A CFD Model for Prediction of the Role of Biomass Growth and Decay on the Aerobic Biodegradation of BTEX fate and Transport in an Unconfined Aquifer System

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ABSTRACT: This paper investigates the importance of considering biomass growth and decay for predicting a field scale microbial degradation of BTEX plume in an unconfined aquifer system in the Pump station area of Tehran oil refinery (TOR), Iran. A two-dimensional finite volume model has been presented to predict multi-species reactive transport incorporating physical, chemical and biological processes in the saturated zone of the aquifer. A multi-purpose commercial software called PHOENICS was modified to solve model equations. A complex Monod approach considering microbial growth and decay employed to describe the biodegradation of BTEX. The results of Monod approach was compared to those results obtained by three kinetics models including zero-order, first-order and Michaelis-Menten expressions that do not support biomass growth and decay. Monod approach predicted a further spreading of the plume. Other kinitics models underestimated the concentrations of BTEX plume, due to neglecting a high bacterial population and increased uptake rate. They are not appropriate to simulate tansport of biodegradable BTEX in the study aquifer. The model predictions agree well with the field measurements with an average error of 5%; describing that the Monod kinetics was well able to simulate the behaviour of the BTEX plume due to supporting bacterial population and considering oxygen as the electron acceptor.

INTRODUCTION

The discharge of organic pollutants into the groundwater aquifers can activate multiple biogeochemical reaction processes including biodegradation which controls the fate and transport of organic pollutants in groundwater system. Hence, biodegradation process is often simulated by various simplie mathematical expressions (Schafer *et al.,* 2005). Many researches have been carried out over the past several years describing the fate and transport of biodegradable substrates considering the growth and decay of microorganisms. These studies have provided useful information to develop appropriate site bioremediation techniques to clean-up the contaminated groundwater. Monod kinetics model is widely used to describe biodegradation rates of organic contaminants in aquifer systems (Borden and Bedient; 1986; Molz *et al.,* 1986; Mac Quarrie *et al.,* 1990). Monod kinetics takes into account the changes in microbial population density, maximum uptake

rates and liner dependency yield on substrate (Schafer *et al.,* 2005).

A simplified shape of Monod kinetics is known Michelis-Menten kinetics. First-order model is the simplest way to mathematically describe the biodegradation of organic compounds. However, this model ignores any dependency of the degradation rate of organic substances on the concentrations of other chemicals or microbial populations (Prommer *et al.,* 2003). Several authors have found that a zero-order model fits well to lab and field data if data show a linear behavior in spase (e.g. Nielsen and Christensen 1994). However, zero-order models encounter problem for prediction because they result in negative concentrations. Considerable efforts have been made to model the growth of microorganisms in porous media. These models incorporate the proper microbial kinetics that can be used for a variety of situations (Borden and Bedient, 1986; Kindred and Celia, 1989; Abriola and Chen, 1995).

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Literature review shows that despite much research related to microbial processes in contaminated aquifers, however, the combination of these processes for the fate and transport of a biodegradable contaminant in a dynamic and reactive system such a the saturated zone of an unconfined aquifer is not fully understood. In this paper, different kinetics approaches were used to model the biodegradation of BTEX. The present work is a further development of the model presented by Schafer et al (2005). The simulation was applied to an unconfined aquifer system in the Pump station area of Tehran oil refinery, Iran. The simulated result for BTEX plume incorporating the biomass growth and decay is compared to the results obtained from other kinetics approaches. It further includes BTEX transport, oxygen consumption and variation in bacterial population.

Oil refining operation around the Rey Industrial Area, south of Iranian capital city, Tehran, has resulted in many environmental problems including soil and groundwater pollution by BTEX compound (benzene, toluene, ethylbenzene, xylene) (Environmental investegations in Tehran oil refinery area, 2005-2007). To design an effective remediation and treatment scheme for such a polluted site, prediction of the fate and transport of the pollutants and identifying their exact plumes is a major task. The study area is loacated in the Pump station in the south side of Tehran oil refininery company (TORC) of Iran (Fig. 1). Soil and groundwater pollution by oil containing BTEX compound had been revealed around the Rey Industrial Area in 1970's.

Although many attempts have been made by the Iranian government to control the release of BTEX compound into the groundwater aquifer, however, considerable achievements were not obtained and the effect of pollution is being increased year by year. As a result, the expansion of the pollution plume has cuased a great concern in the area. An environmental investigation has been conducted by TORC in 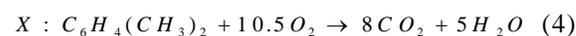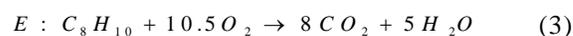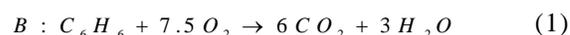the central part of the Rey Industrial Area. This investigation mostly incorpotaes groundwater sampling at the Qanat and water wells inside the site, monitoring the fluctuation of groundwater level and pumping out the groundwater. However, distribution of the pollution had been started earlier than the expectation, and despite these activities, there was no any effective method to monitor the contaminated aquifer and control pollutant leaching into the aquifer due to the lack of equipments and without a proper environmental management program.

Consequently, a serious groundwater pollution problem happened in the Rey Industrial Area. Therefore, because of this matter, it was necessary to take a fundamental action for immediate application of the up-to-date techniques and machinery, in order to perform an effective and accurate environmental investigation. Hence, in response to the request by the TORC, a feasibility study was first carried out by the Japan Corporation Centre and Petroleum (JCCP) in 2002. Consequently, the related investigation plan was prepared in December 2005 and the field investigation was started in February 2006 (Fusione Techno Solutions Co., 2006).

MATERIALS & METHODS

In order to investigate groundwater pollution problem, water samples were taken from the aquifer in the Pump station area. The samples were analysed for physical and chemical parameters (Table 1) (Fusione Techno Solutions Co., 2006).

The oxidation reaction of BTEX can be expressed as follows (modified from Anid et al. 1993, Agah *et al.,* 2011):

$$B : C_6H_6 + 7.5 O_2 \rightarrow 6 CO_2 + 3 H_2O \qquad (1)$$

$$T : C_7H_8 + 9 O_2 \rightarrow 7 CO_2 + 4 H_2O \qquad (2)$$

$$E : C_8H_{10} + 10.5 O_2 \rightarrow 8 CO_2 + 5 H_2O \qquad (3)$$

$$X : C_6H_4(CH_3)_2 + 10.5 O_2 \rightarrow 8 CO_2 + 5 H_2O \qquad (4)$$

Table 1. The physico-chemical parameters of a water sample (Fusione Techno Solutions Co., 2006)

Parameter	temperature	COD-Cr	SS	S^{2-}	TOC	Transparency	pH	Oil content
Unit	^0C	mg/L	mg/L	mg/L	mg/L	cm	-	(mg/L)
P_MW	22.9	30	44	0	15.8	10.5	7.19	75
P_CB								82

Fig. 1. A brief location map of the investigation site (left) and a panoramic view of the investigation site including the Pump station area (right). Groundwater levels distribution around TORC is also shown (Modified after Fusione Techno Solutions Co., 2006)

According to Eq. 1, the Monod kinetics expression describing oxygen limited biodegradation of BTEX and oxygen consumption can be given by the following equations (Schafer *et al.*, 2005; Cirpka and Valocchi, 2007):

$$(5)$$

$$R_{BTEX} = \frac{\partial C_{BTEX}}{\partial t} = -\frac{C_{BTEX}}{K_{BTEX} + C_{BTEX}} \frac{C_{O_2}}{K_{O_2} + C_{O_2}} \frac{\mu_{max}}{Y} f_{BTEX} C_{bio}$$

$$R_{O_2} = \frac{\partial C_{O_2}}{\partial t} = -\frac{C_{BTEX}}{K_{BTEX} + C_{BTEX}} \frac{C_{O_2}}{K_{O_2} + C_{O_2}} \frac{\mu_{max}}{Y} f_{O_2} C_{bio} \quad (6)$$

where, C_{BTEX}, C_{O_2} and C_{bio} are concentrations of BTEX, oxygen and biomass respectively, K_{BTEX} and K_{O_2} are the half-saturation constants of BTEX and oxygen, μ_{max} denotes the maximum specific growth rate, Y represents the specific yield of the reaction, and f_{BTEX} and f_{O_2} are the stoichiometric coefficients of Reactions 1-4.

It is assumed that a population of immobile BTEX oxidising aerobic microbes is present in low concentrations in order to consider the Monod kinetics. Growth of this microbial population follows a double Monod kinetics with two multiplied Monod-terms for BTEX and oxygen and first-order biomass decay. This allows a microbial growth and degradation only if BTEX and oxygen are present. Growth minus decay yields net growth rate, resulting in a permanent consumption of substrates even if biomass is constant (Cirpka and Valocchi, 2007, Mohamed *et al.*, 2010):

$$\frac{\partial C_{bio}}{\partial t} = \frac{C_{BTEX}}{K_{BTEX} + C_{BTEX}} \frac{C_{O_2}}{K_{O_2} + C_{O_2}} \mu_{max} C_{bio} - k_{dec} C_{bio} \qquad (7)$$

where, k_{dec} is the rate coefficient of biomass decay.

Substitution of Eqs. 5 and 6 into the mass transport equations for BTEX and oxygen incorporating linear instantaneous adsorption process, the following equations are obtained:

$$\varphi R_{ret} \frac{\partial C_{BTEX}}{\partial t} - \frac{\partial}{\partial x}\left(D \frac{\partial C_{BTEX}}{\partial x} - u\, C_{BTEX}\right) = R_{BTEX} \qquad (8)$$

$$\varphi \frac{\partial C_{O_2}}{\partial t} - \frac{\partial}{\partial x}\left(D \frac{\partial C_{O_2}}{\partial x} - u\, C_{O_2}\right) = R_{O_2} \qquad (9)$$

$$R_{ret} = 1 + \frac{\rho_d K_d}{\varphi} \qquad (10)$$

$$K_d = f_{oc} K_{oc} \qquad (11)$$

where, D is the dispersion tensor, u denotes the incompressible velocity vector, R_{ret} represents the retardation factor for BTEX, φ is the porosity, ρ_d is referred to the bulk density of porous medium, K_d is distribution coefficient, K_{oc} is the soil organic carbon to water partition coefficient of component, f_{oc} represents the mass fraction of natural soil organic carbon within the soil matrix.

Monod equation assumes that the rate of the transformation increases with the substrate concentration, C_{BTEX}, but as C_{BTEX} grows larger, the rate asymptotically approaches a maximum value defined by $(\mu_{max}/Y)C_{bio}$. Thus, the transformation rate strongly depends on both the biomass concentration and the maximum utilization rate per unit biomass (Bekins *et al.*, 1998). The asymptotic approach to the maximum rate is controlled by the relative values of C_{BTEX} and K_{BTEX}. It is assumed that the biomass remains constant in time and space and a sufficiently large amount of oxygen present. Bekins et al. (1998) were grouped three constants in Eq. 5 into one new constant called the lumped maximum degradation rate defined by $v_M = \mu_{max}C_{bio}/Y$ (mg/L-day). The new simplified equation is similar to the Monod formulation without growth rate (Bekins *et al.*, 1998).

$$\frac{\partial C_{BTEX}}{\partial t} = -v_M \frac{C_{BTEX}}{K_{BTEX} + C_{BTEX}} \qquad (12)$$

Eq. 12 is a Michaelis-Menten kinetics with regard to toluene concentration. The main difference between this model with Monod equation is that Eq. 12 assumes a constant microbial population both in space and time.

Two linear approximations were formulated for Eq. 12 (Bekins *et al.*, 1998; Schafer *et al.*, 2005). The selection of these approximations to be applied for a particular case depends on the relative values of C_{BTEX} and K_{BTEX}. When C_{BTEX} is several times smaller than K_{BTEX} $(C_{BTEX} << K_{BTEX})$, the following first-order equation may be used to approximate Eq. 12:

$$\frac{\partial C_{BTEX}}{\partial t} = -\frac{v_M}{K_{BTEX}} C_{BTEX} \qquad (13)$$

The constants in Eq. 13 are frequently combined to give $k_1 = v_M / K_{BTEX}$ (s^{-1}), where k_1 is the first-order rate constant. When C_{BTEX} is several times greater than K_{BTEX} $(C_{BTEX} >> K_{BTEX})$, then Eq. 12 can be approximated by a zero-order kinetics:

$$\frac{\partial C_{BTEX}}{\partial t} = -v_M \qquad (14)$$

The governing equations describing BTEX biodegradation and oxygen consumption were solved using PHOENICS CFD package. PHOENICS is a general-purpose CFD package which can be used for simulation of fluid flow, heat transfer, and mass transport (Spalding, 1981).

Since Eqs. 8 and 9 contain terms which are not included in PHOENICS general equation, therefore they should be implemented in PHOENICS by introducing the appropriate setting for each term in the Q1 file and applying extra FORTRAN 99 coding in the GROUND subroutine (Doulati Ardejani *et al.*, 2004).

Although not given, PHOENICS model was first verified by data and scenarios provided by Pickens and Lennox (1976) for two dimensional finite element modeling (FEM) of reactive transport problems.

RESULTS & DISCUSSION

After verification of the present model, it was used to predict the fate and transport of BTEX plume considering four different kinetics models including Monod, Michaelis-Menten, first-order and zero-order kinetics for biodegradation process. Most of the model parameters have been taken from Goudar and Strevett, (1998), Park and Juan, (2000), Essaid *et al.,* (2003), Schafer *et al.,* (2005). Other input data are summarised in Tables 2 and 3.

A two-dimensional model was constructed to demonstrate the biomass development and the subsequent removal of organic contaminant (electron donor) inhibited by the lack of oxygen (electron acceptor). The two-dimensional cross-sectional dimensions of the simulated aquifer are 750 m horizontally (x direction) by 40 m vertically (y direction) and this domain is discretised into 35×10 control volumes of size 18 m horizontally $\times$ 4 m vertically.

An immobile NAPL phase of 490 $m \times 8$ is assumed on the groundwater table, dissolving into the mobile pore water through a gradient law (modified from Schafer *et al.,* 2005):

$$\frac{\partial C_{mobile}}{\partial t} = k\left(C_{equilibrium} - C_{mobile}\right) \qquad (15)$$

where, $C_{equilibrium}$ is the maximum solubility and k is a constant called dissolution rate.

For an NAPL mixture (in here gasoline) in contact with water, mixture solubility is equal to the pure maximum solubility component multiplied by the mole (or weight) fraction of the component in the NAPL mixture.

The model was first run for a case of no reactive transport problem. The modelling results are shown

Table 2. Model parameters used in the two-dimensional simulation

Spatial and time discretization	
Model area	750 $m \times 40\ m$
Cells dimensions	18 $m \times 4\ m$
Cell numbers	350
Simulation time	50 *years*
Time steps	50
Flow and transport parameters	
Hydraulic conductivity	8.07 ms^{-1}
dry density of soil	1.7 gr/cm^3
Porosity	0.4
f_{oc}	0.001
Fixed head (left boundary)	34.5 m
Fixed head (right boundary)	31.4 m
Longitudinal dispersivity, α_L	15 m
Transverse dispersivity, α_T	1 m
Stoichiometric coefficient of benzene	1
Stoichiometric coefficient of toluene	1
Stoichiometric coefficient of ethylbenzene	1
Stoichiometric coefficient of xylene	1
Stoichiometric coefficient of oxygen in reaction by benzene	0.41
Stoichiometric coefficient of oxygen in reaction by toluene	0.35
Stoichiometric coefficient of oxygen in reaction by ethylbenzene	0.3
Stoichiometric coefficient of oxygen in reaction by xylene	0.3
Retardation factor for benzene	1.34
Retardation factor for toluene	2.06
Retardation factor for ethylbenzene	3.31
Retardation factor for xylene	3.51
Rate coefficient of biomass decay	$1.175e^{-5}\ s^{-1}$

Table 3. Model boundary and initial conditions

boundary conditions for transport		
Inlet: fixed concentration		Outlet: concentration gradient = 0
C_6H_6	$0\ mg.l^{-1}$	-
C_7H_8	$0\ mg.l^{-1}$	-
C_8H_{10}	$0\ mg.l^{-1}$	-
$C_6H_4(CH_3)_2$	$0\ mg.l^{-1}$	-
O_2	$5\ mg.l^{-1}$	-
Biomass	$0\ mg.l^{-1}$	-
Initial conditions		
C_6H_6		$0\ mg.l^{-1}$
C_7H_8		$0\ mg.l^{-1}$
C_8H_{10}		$0\ mg.l^{-1}$
C_8H_{10}		$0\ mg.l^{-1}$
O_2		$5\ mg.l^{-1}$
Biomass		$1.7 mg.l^{-1}$

in Fig. 2 after 10 years. Organic pollutants considered in the two-dimensional simulations are benzene, toluene, ethylbenzene and xylene. They spreaded into the saturated zone of the aquifer system and diluted in the direction of groundwater flow by the physical transportation processes.

In the next step, simulation was performed to describe the biodegradation process considering the microbial growth by the Monod kinetics expression. For application of the Monod kinetics, a group of the immobile BTEX oxidising aerobic microbes is present in low concentration. Typically, cell numbers in order of 10^6 per gram of aquifer materials was considered.

Using a bulk density of 1.7 gr/cm^3 for aquifer materials, a microbial concenteration of approximately 1.7 mg/l was estimated. Fig. 3 shows the simulation results after 10 years.

The other methods require kinetic parameters, which can not be derived form the Monod parameters. Howeve, these unknown parameters and biodegradation rates maybe found by adjusting their magnitudes until after 10 years of the simulation, the plumes lengths obtained by these methods would become similar to those predicted using Monod kinetics. Subsequently, with the parameterised kinetics, the future behaviour of the plumes was simulated for 36 years time period (modified from Schafer *et al.,* 2005). The predictive capabilities of the different approaches are evaluated by comparing the simulated plumes.

Taking the Monod kinetics into consideration, the highest bacterial population and therefore the main degradation potential develops at the upstream boundary of the contamination, where BTEX and oxygen are mixed by the advection process (Fig. 4). Degradation was only found in the dispersive mixing zone of the plume fringe in downstream of the contaminant source. Outside of the plume, no degradation occurs due to a lack of BTEX. Oxygen is depleted inside of the plume (Fig.4 e).

Fig. 5 compares the field and the simulated concentrations for benzene, toluene, ethylbenzene, xylene and total BTEX applying the Monod kinetics at monitoring well (Table 1, oil content: 75 mg/L) after 36 years. The model predictions correlate well with the field measurements (average error 5%); describing that the Monod kinetics is well able to simulate the behaviour of the BTEX plume. The small difference between the field and the simulated concentrations arisen due to the fact that we considered only BTEX compounds and we ignored the other components present in gasoline.

Although not given, Michaelis-Menten approach, zero- and first- order kinetics models underestimated the BTEX concentrations with respect to the Monod approach. The main reason is that these kinetics approaches do not consider bacterial population and oxygen availability (Agah *et al.,* 2011).
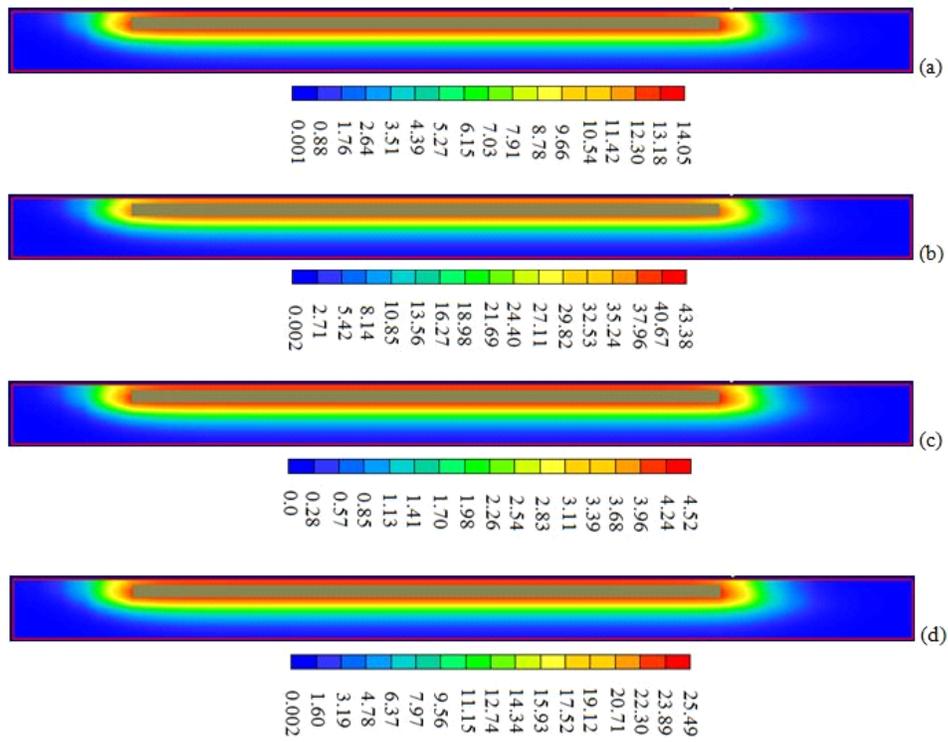
Fig. 2. Two-dimensional simulation results: (a), (b), (c) and (d) are concentration distribution of benzene, toluene, ethylbenzene and xylene after 10 years for a nonreactive transport condition
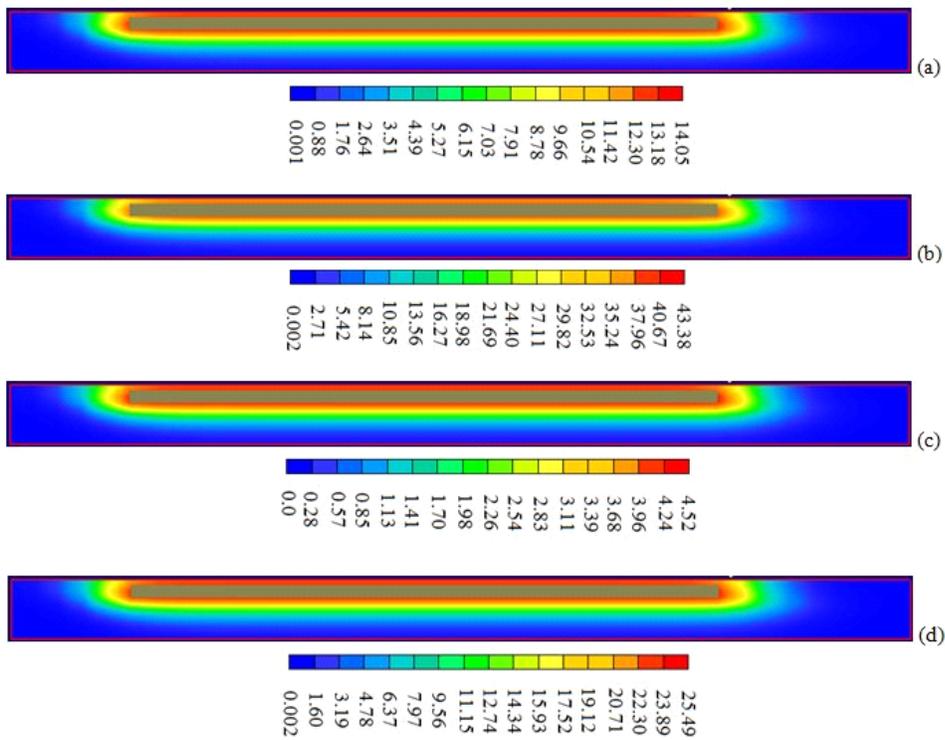
Fig. 3. Two-dimensional simulation results: (a), (b), (c) and (d) are concentration distribution of benzene, toluene, ethylbenzene and xylene after 10 years of the simulation using the Monod approach. (e) and (f) are concentration distribution of oxygen and biomass after 10 years respectively
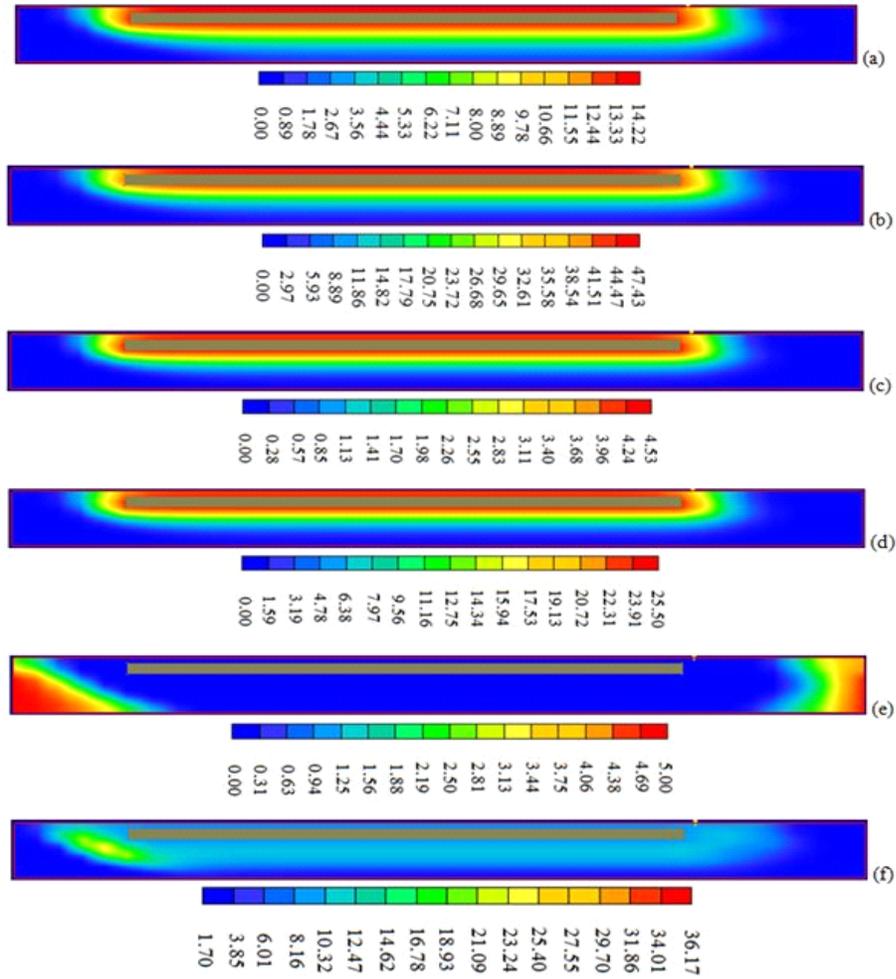
Fig. 4. Two-dimensional simulation results: (a), (b), (c) and (d) are concentration distribution of benzene, toluene, ethylbenzene and xylene after 36 years of the simulation using the Monod approach. (e) and (f) are concentration distribution of oxygen and biomass after 36 years respectively
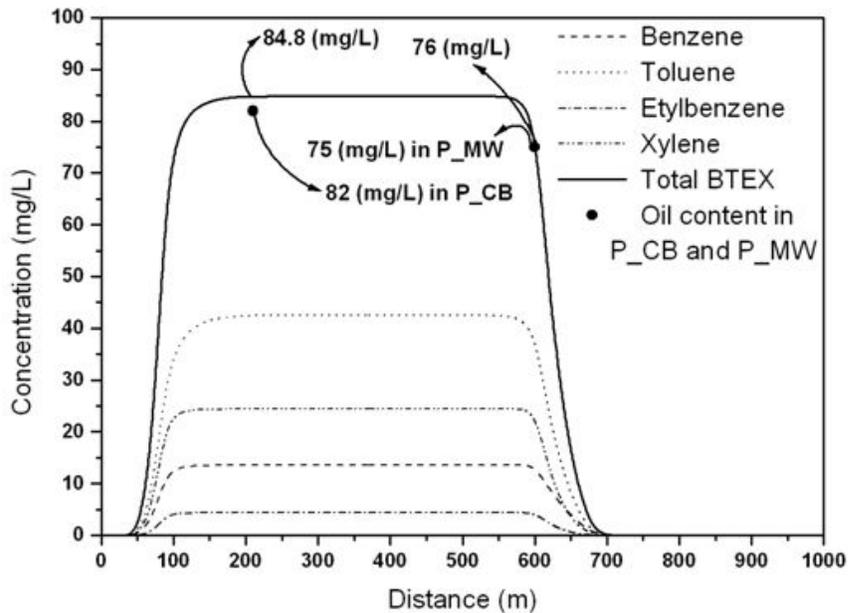

Fig. 5. Comparison of the field observations at monitoring well and simulation results obtained by the Monod kinetics after 36 years

The predictions of all kinetics approaches are evaluated by simulated plume lengths and concentrations. The plumes predicted using the Michaelis-Menten, first-order and zero-order kinetics models are shorter and not as wide as the plume simulated by applying the Monod kinetics. In comparison with the Monod kinetics, all other approaches generally underestimated the plume length. The first-order approach overestimates biodegradation process; resulting in a stationary plume with time.

In the second scenario, the source was removed after 36 years. Therefore, no spill took place but no remediation method was conducted for contaminated soil and groundwater. In this case, contaminated soil above the groundwater table behaves as the only contamination source. Simulation was performed to describe the controlling processes of reactive transport of BTEX. The results show that removal of the contamination source causes some reduction in the concentration of BTEX in comparison with the scenario in which the contamination source is continuous.

In the third scenario, in addition to the elimination of contamination source on the ground surface after 36 years, it is further assumed that the contaminated soil was remediated. Thus, contamination plume reached the aquifer by the physical transport mechanisms over a 36-year period. BTEX decreased significantly by biodegradation and adsorbtion prossess. Comparision of the second and third scenarios shows that the removal of contamination source on the ground surface is itself not enough to reduce BTEX concentration in groundwater and the contaminated soil remediation has to be also considered.

CONCLUSIONS

The results obtained by a two-dimensional finite volume transport model considering Monod kinetics expression show that the highest bacterial population and therefore the main degradation process developed at the upstream boundary of the contamination, where BTEX and oxygen are mixed by the advection process. Degradation was only found in the dispersive mixing zone of the plume fringe in downstream of the contaminant source. Outside of the plume, no degradation occurs due to a lack of BTEX. Oxygen is depleted inside of the plume. Comparison the field and the simulated concentrations of benzene, toluene, ethylbenzene, xylene and total BTEX incorporating the Monod kinetics at monitoring well after 36 years indicates a close agreement with an average error of 5% . The small difference between the field and the simulated concentrations caused due to the fact that the model considered only BTEX and the other components of gasoline were ignored. The numerical model developed here can help in the design and optimisation of the performance of a site remediation and water management system in Tehran oil refinery to control further contamination of groundwater aquifer.

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