NUMERICAL SIMULATION OF CONTAMINANT TRANSPORT IN OIL CONTAMINATED SOILS

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Abstract: The contaminant transport has been a major issue due to the adverse effect of the contaminants on groundwater quality. Effect and movement of the contaminant in soils and groundwater is essential to access and reduce the risk of soil contamination and groundwater pollution. This research investigates contamination transport by modeling the flow in the soil matrix. A two-dimensional numerical model for transport of diluted species was developed under steady and transient state condition using advection-diffusion equation in COMSOL multiphysics by creating a two-dimensional soil matrix profile of 250 cm in the X and Y direction with an oil drop of diameter 30 cm assumed within the profile. The model reveals that at the initial drop of 40 cm under steady state condition the concentration increases as the drop length increases, while in the vertical direction, the peak of the concentration increases with drop. It has been established that the profile developed, provides a good estimation for predicting the effect of a contaminant in a two-dimension soil matrix profile.

Keywords: Contaminated soils, COMSOL multiphysics, crude oil, numerical simulation

Introduction

Contamination of groundwater by inorganic and organic chemicals has become an increasing concern in recent years. Groundwater contamination by petroleum hydrocarbons, organic solvents and other toxic non-aqueous phase liquids are widespread environmental problems that pose serious threat to the groundwater resources. Groundwater contamination includes different kinds of waste such as chemical, bacteria, or radioactive waste. There is so much concern regarding these wastes which are soluble in water and can therefore affect groundwater resources. Infiltration of waste in soils also involves the contaminant transport problem. Pollution of groundwater by contaminants leaching through soils poses a potential hazard to human health. According to Vanderborght and Vereecken (2007), an important effort required to minimize the risk involved is by using various models to adequately assess and predict contaminant transport in soils while Jiang *et al*. (2010), in their study, suggested that both the physical (advection, diffusion and dispersion) and reaction (adsorption and degradation) processes controlling contaminant transport should be analyzed in the numerical model.

Development of the governing equations used in analyzing multiphase flow and multicomponent transport in porous medium was as a result of the interest from the petroleum industry in the 1960's to quantify production and evaluate the efficacy of the recovery method (Panday and Corapcioglu, 1989). Over the years, hydro-environment related problems have been solved using the advection-dispersion equation. According to Fry *et al*., (1993), analytical solutions of the solute transport equations were obtained with rate-limited desorption and decay while Liu and Ball (1998) employed the Green's functions approach in the Laplace domain to obtain analytical solutions for solute diffusion in a semi-infinite two-layer porous medium for arbitrary boundaries and initial conditions. Liu *et al*. (2000) in their study, solved a one-dimensional advection-dispersion equation in a heterogeneous porous media coupled with linear and nonlinear sorption or decay using the generalized integral transforms technique. Khalifa (2003) applied the transformation group approach using the advection-dispersion governing equations to solve a cylindrical geometry and parallel plate model contaminant transport in a main fracture surrounded by a two-dimensional rock matrix. Maniliadis (2000) in his study applied the Runge-Kutta Gill algorithm to analyze a soil water model of one-dimensional flow while Moreira *et al.* (2005) presented an analytical technique for the advection-diffusion equation for passive contaminants in the planetary boundary layer. The Laplace transformation technique was also used by Moreira *et al.* (2006) to solve a non-stationary two-dimensional advection-diffusion equation; they presented a range of analytical solutions to simulated pollutant dispersion. The Analytical solutions of Convective Diffusion Equation with respect to an exponentially decaying and sinusoidal input functions were obtained by Chen and Liu (2011).

Gao *et al*. (2013) studied a one dimensional model convective diffusion in soil contaminant transport. The study obtained an analytical solution for constant reaction coefficient, depth dependent reaction coefficient and time dependent inlet boundary condition while Chegenizadeh *et al*. (2014) used a two-dimension convection dispersion equation to investigate the soil contaminant transport subjected to time dependent boundary conditions.

Problem Statement and Methodology

This study considers a contaminant transport problem in a vertical direction and analyzed by two dimensional advection diffusion equations (ADE) with constant water content, dispersion coefficient and velocity.

A two-dimensional soil matrix was created on COMSOL multiphysics with an assumption of a circular oil drop contaminant. The diffusion and impact of the contaminant will be varied at different center position of the oil drop as it moves downward in the soil matrix with a two-dimensional cut analysis. The contaminant undergoes depth-dependent local reactions; the solute adsorption is described with a linear isotherm, and solute degradation is assumed to be a first-order process. The governing equations for this contaminant problem are expressed as:

$$R(x)\frac{\partial C}{\partial t} = D\frac{\partial 2_C}{\partial x^2} - v\frac{\partial C}{\partial x} - \mu(x)C \quad (1)$$

$$R(y)\frac{\partial C}{\partial t} = D\frac{\partial 2_C}{\partial y^2} - v\frac{\partial C}{\partial y} - \mu(y)\,C \quad (2)$$

$$R(x) = 1 + \frac{\rho_b K_d(x)}{\theta} \quad (3)$$

$$R(y) = 1 + \frac{\rho_b K_d(y)}{\theta} \quad (4)$$

$$K_d(x) = K_0\,cosh^{-2}\left(\frac{x}{x_0}\right) \quad (5)$$

$$K_d(y) = K_0\,cosh^{-2}\left(\frac{y}{y_0}\right) \quad (6)$$

With the associated boundary conditions;

$$C(x,0) = 0 \quad 0 \le x \le L \tag{7}$$

$$C(y,0) = 0 \quad 0 \le y \le L \tag{8}$$

$$\frac{\partial C}{\partial x}(L,t) = 0 \quad 0 < t < \infty \tag{9}$$

$$\frac{\partial C}{\partial y}(L,t) = 0 \quad 0 < t < \infty \tag{10}$$

Where

C is the resident solute concentration (ML^{-3})
θ is the volumetric water content
D is the hydrodynamic dispersion coefficient (L^2T^{-1})
v is the average pore-water velocity (LT^{-1})
ρ_b is the soil bulk density (ML^{-3})
K_d (x) is the depth-dependent adsorption coefficient ($M^{-1}L^3$)
K_d (y) is the depth-dependent adsorption coefficient ($M^{-1}L^3$)
μ (x) is the depth-dependent degradation rate (T^{-1})
μ (y) is the depth-dependent degradation rate (T^{-1})
x is spatial coordinate (L)
y is spatial coordinate (L)
t is time (T).

The space is varied between 0 and 2.5 m in the X (horizontal) direction and negative Y (vertical) direction, the coefficients were assumed to be equal. The adsorption rate, K and degradation rate, μ were considered to be depth dependent and time independent. Moreover, both the vertical and horizontal directions were assumed to have the same physical properties.

Simulation parameters

A number of parameters were considered to run the simulation. The simulation parameters are presented in Table 1.

Table 1: Parameters description values symbol

Parameters Description	Values	Symbol
Finite spatial domain length	250 cm	L
Volumetric water content	0.4 cm3/cm3	Θ
Bulk Density	1.2 g/cm	P
Average pore-water velocity	20 cm/d	N
Hydrodynamic dispersion coefficient	400 cm3/g	D
Retardation factor in top soil	2	R
Adsorption coefficient in topsoil	1/3 cm3/g	K
Degradation rate	0.2	M
Observed time for concentration profiles	5 day, 10 day, 20 day, 30 day	T

A model was created with the aid of the software wizard. In order to study the flow under the influence of oil droplet, the chemical species transport physics was selected. A rectangular geometry was created by selecting the "geometry" link in the model builder window and selecting "rectangle' from the drop box. The tool was used to create a 2D matrix of width 250 cm and height 250 cm, and it was also used to create the circular geometry of diameter 30 cm assumed to be within the rectangle, which is assumed to be an oil drop. The centre of oil droplet was first placed at 40 cm along the width and the effects were carefully studied. The process was repeated for the oil droplet placed at 40, 100, 180, and 200 cm along the vertical direction, and the effects where studied respectively. A 2D plot group was also created to plot surface contours of concentration and by default, the parameter to be contoured is concentration (c) against the lateral and horizontal coordinate.

Results and Discussion

The simulations was carried out with the aid of the COMSOL multiphysics, it was post processed and categorized into two major sections. Initially, the fluid flow campaign for the effects of changing the position of the drop and the impact on fluid flow within the 2D matrix was showcased. Also, the effect of the 2D cut line campaign, which involves dissecting the soil matrix along the vertical direction (and along the horizontal direction), was investigated. The diffusion study on the 2D soil matrix with different center position showed a general trend which is, as the center position decreases along the vertical direction, the region with the maximum concentration decreases gradually.

The concentrated contaminant moves in a vertical direction. The contamination is expanding in space which can only be observed in a two dimension modeling as it is completely hidden in a one dimension analysis.

Figs. 1 to Fig. 4 present the contamination profile in two dimension matrix at stationary state. Fig. 1 shows the position of the drop at 40 cm as the contamination spread through the 2D space with the peak pronounced from 70 cm downward. Fig. 2 depicts that, with the drop at 100 cm assumed to be below the ground surface, the concentration level dropped to 80 cm. Also, from Fig. 3, it was observed that at the distance of 180 cm downward of the channel; the peak was dropped to 120 cm. Fig. 4 shows the concentration when the drop is at the bottom of the 2D matrix with the centre of the drop at 200 cm, the concentration is noticed to decrease and expand in the space.

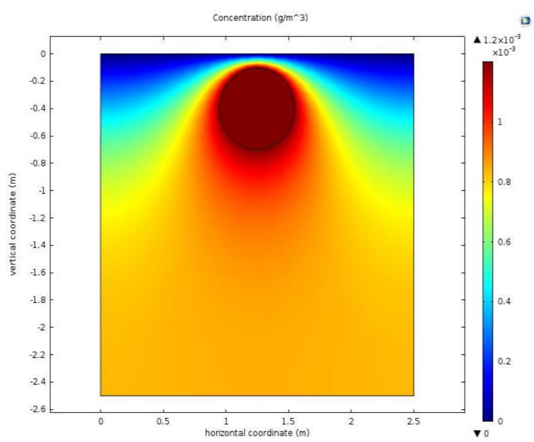

Fig. 1: Concentration profile at 40 cm

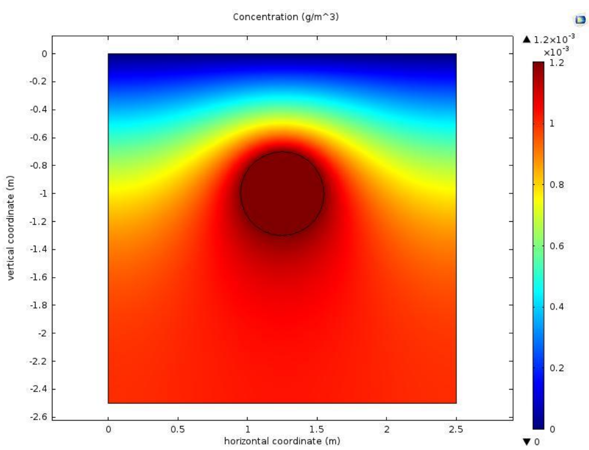

Fig. 2: Concentration profile at 100 cm

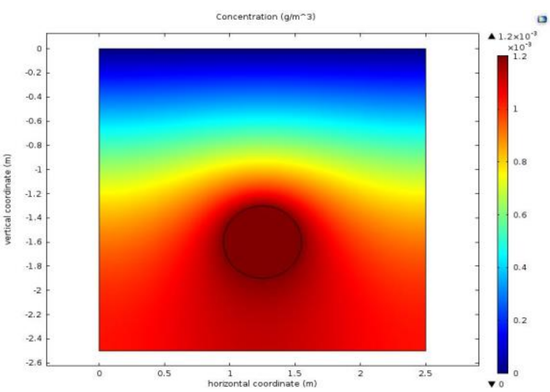

Fig. 3: Concentration profile at 180 cm

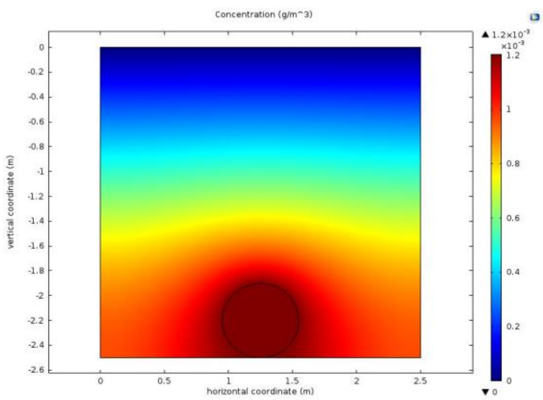

Fig. 4: Concentration profile at 200 cm

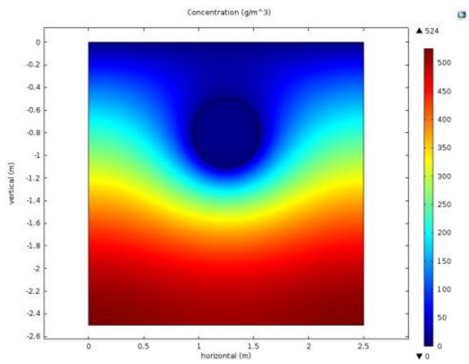

Fig. 5: Concentration profile at 80 cm

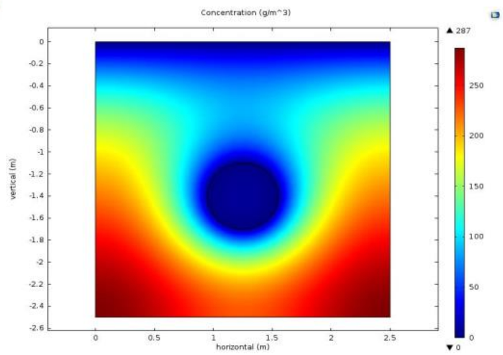

Fig. 6: Concentration profile at 140 cm

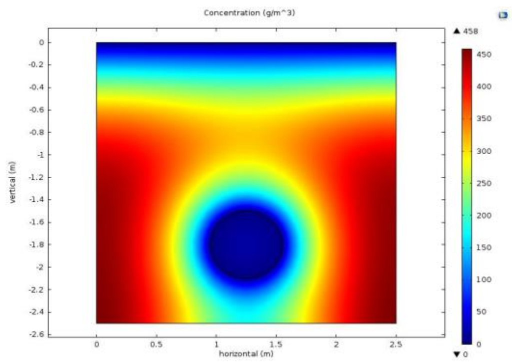

Fig. 7: Concentration profile at 180 cm

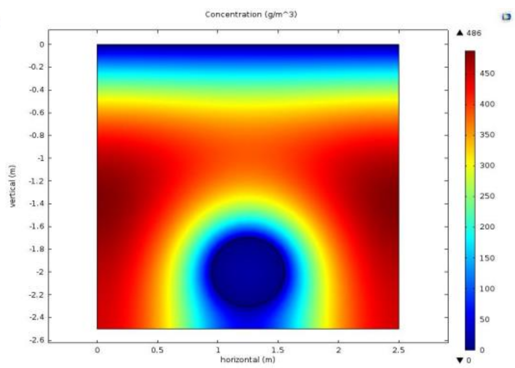

Fig. 8: Concentration profile at 200 cm

The contaminant profile in Figs. 5 and 6 present the concentration at various distant with the reaction. It is observed that as we move downward in the profile, the concentration tends to decrease which is due to the reactant introduced into the model. Fig. 8 depicts that, at the distant of 200 cm, the contamination around the drop reduced, thereby disintegrating the concentration at the bottom. This process can be employed when the concentration is to be reduced at any instance.

Transient State of the Model

Figures 9 to 12 present the transient state of the concentration profile at 80 cm for different time range. The results show that after 5 days, the concentration region is small as shown in Fig. 9 and it is observed that this concentration increases with time after 30 days as depicted by Fig. 12. It is also important to note that the region of concentration is high.

The effects of the concentration at 200 cm are also shown in Figs. 13 to 16 for different time variation. This shows that the range of high concentration is small compare with the 80 cm. it is noticed in Fig. 13 that, after 5 days the concentration region is small and this grows with time; but according to Fig 16, it is observed that after 30 days, the region with less concentration is higher than the region with high concentration.

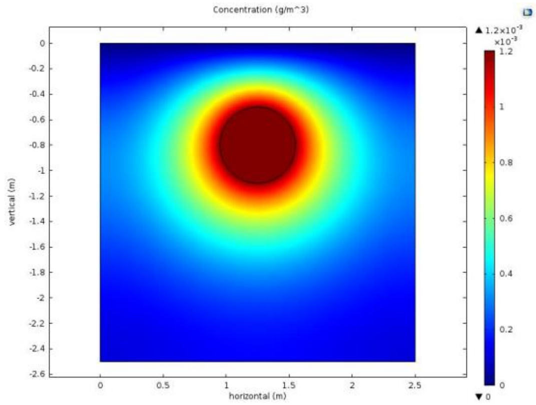

Fig. 9: Concentration profile (80 cm) after 5 days

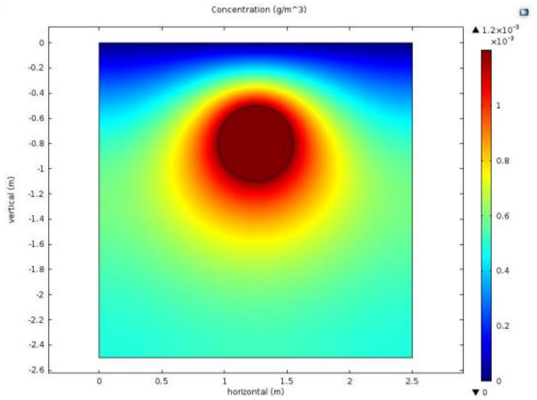

Fig. 10: Concentration profile (80 cm) after 15 days

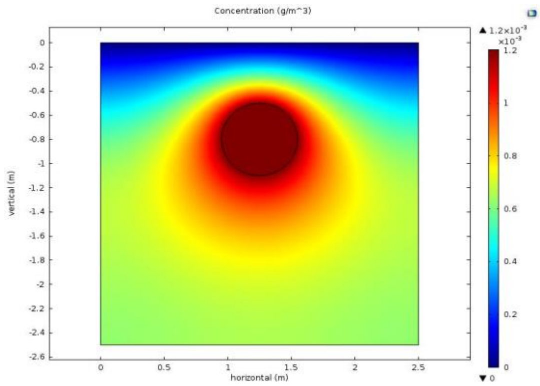

Fig. 11: Concentration profile (80 cm) after 20 days

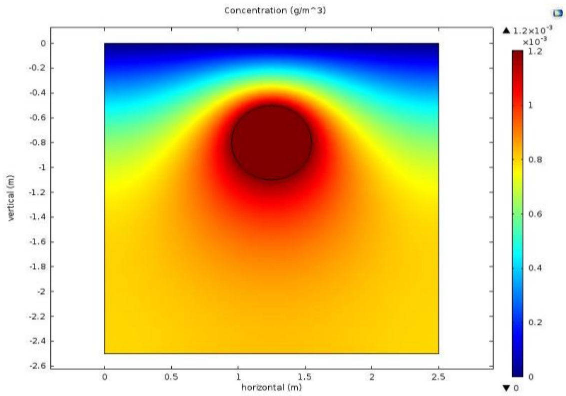

Fig. 12: Concentration profile (80 cm) after 30 days

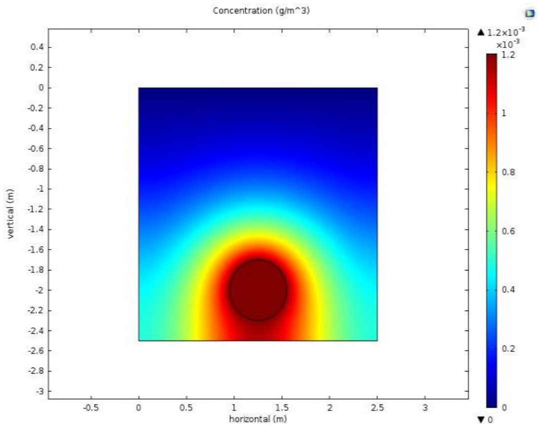

Fig. 13: Concentration profile (200 cm) after 5 days

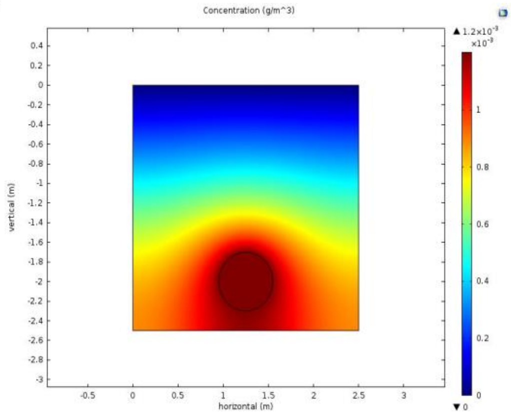

Fig. 14: Concentration profile (200 cm) after 15 days

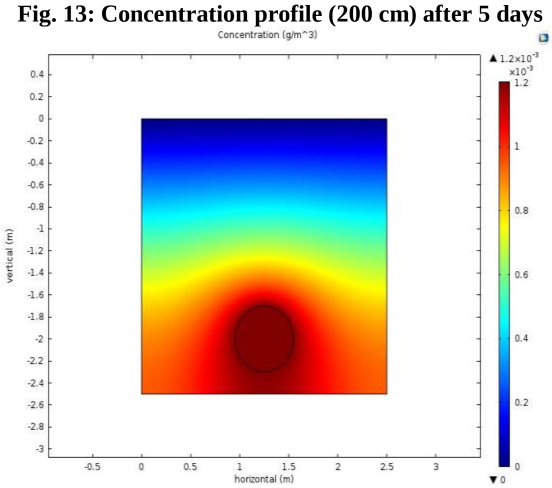

Fig. 15: Concentration profile (200 cm) after 20 days

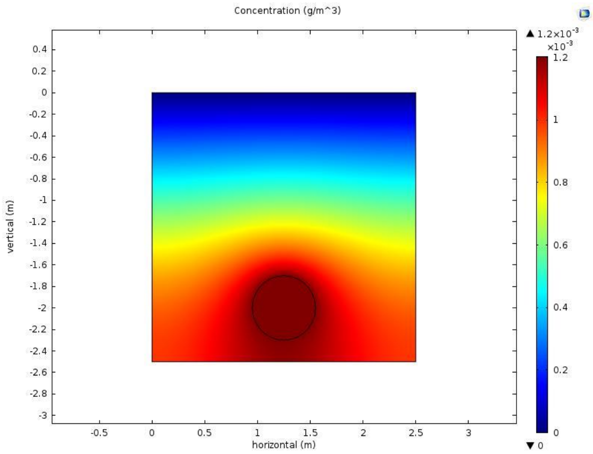

Fig. 16: Concentration profile (200 cm) after 30 days

Conclusion

The numerical simulation of contaminant transport in oil contaminated soils has been studied. The study examined the contaminant transport in soil under the steady and transient state conditions by varying the model from 0 day to 30 days. The model presented a numerical modeling of the contaminant transport in soil by applying a two dimension advection diffusion equation. From the present study, the following conclusions may be drawn:

(i) It is observed that as we move downward in the profile, the concentration tends to decrease which is due to the reactant introduced into the model.

(ii) It is noticed that at the distant of 200 cm, the contamination around the drop reduced, thereby disintegrating the concentration at the bottom.

(iii) It has been established from the transient state of the model that after 5 days the concentration region is small and grows with time but after 30 days, the region with less concentration is higher than the region with high concentration.

(iv) The model established a fast prediction of the evolution of the rate of oil penetration into soil and can be used to estimate a window of opportunity for emergency action.

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