v. 3, n. 38, 2023

Journal of
Engineering
Research

APPLICATION OF THE BIOSCREEN MODEL TO SIMULATE BTEX CONCENTRATION IN FEATHER: A CASE STUDY

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Abstract: The contamination of groundwater by petroleum-derived fuel has been the subject of increasing research in Brazil. The compounds, benzene, toluene, ethylbenzene and xylenes (BTEX), present in these fuels, are extremely toxic to human health and the environment. The remediation of contaminated aquifers and soils depends on knowledge of the physical and chemical parameters of each site to quantify the flows and transport of contaminants in groundwater. This quantification has been done through mathematical modeling used in computational models, one of these most used models is BIOSCREEN. The objective of this work is to evaluate the use of the BIOSCREEN model to monitor the evolution of the contaminant plume, the extent of the affected area and the prediction of the time for restoration of water quality in the studied region. The case study discussed in this article refers to an accidental leak that occurred at a service station located in the neighborhood of Brisamar, municipality of Itaguaí/RJ. The aforementioned station has one alcohol tank, two gasoline tanks and two diesel tanks, each of these tanks with a capacity of 15,000 L. It was concluded that: after carrying out the study, it was not possible to evaluate the evolution of the contaminant plume for this site through the BIOSCREEN computational model due to the limited number of experimental parameters.

Keywords: contamination, BTEX, BIOSCREEN and bioremediation.

INTRODUCTION

In leaks from automotive gas stations, the biggest groundwater contamination problems are attributed to monochromatic hydrocarbons, which are the most soluble and mobile constituents of gasoline, such as: benzene, toluene, ethylbenzene and xylenes (known as BTEX). These compounds are powerful central nervous system depressants, presenting chronic toxicity, even in small concentrations (on the order of μg L^{-1})). Benzene is recognized as the most toxic of all BTEX.

It is a proven carcinogenic substance (which can cause leukemia, that is, cancer in the tissues that form blood lymphocytes) if ingested even in low concentrations for not very long periods of time. Acute exposure (high concentrations in short periods) through inhalation or ingestion can even cause death. While the benzene potability standard established by the Ministry of Health (MS) is 5 μg L^{-1}, its concentration, when dissolved in water in contact with gasoline, can reach 3 x 104 μg L^{-1}.

Groundwater contamination due to gasoline leaks from underground storage tanks (TAS) is a major concern due to its environmental and human health risks. This problem is associated with the end of the useful life of the TAS, which is on average 25 years and, as most gas stations here in Brazil were opened in the 70s, it is to be expected that many of these TAS are having problems with leak, despite there being no data on the subject.

The main concern, after a fuel leak, is centered on detecting it as soon as possible, in order to limit it to the smallest possible area, thus facilitating remediation work, thus reducing environmental impacts and costs in recovering the area. achieved.

The objective of this work is to evaluate the use of the model (BIOSCREEN) to monitor the evolution of the contaminant plume, the extent of the affected area and the prediction of the time for restoring water quality in the studied region.

DESCRIPTION

SITE CHARACTERISTICS

The case study discussed in this article refers to an accidental leak that occurred at a service station located in the neighborhood of Brisamar, municipality of Itaguaí/ RJ. The mentioned station has one alcohol tank, two gasoline tanks and two diesel tanks, each of these tanks with a capacity of 15,000 L.

The fuel leak was noticed by two residents neighboring the station, when they detected the flow of pure gasoline, in the free phase, from their taps. One week after reporting the leak, the product was pumped into the free phase and the damaged tank was drained.

Collections were made in the monitoring wells with the aim of evaluating the quality of the groundwater in terms of the presence of BETEX, the analysis of nitrate, sulfate and Fe^{2+}, pH, temperature, conductivity, chemical potential, turbidity and dissolved oxygen.

The available field data, referring to local hydrogeology, were only those provided by the distributor [8] and are listed in Table 1.

PARAMETERS	MINIMUM	MAXIMUM
Hydraulic gradient	0,03%	1%
Hydraulic conductivity (cm s^{-1})	1,43 x 10^{-5}	2,98 x 10^{-5}
Effective porosity for flow	45%	12%
Average linear speed (cm day^{-1})	0,03%	0,21%

Table 1 - Hydrogeological data of the site

The lithology of the area, according to the Hidroplan report [8], is monotonous and allows us to assume that the aquifer is homogeneous for the area of interest in this work. The aquifer was assumed to be isotropic. The length of the plume is of the order of 83.85 m^2.

Local potentiometry indicates groundwater flow to the south, with equipotential lines appearing approximately east-west in orientation. Hydraulic conductivity was determined by carrying out three Slug tests.

Dispersion and adsorption data were extracted from the literature(2) based on sites with similar characteristics.

To simulate contaminant transport, longitudinal, transversal and vertical dispersivity values were obtained from equations 19, 20 and 21(7) (Anexo 1). According to Gelhar(7), the longitudinal dispersivity can be estimated as a value of 10% of the plume length.

Equation 19	$\alpha_{x=}$ 0,10 Lp
Equation 20	$\alpha_{x=}$ 0,10 α_x
Equation 21	$\alpha_{x=}$ 0,010 α_x

Appendix 1 - Equations 19, 20 and 21

The biodegradation values considered were the average electron acceptor values suggested by Newell presented in Table 2. The delay factor considered was equal to 1, which means that the velocity of the contaminants is equal to that of groundwater.

ELECTRON ACCEPTOR	CONCENTRATION (mg L^{-1})
Dissolved oxygen	5,8
Nitrate	6,3
Sulfate	24,6
Methane	7,2
Fe^{2}	1,6

Table 2 – Average electron acceptor values suggested by the BIOSCREEN manual

THE BIOSCREEN COMPUTATIONAL MODEL

In order to assess the environmental risks involved in the leak, a simulation of contaminant transport was carried out using the BIOSCREEN software. THE BIOSCREEN(10) is based on Domenico's analytical solution(5) and(4) for the solute transport model, and has the ability to three-dimensionally simulate the transport of dissolved hydrocarbons considering the processes of advection, dispersion, sorption and biodegradation (first order decay and instantaneous reaction). The original model assumes a one-dimensional vertical penetration of the contaminant, oriented perpendicularly from the source to the groundwater flow, aiming to simulate the leakage of organic compounds moving with the groundwater flow. In this program, Domenico's solution is adapted to promote the representation of three types of models:

1) Solute transport without decay – Suitable for predicting the movement of conservative (non-degradable) solutes, such as chlorine.

2) Solute transport with biodegradation process with first order decay – In this model, the degradation rate of the solute is proportional to its concentration.

3) Solute transport with biodegradation reaction – The biodegradation of organic compounds in groundwater is much more difficult to quantify when using a decay reaction, since, in this case, the limitation of electron acceptors is disregarded, and these effects are more accurate when incorporated into the instantaneous reaction equation. in the transport model. This is how the BIOSCREEN instant reaction model is based.

BIOSCREEN has been widely used as an evaluation model to determine the viability of RNA (Remediation through Natural Attenuation) on the site, it can also be used as a primary RNA model in groundwater on small sites.

As an analytical model, BIOSCREEN assumes simple flow conditions for groundwater and must not be applied where pumping systems are created to complicate

Journal of Engineering Research ISSN 2764-1317 DOI 10.22533/at.ed.3173382321113

field flow. In addition, the model cannot be applied where vertical flow gradients affect contaminant transport. It must not be applied where the expected results are extremely detailed, which are closely linked to the required site conditions. In these cases, more sophisticated and comprehensive models must be used.

BIOSCREEN was used with the aim of three-dimensionally simulating the transport of dissolved hydrocarbons considering the processes of advection, dispersion, sorption and biodegradation (first order decay and instantaneous reaction). The model applies the Domenico equation (equation 18). In this work, the model was applied to evaluate the time taken to restore water quality to potable levels, transport processes and the attenuation of contamination by intrinsic bioremediation.

MATHEMATICAL MODELS AND REMEDIATION

The protection and cleaning of aquifers depends on knowledge of the physical and chemical parameters of each site to quantify the flows and transport of contaminants in groundwater. This quantification can be done in several ways, including field measurements and mathematical modeling. The approach through field measurements is the most direct, however, it is rarely used exclusively, due to its high costs and long deadlines (groundwater moves very slowly, and may require several years to characterize its behavior), or in certain cases, inapplicability (for example: the impact of an industrial lagoon designed, but not yet built, which needs to be assessed). The quantitative approach most frequently used by government agencies and consulting companies is modeling. The models used can be physical or computational, the latter being the most popular since the 1960s.

As the name suggests, a computational model is an equation or series of equations that simulate and predict physical-chemical responses of an aquifer subject to disturbances, such as injection or extraction wells or the migration of a toxic waste [5]

Among these computer programs, we can mention MODFLOW[9] , used for flow analysis, and the programs: BIOSCREEN[10], BIOCHLOR[1], BIOPLUME III[11], MT3D[12], RT3D[6] and FemPol[4], used in contaminant transport simulation. All of these models are sophisticated and must be used when the expected results must be highly accurate. In cases where it is desired to use simpler models, the Houston Groundwater Service developed the BIOSCREEN model (1996). This is a simple, easy-to-use model that simulates remediation through natural attenuation in sites where oil spills or oil derivatives have been detected. Its data are very close to those used in BIOPLUME, and in BIOSCREEN it does not consider vertical interference in the underground flow, which makes it simplified when compared to the other models mentioned above. However, it is of great use in environments where the subsurface flow does not suffer these types of interference[6].

APPLICATION OF THE BIOSCREEN MODEL ON THE WEBSITE

Three simulations were carried out applying the BIOSCREEN model. With simulations 1 and 2, attempts were made to reproduce the BTEX concentrations at the time of the accident. Simulation 3 imagines a scenario where a TAS (underground storage tank) accident occurs in the municipality studied (municipality of Itaguaí). This simulation was carried out in an attempt to evaluate, according to the modeled area and the leak time, which water collection points could be reached by the contaminant plume.

Simulation 1 was an attempt to reproduce BTEX concentrations at the time of the accident based on the field data presented in tables 1 and 2. The modeled area, 62 m long by 30.5 m wide, covers the affected points by the leak, including the first capture point, 30 m from the source of contamination. From the length of the plume, Lp = 62 m (200ft) and equations 19, 20 and 21, the following were calculated: the longitudinal dispersivity, α_x = 6,2 m (20ft), the transverse dispersivity, α_y = 0,6 m (2 ft) and vertical dispersivity, α_z = 0,06 (0,02 ft). Source data were estimated according to information from HIDROPLAN (1999), which after pumping the gasoline-free phase, reported a residual concentration of BETEX in the monitoring well closest to the source.: 16,6 mg L^{-1} and size: 15 m^2.

In simulation 2, the BIOSCREEN model was calibrated in an attempt to reproduce the BTEX concentrations at the time of the accident. The hydrogeological data, biodegradation, modeled area and BTEX concentration data were the same as those used in simulation 1. However, in this simulation the dispersion and source area data were overestimated. The values used were: longitudinal dispersivity, α_x = 96 m (306 ft), transverse dispersivity, α_y = 9,6 m (30,6 ft) and vertical dispersivity, α_z = 0,96 m (0,3 ft) and 150 m^2 to the fountain area.

Simulation 3 was carried out in an attempt to evaluate, according to the modeled area and the leak time, which water collection points could be reached by a plume of contaminants, in the event of a fuel leak in one of the installed TAS. In this simulation, the following were considered: the modeled area, 60 m (300 ft) x 30.5 m (120 ft), time of 2 years after the start of the leak, the area of the contamination source, 15 m^2, and the velocity of the contaminant plume, 8 m $year^{-1}$ (26 ft ano^{-1}).

For safety reasons, the plume velocity value was calculated to be 10 times greater than the field parameters. From the length of the feather, Lp = 100 m (330 ft), that of the equations ($\alpha_x = 0{,}10$ Lp, $\alpha_y = 0{,}10\, \alpha_x$ e $\alpha_z = 0{,}010\, \alpha_x$), values were obtained for longitudinal dispersivity, α_x = 10,0 m (33 ft), transverse dispersivity, α_y = 1,0 m (3,3 ft) and vertical dispersivity, α_z = 0,1 m (0,3 ft). Regarding the concentration of BETEX from the source, the value adopted corresponds to the solubility of the compounds in water, which is 164 mg L^{-1}.

This value was taken from Brost and Beckett(3), as the value corresponding to the solubility of Brazilian gasoline was not found in the literature, which, due to the addition of ethanol to its composition, causes the solubility value to be greater than that of the pure product. There was no consideration in the free phase, because as previously mentioned, its speed can only be determined indirectly, considering the monitoring.

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