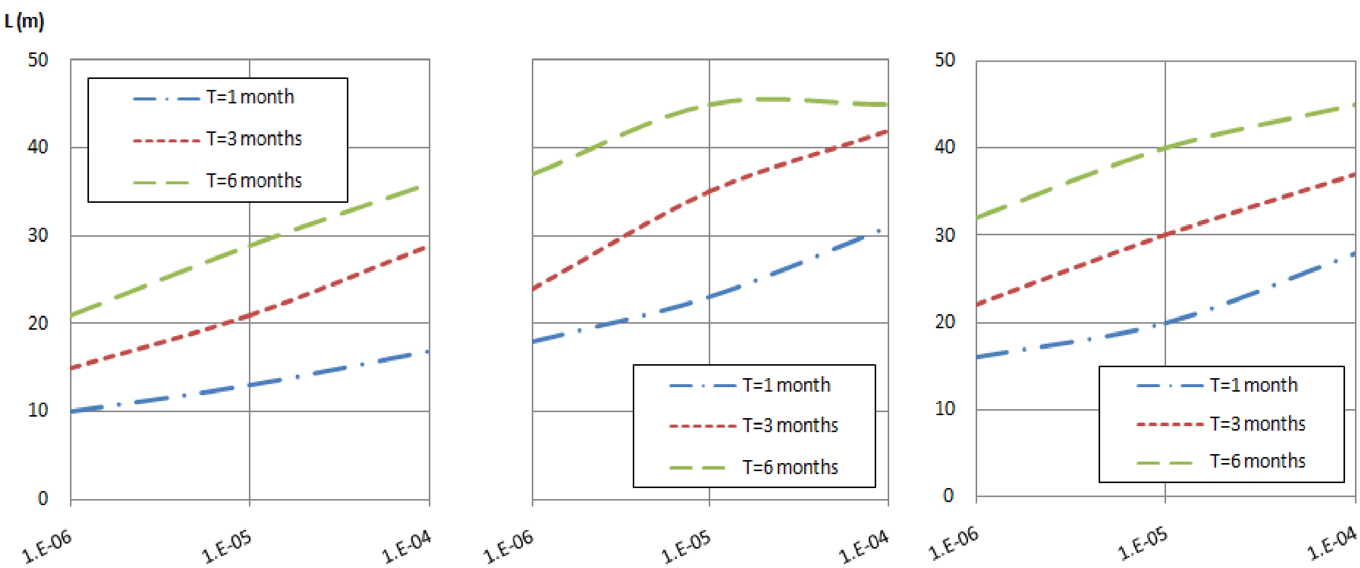
Figure-12: Length variations of contamination in fine soils according to changes in the inflow discharge of the contaminant in fine soils with different permeability.

The effect of relative density of pollutants and water table: For investigating the pollutant density of 0.8, which represents the pollutants lighter than water to 1.4, indicating contamination heavier than water has been changed (Figure-13).

In this part of the research, the effects of water level changes on emissions and in particular the changes in surface and depth emissions have been studied. Therefore, the modeling done for both fine and coarse soil environment, it is assumed that the underground water level in the depth of three values: 5, 10 and 15 meters from the ground. (Figure-14)

The diagram related to the depth variation of the contamination due to subtle changes with the change of water level has not been drawn (relative density=0.8) (Figure-15).

The effect of Diffusion coefficient and Dispersion coefficient: In this section we study the effects contamination on the distribution pattern of Dispersion coefficient, the Dispersion coefficient of the several models with 8-10×1 to 4-10×1 simulated. Output parameters in these models, area pollution are published in the soil profile. For both fine and coarse soil, the contamination spread area changes according to the different distribution coefficient is drawn (Figure-16).



(a) k=1E-5(m/s) (b) k=1E-7(m/s) (c) k=1E-9(m/s)

Figure-13: Depth variations of contamination in fine soils according to changes in the inflow discharge of the contaminant in fine soils with different permeability.

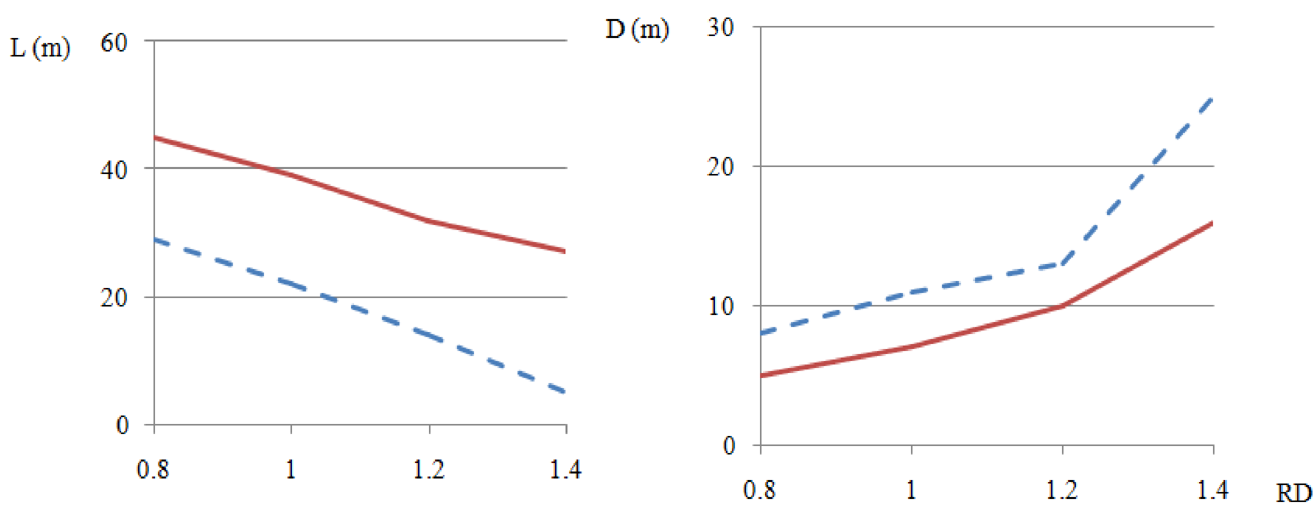


Figure-14: Changes in Length (L) and depth of pollution (D) according to changes in contaminants relative density (RD).

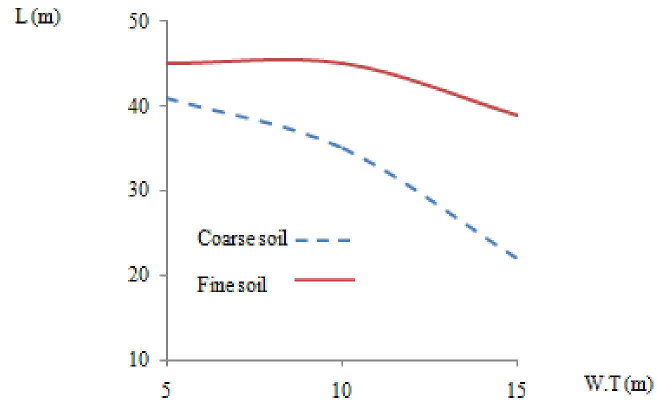


Figure-15: Changes in pollution (L) based on water level changes (WT) for contaminants with a relative density of 0.8.

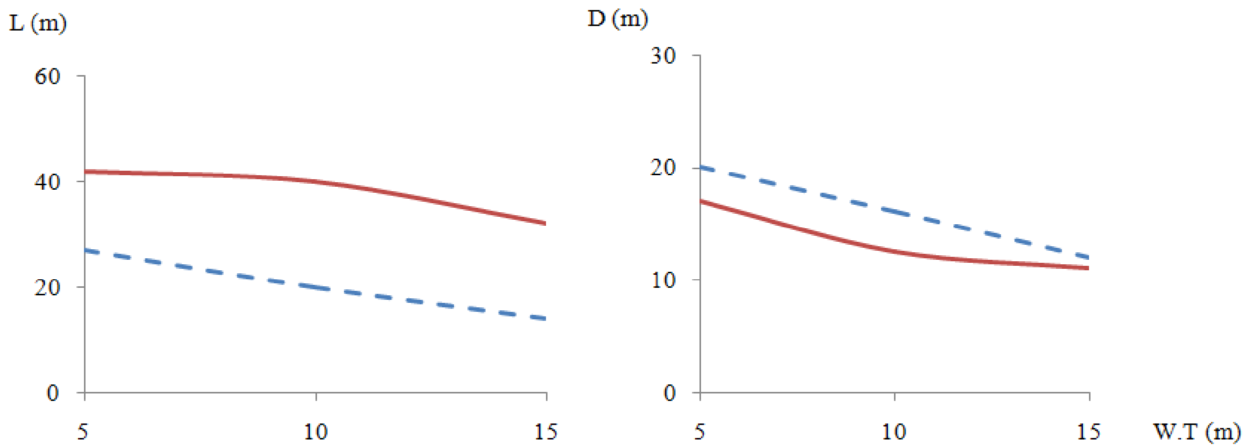


Figure-16: Changes in length (L) and depth (D) of pollution based on water level changes (WT) for contaminants with a relative density of 0.8.

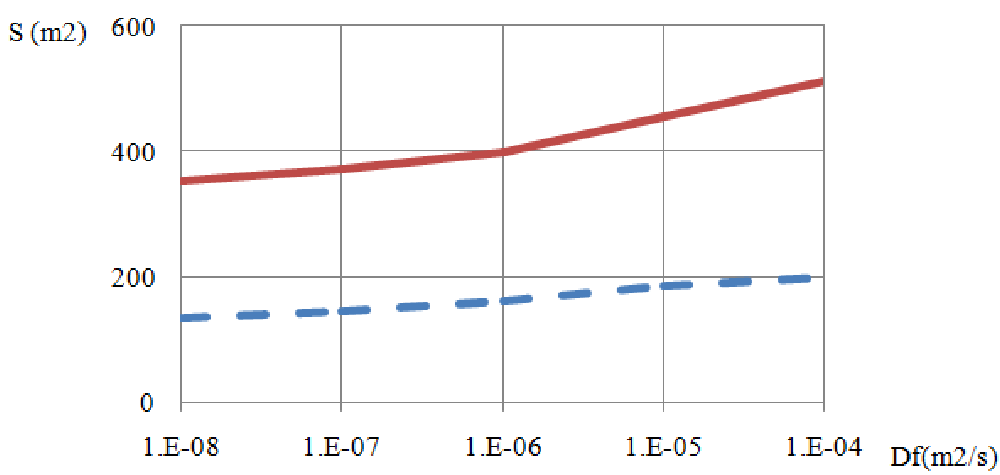


Figure-17: The effects of changes diffusion coefficient (Df) spreading over an area of section of contamination (S).

In this part to investigate the dispersion coefficient of variation of this parameter in the pattern pollution has been used in similar models. Longitudinal dispersion coefficient values are assumed: 2, 3, 4, 5, 10 meters and transverse dispersion coefficient are: 0.5, 1, 2, 3, 4 and 5 meters. The results for these two parameters change in the length and the depth of contamination is given.

The effect of ion exchange capacity on the movement of heavy metals: In order to investigate on the effect of ion exchange capacity of the soil on heavy metals movement, 3 soil columns in a saturated environment and under constant hydraulic gradient was simulated with a height of 8cm that Pb was impregnated its first 1cm and 7cm residue was no Pb. ion exchange capacity of the soil column were assumed to 0.001, 0.01, 0.05 and 0.1 and the Pb leachate were measured during a period of 100 days.

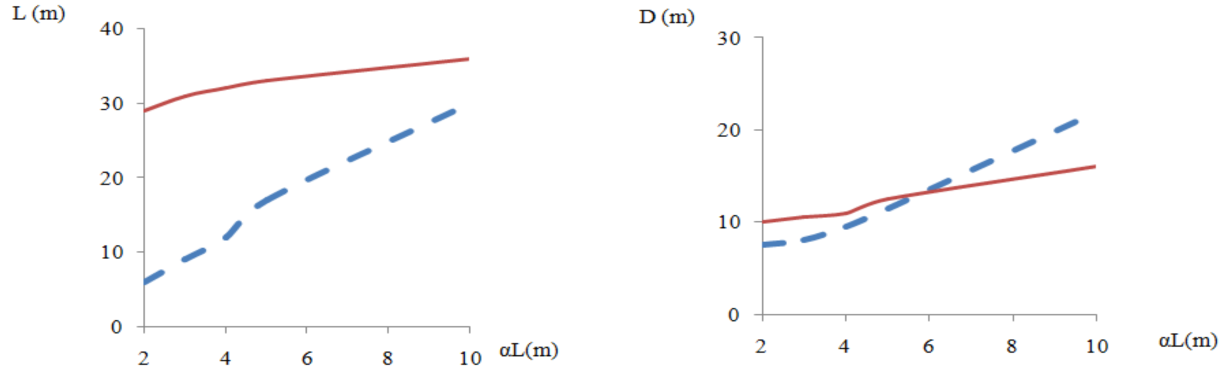


Figure-18: Changes in emission levels (L) and the depth of contamination (D) based on changes in the longitudinal dispersion coefficient (α_L).

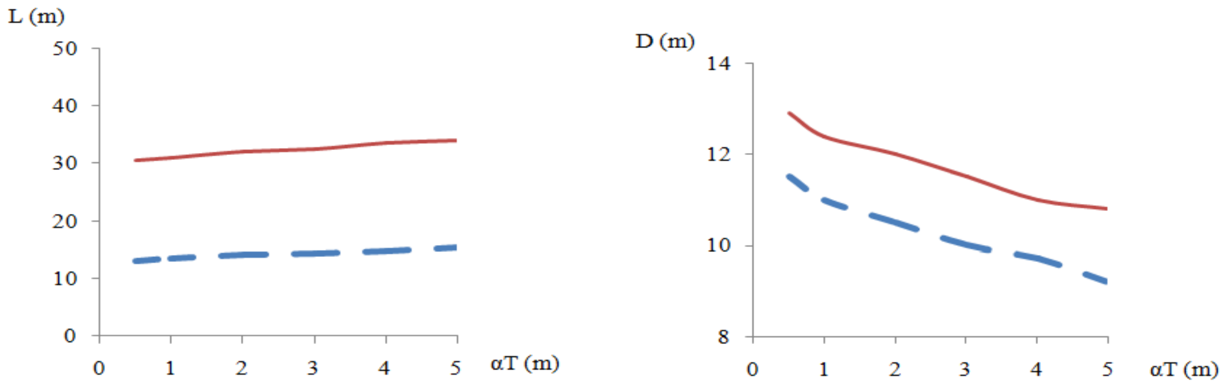


Figure-19: Changes in emission levels (L) and the depth of contamination (D) based on changes in the transverse dispersion coefficient (α_T).

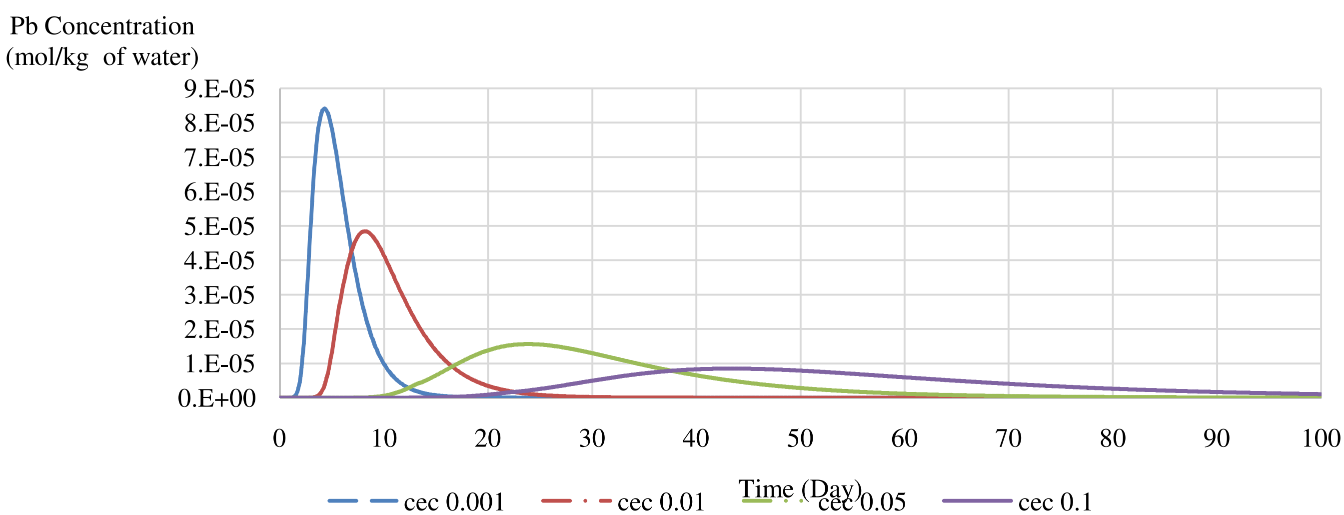


Figure-20: Pb concentration in the soil with different ion exchange capacity.

With the increase in ion exchange capacity, the maximum amount of Pb output is reduced. So that the ion exchange capacity of the soil with minimum, maximum Pb concentration output value of 85μmol/kg of water and in the soil with the highest ion exchange capacity, the lowest concentration of Pb output 9μmol/kg of water can be seen. In the Figure-19(a) and (b), the concentration of contaminants in the soil profile in 0/1, 10, 30, 60 and 180 days in two soils with different ion exchange capacity is shown.

The effect of alkalinity (PH) on the movement of heavy metals: In this simulation, the movement of major cations such as sodium, potassium, calcium and magnesium and three heavy metals include cadmium, zinc and lead in a soil column during 1 year under unsaturated flow is investigated. The top layer of soil contaminated by heavy metals and the underlying layer is without heavy metal.

In this analysis, an acidic solution with three different alkalinity 3.5, 7 and 10 as the upstream boundary conditions is considered. Assuming that the ion exchange capacity of organic materials is 6meq/g, the ion exchange capacity of soil column in different parts of 0.002 to 0.01mEq/kilogram of soil is considered (Figure-22).

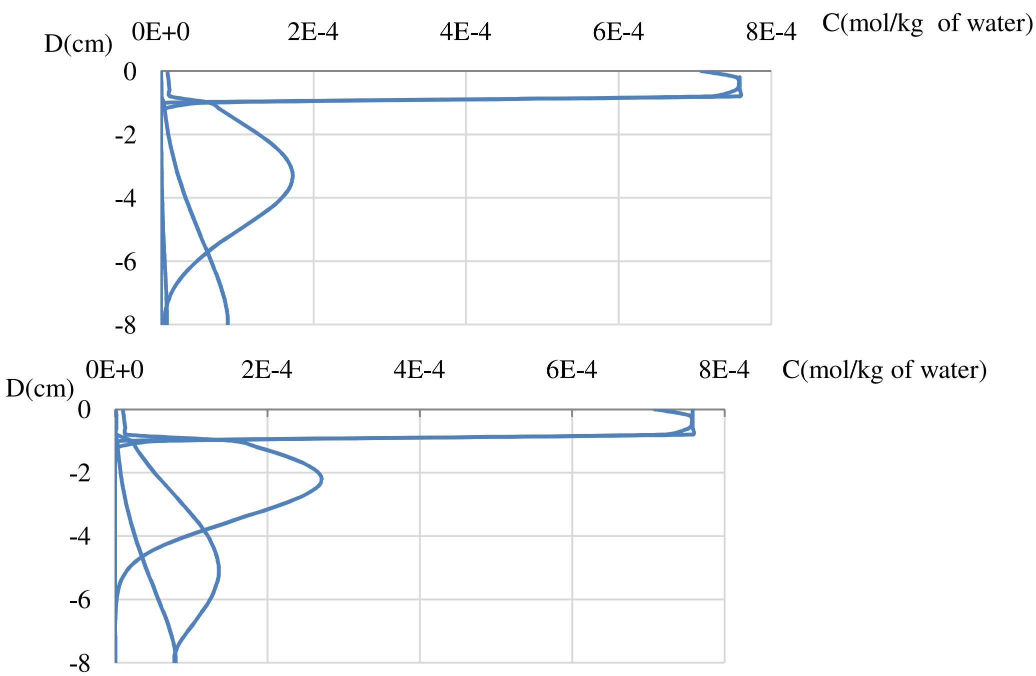


Figure-21: concentration of contaminant (C) in the soil profile (a) CEC=0.5 (b) CEC=0.1.

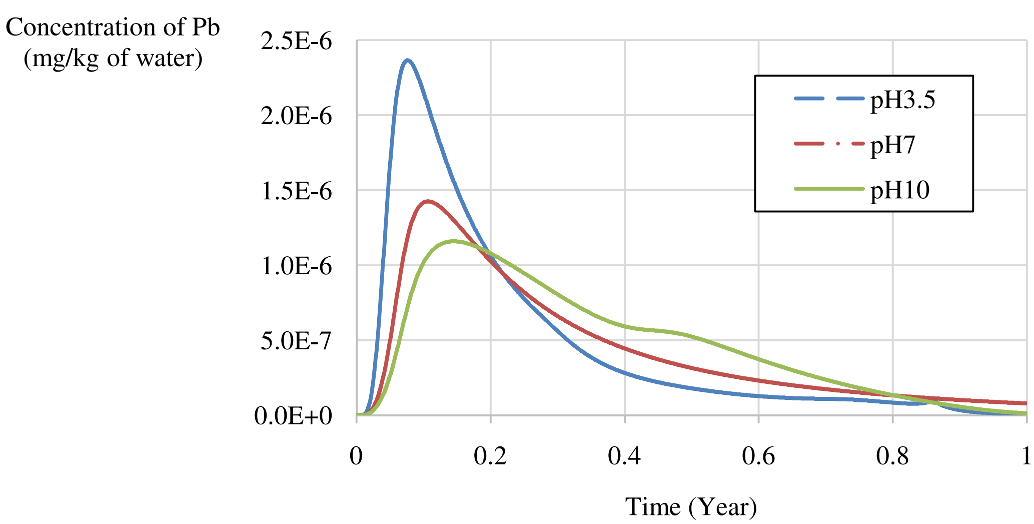


Figure-22: Output concentration of Pb from soil column.

Conclusion

Pollutant origin moves progressively to the depth and length of the permeable medium due to its density and because of gravity force and propogation impelled by mechanical and molecular movement, with the disposition of contaminant on the solid matrix surface as well as in saturated zone, it moves due to convective water flow. Hence, the contaminant concentration in a porous medium at a given depth increases until a peak is reached and then falls gradually to zero.

The two-dimension hydrodynamic dispersion coefficients hasten the movement processes of the contaminant in the vertical direction and the diffusion in the horizontal direction, resulting in a dramatic increase in the contaminant concentration in a short time. Some factors -include permeability and inflow discharge of contaminant- have a straight and great effect on contaminant transport that move in the same direction.

Density and level of underground water have a key role in contaminant transport. For example, in both fine and coarse soil with 20% increase in the density of contaminants, due to the weight force, we expect more penetration in depth of soil and see 50% increase in depth and 30% reduction in length of pollution. As well as by reducing the level of underground water from 15 meters to 5 m, in both fine and coarse soil, increased level of pollution in the environment. This issue in coarse soils has more uniform manner and reach from 22 m to 41 m and in fine soils by increasing the groundwater level, increasing has less intensity. The total amount of the pollution in the soil density of 1.2 to 0.8 with the same amount of contaminants density in the state is facing a 40 percent reduction.

Summary: The most important factors that affect movement of oil hydrocarbons and heavy metals in unsaturated soils were investigated in this article. Factors related to soil environment or contaminant characters. The common solutions for transport of contaminants in an unsaturated semi-infinite permeable soil are derived using the Advection-Dispersion equation. Also, the specifications of one-dimensional leakage flow and the two-dimensional dispersive force are considered. Based on the fundamental solution of an instantaneous point contaminant source, the numerical investigations of the contaminant concentration in a porous medium subjected to a local contaminant source are derived by CTRAN/W.

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