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2D Simulation of Dynamic Transportation of Volatile Hydrocarbons in Vadose Zone of Tehran Oil Refinery and Industrial area of Ray, Tehran, Iran

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Abstract

This work investigates the reactive transport of volatile hydrocarbons in the unconfined aquifer system of Tehran oil refinery and the industrial area of Ray, Tehran. A 2D finite volume model is presented to predict the soil gas contamination caused by LNAPL traveling on the phreatic surface through the vadose zone of the aquifer incorporating physical, chemical, and biological processes. A multi-purpose commercial software called PHOENICS is modified by incorporating extra codes to solve the model equations numerically. The model predictions closely agree with the field measurements, showing that the LNAPL migration is typically affected by the volatilization process. LNAPLs represent a potential long-term source of soil and groundwater contamination in the studied site. A comparison of the simulation results in a time step of 36 years with the results of field studies shows that the presented numerical model can simulate the reaction transfer of evaporated hydrocarbons in the unsaturated region. The concentrations have decreased in the time step of 36 years compared to the values shown in the time step of 50 years. This decrease in the hydrocarbon gas-phase concentrations in the unsaturated zone is due to excavations at the site for field studies. Through these excavations, a significant volume of the gaseous phase trapped below the earth's surface is released into the atmosphere, which reduces the accumulation of volatile gases beneath the earth's surface.

1. Introduction

Non-aqueous phase fluids (NAPLs) are the most prevalent among the most frequent and extensively dispersed pollutants in the environment. Numerous locations throughout the globe are potential long-term contributors to ongoing soil and groundwater pollution [1, 2]. Waterless light fluids (LNAPLs) are NAPLs that are more frivolous than water. These fluids cannot be combined with water and are non-aqueous phase liquids. Aqueous solutions of these compounds, on the other hand, are exceptionally weakly soluble and emerge as a distinct liquid phase. In order to determine their effect, it is essential to understand how NAPLs arise from different point origins, enter the underground ecosystem, and move via the groundwater flow channel. Evaporation from a supply region and gas transport away from the source by convection and scattering mechanisms are causes for the dissemination of volatile contaminants from remaining LNAPL with high vapor pressure components [3]. A hydrocarbon source has been described in the vadose zone of an unconfined aquifer using a theoretical model that describes physical transportation pathways and degradation (attenuation) processes [3]. According to their vapor pressure and solubility, LNAPL components may partition into the soil gas phase or groundwater before biodegradation without penetrating the aqueous phase [4-6]. The complexity of the LNAPL distribution in the subsurface, partitioning features of the LNAPL components, physical characteristics of the medium, ambient fluid flow conditions, types of microorganisms and their predators, accessibility

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of electron acceptors and nutrients, and environmental parameters such as temperature and pH are some factors affecting the rate of natural source depletion [7-11].

Over the last several decades, many analytical solutions and numerical models have been created to explain and characterize the transport mechanisms incorporating species and different phases [12-27]. Hers *et al*. used the BioVapor model to model vapor transport of ethylene dibromide (EDB) [28]. BioVapor is an analytical vapor diffusion model that simulates one-dimensional diffuse vapor transfer to indoor air and involves oxygen-limited biodegradation in the vadose area. Huang proposes a three-dimensional mathematical model for transporting volatile organic compounds in a coupled vadose-saturated zone system [27]. He incorporated subsurface processes including dispersion, advection, diffusive mass exchange, and interphase mass transfer between two horizontal porous media formations, as well as the time-dependent mass loading from a source zone into his model. This model facilitates the use of this technology in a broader range of contaminated sites and overcomes the limitations of previous interpretation models for the transport of vapors and soluble contaminants. Kondo *et al*. developed a model for forecasting the evaporation flux of volatile chemical substances at the subsurface [29]. The factors included in their model were multiphase flow containing NAPLs, water, and gases associated with rainfall infiltration into surface soil, evaporation/condensation of volatile chemical substances, and adsorption/desorption of volatile chemical substances. This newly developed prediction model can estimate dynamic changes in flux under natural environmental conditions. Qi *et al*. developed a nonequilibrium multiphase flow and transport model to study the effect of atmospheric pressure fluctuations on volatile organic compound emissions from groundwater to the atmosphere [30]. In the model they proposed, kinetic mass transfer processes between vapor and liquid phases and between liquid and solid phases were considered. In one study, the COMSOL multi-physics model was used to perform coupled simulations of soil gas transfer and hydrocarbon and oxygen reactions [26].

Several studies have addressed the issue of NAPL movement and the vaporization and dissolution of the LNAPL sources. However, there are limited studies on the vaporization and dissolution of the residual NAPLs [31, 32].

Numerous environmental approaches depend on the simulation of the underground degradation of NAPLs. For example, several samples of biodegradation and natural attenuation of pollutant plumes across groundwater aquifers [33-41] and the intrusion of degradable vapor organic compounds into buildings through the vadose zone [42-44] and enhanced petroleum recovery [45, 46] is available.

This study presents a two-dimensional numerical model for the reactive transport of volatile hydrocarbons in the vadose zone of an unconfined aquifer. To perform this modeling, a numerical finite volume model has been developed by modifying a general multi-purpose commercial package called PHOENICS [47]. The relevant settings for mathematical expressions associated with the chemical and biological reactions were performed by creating a PHOENICS input file (Q1) and supplying extra coding in FORTRAN in the GROUND subroutine [10, 48, 49]. These FORTRAN codings for all non-standard computations were used by the PHOENICS solver during the solution process.

2. Site-delineation and environmental effects

Oil contamination of groundwater sources began in the 1970s in the Ray industrial area, and started to significantly impact the lives of the local population in the 1980s. Although the Iranian government has developed several remedies, little progress has been made, and the contamination has grown. A great deal of concern has been expressed about the spread of this contamination. As a result, the groundwater contamination in the same region was investigated again in 1997. Nevertheless, this effort was also abandoned. Consequently, to conduct an efficient and accurate inquiry, it is essential to examine basic steps for the immediate deployment of the latest analytical methods and equipment. As a result of detecting volatile organic compound (VOC) gas intensity, evaluating the amount of petroleum within the soil and pits, measuring the oil layer thickness in the wells, and analyzing the components of the contaminating oil, this technique may be used to estimate contamination levels and sources.

In each observation period, the distribution of VOC gas concentrations is nearly identical, and the only thing that differs is the density.

Comparing the VOC gas density observed in three companies on the southern side with the VOC gas density detected in the other areas of four companies on the northern part (Area 1: Research institute of petroleum industry, Area 2: Oil exploration operations company, Area 3: Commercial storage, Area 4: Iranol company), it was found that the values of gas density in the four northern companies were considerably lower.

In addition, a high density of VOC gas was observed around the places where the leakage of oil had been confirmed during the site survey. In these locations, there are some points where the oil is leaking such as the accumulation point of sludge discharged from oil tankers or from the pipeline outlet, which transfers the oil to the tank trucks, and so on. This leaked oil permeates into the ground, and due to its vaporization, the formation of a region with a high density of VOC is presumed.

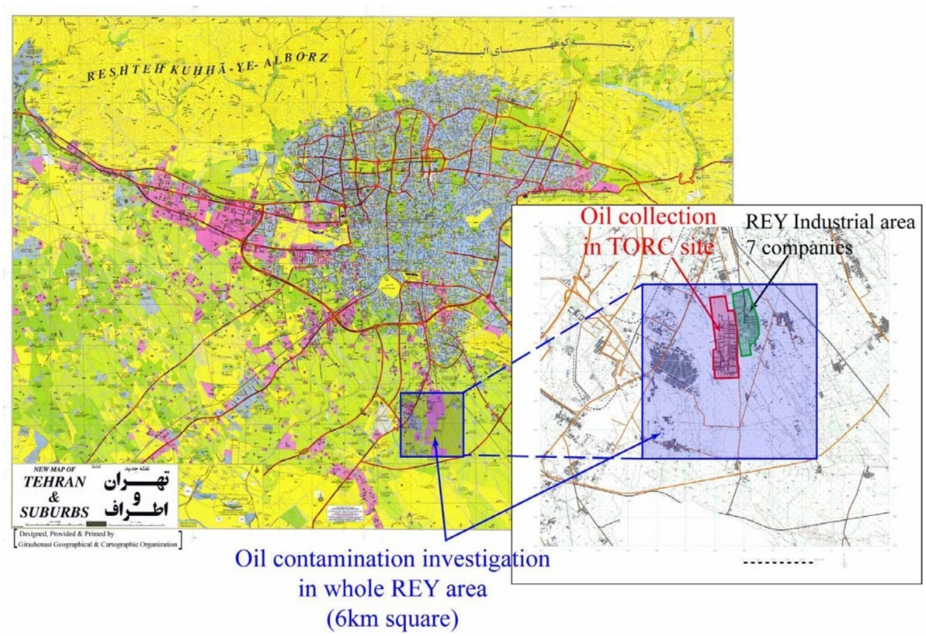


Figure 1. Geographical location of Shahr-e-Ray industrial area and studied area [50].

When the density of VOC gas is measured around the storage tanks, high-density test results are expected at the first stage since there are many drain pits. However, actual test results show significant differences in density values ranging from high to low. This result indicates that the points with high VOC gas density are limited partially, and waste oil in drain pits is apt to permeate into the ground vertically.

Furthermore, as the oil content of the polluted soil can be vaporized by the temperature rise, it was thought that the density of the measured gas should be higher at higher temperatures. However, considering the results obtained from these three measurement periods, a clear tendency to increase the density of VOC gas was not found by the increase in temperature.

The effect of the following two points can be considered in this regard:

1. At high temperatures, the evaporated gas in the tubes that have been pressurized can be vented off by opening the cap for performing the measurement, i.e., the reduction of gas density inside the tube during measurement time can be considered a result of this matter.
2. As the operation time of measurement was not long enough, precise data of seasonal variations could not be found in such a short period of measurement (four months from February to June).

High density and vast pollution were confirmed over a broad region of the Rey industrial area, including Tehran Oil Refinery Company (TORC). This pollution range seems to be continued in the southwestern direction. On the other hand, groundwater flow is also in the southwest direction. If it is oil in the well, it is thought that the pollution range spreads out by the flow of groundwater. However, if it is the pollution in the vicinity of the ground surface, the relationship with groundwater flow is low. However, the relationship between the pollution in the vicinity of the ground surface and groundwater flow is unclear.

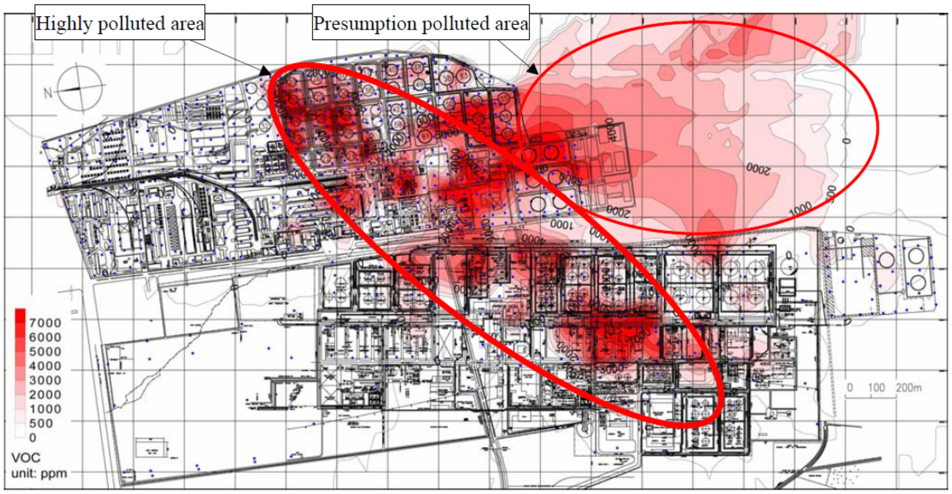


Figure 2. Distribution of volatile organic compounds (VOCs) at a depth of 4 m in Tehran oil refining company, seven other companies in Rey industrial zone, and a pumping station [50].

3. Model development/Governing equations

3.1. Transport equation

The nature of the sub-surface environment in an unconfined aquifer is typically divided into two saturated and vadose zones or the so-called unsaturated region. The saturated area is where all pores and rock cracks are filled and its pressure exceeds the atmospheric pressure, whereas the pores throughout the vadose region contain water and air. The soil water pressure throughout this region is smaller than the atmospheric pressure (negative pore water pressure). In addition to the atmosphere, the NAPL and saturated zones interact with the vadose area [51]. In order to evaluate the effect of NAPL contaminants, it is critical to clarify how they move through the sub-surface environment. Separate phases of residual NAPL, often with constituents of high vapor pressure, are the significant sources of spreading volatile pollutants by the volatilization process from a source zone and gas transport away from the source by dispersion and advection processes. According to the theory of mass conservation, the reactive transport scenario for volatile contaminants throughout the vadose area given gas-phase concentration appears as follows [51]:

$$d\frac{\partial}{\partial t}\left[R\theta_a C_g\right]+\nabla\cdot\left[dq_g C_g - d\left(D_g + D_w H\frac{\theta_w}{\theta_a}\right)\theta_a \nabla C_g\right] = -dR_{g,bio} + E_N^g - E_g^a + E_w^g \quad (1)$$

$$R = 1 + H\frac{\theta_w}{\theta_a} + k_d H\frac{\rho_b}{\theta_a} \quad (2)$$

$$D_g = \frac{\theta_a^{7/3}}{\theta^2} D_g^b \quad (3)$$

$$D_w = \frac{\theta_w^{7/3}}{\theta^2} D_w^b \quad (4)$$

$$R_{g,bio} = \lambda H\theta_w\left(1 + k_d\frac{\rho_b}{\theta_w}\right)C_g \quad (5)$$

where d is the depth of the vadose region, R is the retardation factor of the contaminant plume throughout the gaseous phase of the soil, θ_a is the volumetric content of soil gas, θ_w is the volumetric content of water in the NAPL region, C_g is the contaminant level in the soil gas, H is the dimensionless Henry's constant, q_g is the volumetric flow of soil gas, D_g is the efficient diffusion coefficient of contaminants in soil gas, D_w is the efficient dispersion factor of contaminants in the aqueous phase of the vadose region, D_g^b is the pollutant diffusion coefficient in block air, D_w^b is the pollutant diffusion coefficient in block water, $R_{g,bio}$ is the general consumption due to biodegradation in the solid phase, λ is the degradation factor of the contaminant throughout both aqueous and sorbed phases of water and gas of the vadose region, k_d is the distribution factor, and ρ_b is the mass density of dry soil.

Then the mass flux from NAPL to groundwater, E_N^w, can be defined as follows:

$$E_N^w = -\theta_w D_D \frac{\left(C_w - C_w^s\right)}{l_c} \quad (6)$$

where C_w^s is the contaminant solubility, and l_c is the density of the capillary border just above the phreatic layer.

The dispersion mechanism via the capillary fringe is believed to regulate the mass transport from groundwater to soil gas at the interface [51]. Then the mass flux from groundwater to soil gas E_w^g can be expressed as follows:

$$E_w^g = -\theta_w D_D \frac{\left(C_g - C_w/H\right)}{l_c} \quad (7)$$

If the ground surface is hypothesized to be impermeable, E_g^A in Eq. (1) is set to zero, and E_N^g can be taken as a constant as given below:

$$E_N^g = E_v \quad (8)$$

where E_v is a constant for volatilization rate.

Eq. (1) is not employed for permeable ground surfaces, and the vadose area depth is utilized as a diffusion length for calculating emissions to the atmosphere without taking contamination into account. The mass flux, E_N^a, from the NAPL phase to the air through the vadose region can be described as follows:

$$E_N^a = \left(\theta_a D_a + \theta_w D_w H\right)\frac{\left(C_g^S - C_a\right)}{d} \quad (9)$$

where C_g^s is the vapor-phase saturation of contaminants in equilibrium with the NAPL phase and C_a is the contaminant level throughout the air.

4. Modeling setting and performance

Across the Rey industrial zone, a two-dimensional model was developed to predict the dynamic movement of volatile hydrocarbons throughout the vadose region of an unconfined aquifer. Modeling of the top view was run (plan view).

The dimensions of the two-dimensional model are 3000 m horizontally and 4000 m vertically, which includes 121680 control volumes.

The impervious section of the aquifer was simulated by providing a no-flow boundary condition to the bottom border of the simulation. On the left and right sides of the model, constant head boundary values of 34.5 m and 31.4 m were set, respectively.

The flow system initially contained no NAPL compound, so a zero value was maintained ($C(\infty, t)=0, \quad t \geq 0$). A constant concentration equal to the concentration of pollutants at the inlet of the model was considered ($C(\infty, t)=0, \quad t \geq 0$). A constant concentration equal to zero was determined at the outlet of the model ($C(\infty, t)=0, \quad t \geq 0$).

Assumptions were made that the groundwater flow mechanism was in a steady-state condition. Therefore, the concentrations were measured in mg/L. Table (1) shows the design input data.

5. Model validation

Analytical data from Sun *et al*. [52] on the reactive transportation of volatile contaminants throughout the vadose region were utilized to validate mathematical forecasting accuracy. With the help of PHOENICS, a one-dimensional simulation was conducted. The 1.2-meter-long one-dimensional model was split into 24 equal-sized control volumes, each with a different dimension. The orientation of the flow was adjusted on the z-axis. At the model's input boundary, a first-type or Dirichlet boundary condition was chosen. Initially, the concentration in each simulation cell was zero, and a set value of zero was used at the model's output. The model utilized twenty-time steps and 100 iterations. The simulation was developed over a long period of 200 days (Figs. 3-5). The input parameters of the model were taken from Sun et al. [52] and are presented in Table 2.

Table 1. Model parameters utilized in two-dimensional simulation in this work.

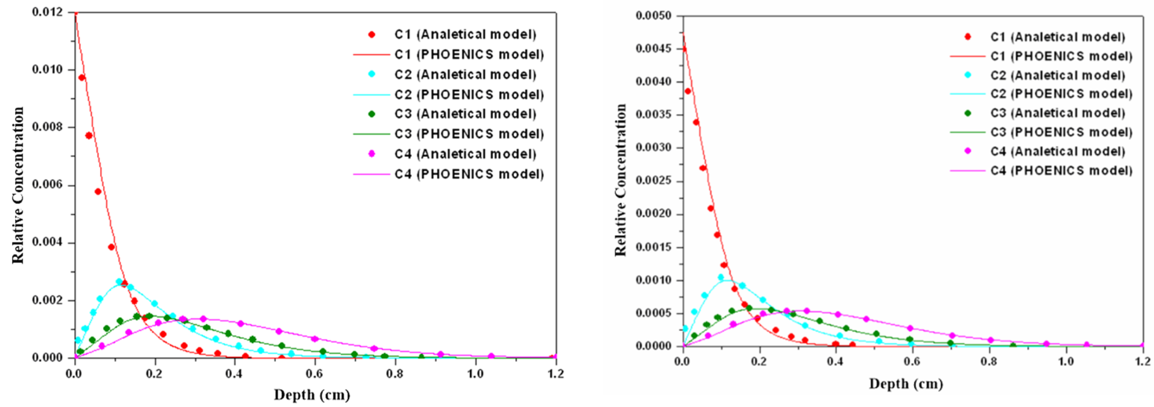
Symbol	Term	Unit	Value
	Spatial and time discretization		
	Model dimension	$m \times m$	3000 × 4000
	Cell numbers		121680
	Simulation time	*years*	50
	Time steps		50
	Flow and transport parameters		
K_x	Hydraulic conductivity in the x-direction	*m/s*	8.07×10^{-6}
K_y	Hydraulic conductivity in the y-direction	*m/s*	8.07×10^{-7}
θ	Porosity		0.41
	Fixed head (left boundary) Dirichlet b. c*		
	Fixed head (right boundary) Dirichlet b. c		
R	Retardation factor		2
l_c	Capillary fringe thickness	*m*	0.07
λ	Decay coefficient of the pollutant	*1/day*	0.00005
D_g	Effective diffusion coefficient of pollutants in soil gas	cm^2/s	1×10^{-1}
D_w	Effective diffusion coefficient of pollutants in the water of the vadose area	Cm^2/s	1×10^{-5}
θ_a	Volumetric soil gas content		0.07
θ_w	Volumetric water content in the NAPL zone		0.2
H	Henry's constant		0.23
d	Vadose zone thickness	*m*	12

Table 2. Input parameters for model validation [52].

Symbol	Term	Units	Value
φ	Porosity	cm^3/cm^3	0.5
a	Air content	cm^3/cm^3	0.2
θ	Water content	cm^3/cm^3	0.3
ρ_b	Bulk density	g/cm^3	1.35
k_d	Soil–liquid partition coefficient	cm^3/g	61.1
k_h	Henry's law constant		0.397
k_1	1st-order reaction rates of species 1	1/d	0.05
k_2	1st-order reaction rates of species 2	1/d	0.03
k_3	1st-order reaction rates of species 3	1/d	0.02
k_4	1st-order reaction rates of species 4	1/d	0.0001
y_2	Yield factor from species 1 to 2		0.79
y_3	Yield factor from species 2 to 3		0.74
y_4	Yield factor from species 3 to 4		0.64
D_g	Gaseous diffusion coefficient	cm^2/d	508
D_l	Liquid diffusion coefficient	cm^2/d	0.0155
J_g	Air velocity	cm/d	0
J_w	Groundwater velocity	cm/d	10

The results of modeling by PHOENICS and those obtained from Sun *et al.*'s [52] simulation show close agreement (Figs. 3-5). Thus, by making a few changes in the PHOENICS program, the existing mathematical simulation may be used to accurately simulate the dynamic transportation of volatile contaminants throughout the vadose area of a polluted unconfined aquifer.

In this simulation, the transport of four sequentially reactive species with transport from the ground surface down to the groundwater table was investigated in the study area. Figs. 3 and 5 show the concentrations of four species in the liquid and gas phases, respectively. Both figures are graphically the same; however, the values of the concentrations are different. Since the four simulated species are volatile, the concentration values of these species in the gas phase are higher than their concentrations in the liquid phase. The ratio of the concentration of a single species to the concentrations of other species in a single phase is controlled by the first-order reaction rates and stoichiometrically yield factors, whereas the ratio of the concentration of a single species in one phase to its concentration in other phases is dominated by partition coefficients [52].



(a) **(b)**

Figure 3. A comparison of model predictions (lines) and analytical solutions (dots) presented by Sun *et al*. [52] for concentration profiles of four chemical species in (a) aqueous phase (b) gas phase (c) for 200 days.

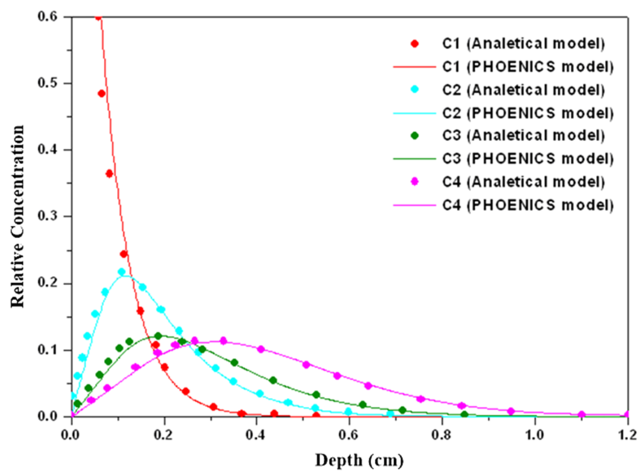


Figure 4. A comparison of model predictions (lines) and analytical solutions (dots) presented by Sun *et al*. [52] for total concentration profiles of four chemical species for 200 days.

6. Simulation results

The model assumed that the NAPL phase was absent throughout the vadose area. Instead, it is an area that consists of water, gas, and solid phases, and is subjected to interactions with the atmosphere, the NAPL, and the saturation domain. When the vadose region is polluted by NAPL volatile chemicals or if the contamination occurs in the saturated area, a local equilibrium partitioning the pollutants between the phases is presumed. Eq. (1) was used for two-dimensional modeling of VOCs transport in the vadose zone. The model was implemented considering the above assumptions. The simulation results for two elapsed times of 36 and 50 years are shown in Figs. 6 and 7, respectively.

A comparison of simulation results and field data for 36 years (Figure 2) shows that the numerical model presented here simulated the reactive transport of volatile hydrocarbons in the vadose area of an unconfined aquifer successfully so that the model results show close agreement with field data. The close agreement between the simulated and calculated profiles illustrated in Figure 6 indicates that PHOENICS can reliably simulate solute transport problems in porous media (an average error of 10.65%).

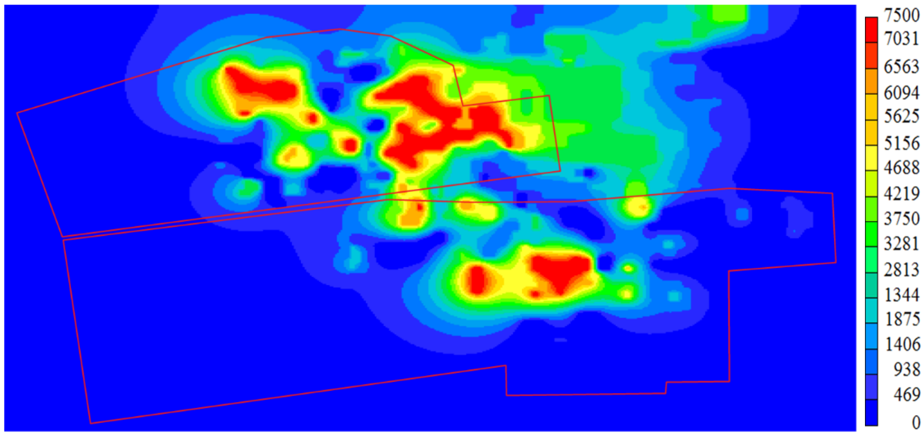


Figure 5. Distribution of volatile organic compounds (VOCs) for 36 years.

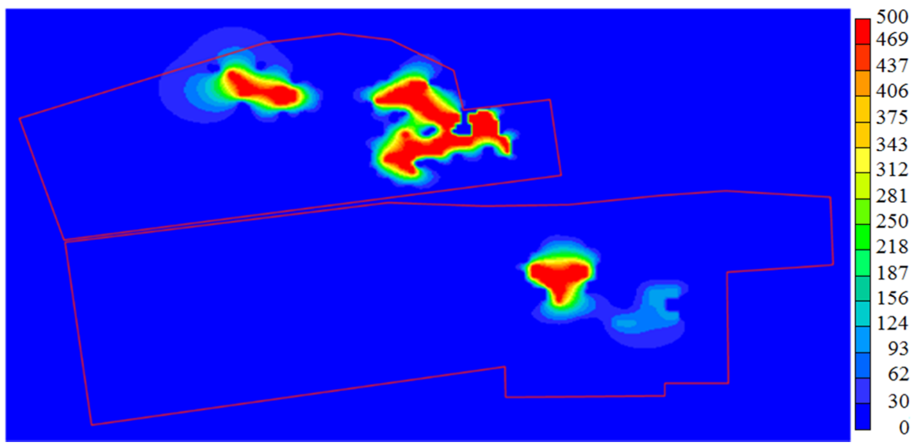


Figure 6. Distribution of volatile organic compounds (VOCs) for 50 years.

As shown in Figure 6, the concentrations of VOCs have decreased compared to those shown in Figure 5. This decrease in concentrations of volatile hydrocarbon compounds in the vadose zone is due to excavations made at the site for field studies. Through these excavations, a substantial volume from the hydrocarbon gas phase confined underneath the ground surface is released into the atmosphere, which reduces the accumulation of volatile gases.

7. Conclusions

In this research work, the risk of VOCs throughout the vadose region of Tehran oil refinery and Rey industrial area in Tehran, Iran was investigated using the mathematical simulations. For the first time, the simulation was verified using the data and findings from Sun *et al.*'s [52] one-dimensional analytical method. The dynamic transportation of volatile hydrocarbons throughout the vadose region of an unconfined aquifer was, therefore, simulated in the validated model. The dynamic model for transportation simulates dispersion, rate-limited mass transfer, the first-order decay between phases of the vadose area, and coupling diffusive mass transfer through the water table. The initial distribution of concentration within the region selected was incorporated into the simulation. The interactions between the vadose region and the atmospheric borders were also included in the model. The model gave an appropriate estimation for the gas distribution across the vadose region reported on location in 2004. The modeling provides insights into the interactions among gas transfer and degradation processes within polluted grounds in the vadose area. In order to reproduce the situations representing current measurements, the transient development of the system was modeled. The non-uniqueness of the simulations may be ascribed to the interactions between parameters that were utilized to build the model, including the effective diffusion coefficients for gaseous transfer and the kinetics of reactions.

Using a two-dimensional finite volume model, the researchers discovered that the mathematical model provided in this work could simulate the dynamic movement of volatile hydrocarbons throughout the vadose region of an unconfined aquifer. For 50 years, the quantities of VOCs have been lower than the expected values over 36 years. This reduction is related to digging carried out during field investigations on volatile hydrocarbon compounds throughout the vadose region. Because of these drills, underground gaseous hydrocarbons may be released into the air, which reduces the accumulation of volatile gases.

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Conflict of interest

The authors claim that they have no conflict of interest.

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چکیده:

این کار به بررسی انتقال واکنشی هیدروکربن‌های فرار در یک سیستم آبخوان آزاد پالایشگاه نفت تهران و منطقه صنعتی ری، تهران می پردازد. یک مدل حجم محدود دوبعدی شامل فرآیندهای فیزیکی، شیمیایی و بیولوژیکی برای پیش‌بینی آلودگی گاز خاک ناشی از انتقال واکنشی LNAPL بر روی سطح آب زیرزمینی از طریق ناحیه هوادار آبخوان ارائه شـده اسـت. یک نرم افزار تجاری چند منظوره به نام PHOENICS با اعمال کدهای اضـافی برای حل معادلات مدل به صـورت عددی ا صلاح شده ا ست. پیش‌بینی‌های مدل کاملاً با اندازه‌گیری‌های میدانی همخوانی دارند، و ن شان می‌دهند که مهاجرت LNAPL معمولاً تحت تأثیر فرآیند تبخیر قرار می‌گیرد. LNAPL ها منبع بالقوه طولانی مدت آلودگی خاک و آب‌های زیرزمینی در منطقه مورد مطالعه هسـتند. مقایسـه نتایج شـبیه‌سـازی در یک گام زمانی ۳۶ سـاله با نتایج مطالعات میدانی نشـان می‌دهد که مدل عددی ارائه‌شـده می‌تواند انتقال واکنش هیدروکربن‌های تبخیر شـده را در ناحیه غیراشـباع شبیه‌سازی کند. غلظت آلاینده‌ها در مرحله زمانی ۳۶ سال نسبت به مقادیر نشان داده شده در مرحله زمانی ۵۰ سال کاهش یافته است. این کاهش در غلظت فاز گاز هیدروکربن در ناحیه غیرا شباع به دلیل حفاری در محل برای مطالعات میدانی ا ست. از طریق این حفاری‌ها، حجم قابل توجهی از فاز گازی محبوس شده در زیر سطح زمین در جو آزاد می‌شود که باعث کاهش تجمع گازهای فرار در زیر سطح زمین می‌شود.

کلمات کلیدی: انتقال هیدروکربن‌های فرار، شبیه‌سازی دو بعدی، مکانیسم‌های بیولوژیکی، پالایشگاه نفت.