



Temporal Transport Simulation of Heavy Metal Pollutants in Eleme Industrial Area of Rivers State, Nigeria

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Authors' contributions

This work was carried out in collaboration with between all authors. Author OLG designed the study, wrote the protocol, managed the literature and wrote the first draft of the manuscript. Authors DCO and CUO managed the analyses of the study. All authors read and approved the final manuscript.

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ABSTRACT

The temporal transport of heavy metals like Iron (Fe), Manganese (Mn), Zinc (Zn), Lead (Pb), Copper (Cu), Chromium (Cr), Cobalt (Co) and Cadmium (Cd), deposited in the soil of Eleme in Rivers state Nigeria due to industrial activities was studied. Advection-Dispersion equation was used to determine the possible displacement of these metals laterally and transversely with time towards the water table. The results show a flow towards and lateral to the water table. A diffusion coefficient of 10^{-9} to 10^{-10} m²/s the pollutants drift faster towards the water table. Also, from the steady-state analysis made, the results show that these pollutants are also displaced vertically to as much as 9.6m of the static water level of 12.0metres in the study area. This level of pollution and flow of heavy metals in the area should call for a remediation strategy by the companies and other authorities concerned.

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1. INTRODUCTION

Flow and solute transport in the subsurface involve a series of complex processes that work in accordance with the conservation laws to determine the movement of contaminants along with the flowing water towards the water table. Water flow is in response to recharge to the soil matrix, mainly from meteoric water sources in the form of precipitation as rainfall. The precipitation that falls to the land surface is dispersed in several ways and direction according to the hydrological cycle [1,2]. The interrelationships between the infiltrated/percolated water, the presence of contaminants within the catchment area under consideration and the catchment properties of the soil determine the degree of transport of the contaminants from the land surface towards the water table and consequently, the quality of the catchment underground water.

The vertical transmission of water within the subsurface is described with respect to two major subsurface layers divided by an irregular surface called water table into the Unsaturated (or vadose Zone) and the saturated Zone. The vadoze Zone is the zone lying immediately below the land surface and contains water and air in its pore spaces. The presence of pores containing air and water lays the foundation for a series of complex array of time-dependent physical, chemical and biological activities and processes which are found to be taking place in this zone [3]. These processes control the transfer of heat, mass and momentum between the atmosphere and water table.

The saturated zone underlies the vadose, and it is the zone in which all the pores and rocks are filled with water.

The water table is the locus of points where hydrostatic pressure equals atmospheric pressure. There are variations of flow patterns in each of these two zones according to the appropriate flow characterisation.

Bear [4] defined the vadose zone of the subsurface as having a pressure head less than zero. This means that the pressure head is negative in this zone (soil tension or suction) and water is being sucked into dry soil.

The vadose zone often contains more significant amounts of organic matter and metal oxides due to its closeness to the land surface. One of the major characteristics of this zone is the presence of air/gas in its pore spaces, a phenomenon known to facilitate the activities of numerous microorganisms, resulting in the occurrence of complex subsurface chemical reactions. Hence, the unsaturated portion of the subsurface is seen as an important pathway for transport of gasses and volatile organics [5]. Three regions of subsurface water have been identified resulting in three subdivisions or belts: the zone of soil water, the intermediate zone and the capillary fringe [6].

The zone of soil water is the uppermost zone extending from the land surface to a depth where moisture changes are minimal (the root zone of plants). Infiltration and evapotranspiration take place here, and through it the water table is recharged. The capillary fringe is at the base of the vadose zone and extends upwards from the water table until there is a decrease in soil moisture. Here, water is always raised by capillary and portions of this zone can be at 100% saturation. This zone changes as recharge/discharge cause the water table to fluctuate.

The intermediate zone lies between the soil water zone and the capillary fringe. The soil in this zone has an average moisture content, which remains constant. Moisture in the soil usually is in the form of gravity water in large pore spaces, while in small, poor spaces it exists in the form of capillary water.

Fluid flow in the unsaturated zone is due to gravity or soil moisture gradient, with the mechanism of water movement being a transmission from pore to pore [7]. The rate of movement depends on the temperature gradient, relative humidity, pore size/continuity as well as the amount of available water.

The saturated (phreatic) zone lies below the water table, with the interstices usually filled with water. All water movement beneath the water table is of the saturated flow type.

Characterised by flow and transport in the saturated zone is done in like manner to the vadose zone. Herein, the relative conductivity is equal to or nearly equal to one and the moisture content is equal to the saturated moisture

content since the effective moisture content is unity.

$$K(h) = K_r K_s \quad (1a)$$

Where K_r is the relative conductivity ($0.0 \leq K_r \leq 1.0$),
 K_s is the saturated conductivity, h is the hydraulic head

$$K_r = 1, \theta_e = 1 \text{ and } \theta_w = \theta_s \quad (1b)$$

It can be observed that groundwater is always in motion from areas of natural flow direction and artificial recharge to areas of natural and artificial discharge. Under natural conditions groundwater moves very slowly, its velocity ranging from fractions of a centimetre per year (cm/yr) to several cm per day (cm/day). Solute transport describes the displacement of solute contaminant along with flowing water from the land surface into the soil matrix and towards the water table. The transport of solute through the vadose and saturated regions of the subsurface is represented mathematically via the conservation equations of mass, momentum and energy with their constitutive relations for the process variables, all coupled into the Fick's law. Fick's Law gives a relationship between the fluxes of the contaminant within the given volume. There are two major mechanisms responsible for the transport of pollutants in the soil/aquifer: Advection/convection and Hydrodynamic dispersion.

2. TRANSPORT BY ADVECTION/ CONVECTION

Advection is the movement of particles of a contaminant by the fluid velocity. The fluid velocity under consideration, in this case, is the groundwater velocity. In soils and aquifer, the flows are nearly always laminar and, generally, it is either impossible or impractical to determine all aspects of a particular velocity field. Therefore, advection usually refers to the transports due to the mean velocity field of the fluid.

The advective flux, except in a mass-balance equation, is exactly the same as convection flux, with the only exception being that in the later, the individual densities of the particles are taken into consideration.

2.1 Hydrodynamic Dispersion

Hydrodynamic dispersion is the mixing of fluid or the transport of pollutants due to the effects of

unresolved heterogeneities or concentration gradients in the permeability distribution. Hydrodynamics dispersion usually occurs via two main processes: Mechanical dispersion and Molecular diffusion. Mechanical dispersion is the process that results in the distribution of contaminants along flow path due to velocity gradient while Molecular diffusion is the process that involves the distribution of mass as a result of fluid thermal kinetic energy and contaminant concentration gradient. In soils and aquifers, the contributions of tortuosity to dispersion are generally much greater than that due to molecular diffusion. Tortuosity (τ) is a factor that accounts for the increased distance a diffusing ion/particle must travel to get around sand grains. Thus, the flow variation portion of the dispersion term is used to describe the effects of shear in the velocity field, and the tortuous path fluid takes within a porous medium. Hence, the coefficient of hydrodynamic dispersion is usually expressed as a sum of two terms, the mechanical dispersion and molecular diffusivity [8].

$$D = D_o \tau + \alpha u \quad (2)$$

D_o is the free solution diffusion coefficient;
 τ , the tortuosity factor; α , the dispersive parameter and
 u is the flow velocity.

The dominant mechanism responsible for transport at any point in time depends on the hydraulic conductivity of the soil/aquifer. This is because, if the hydraulic conductivity is very low, as in some aquifers and clay, then the transport mechanism may primarily be by diffusion, while for high conductivity, advection is the dominant transport mechanism.

Contaminants released into the environment as the result of manufacturing, use of manufactured products and reckless waste disposal, rarely remain at the point of discharge in an untransformed state. In many cases, chemical and biochemical transformations result in significant changes in the nature of the contaminants. In the majority of cases, contaminant mixtures are involved, and individual species may be transported at different rates, with the rates of transport being functions of the degree of saturation of the soil/aquifer and the various biogeochemical processes taking place in the subsurface.

It is also important to note that some compounds are conservative. This means that they are highly

resistant to transformation, while others are quite chemically or biochemically reactive. Thus, old or un-weathered contaminants are entirely different in makeup compared to recent discharges. Weathering as used here describes the selective loss or disappearance of a contaminant mixture in the soil. Understanding of nature, transport mechanisms and the fate of these pollutants is necessary for successful site remediation and hazardous waste management.

Attempts to simulate the effects of natural phenomena are referred to as modelling, which are representations of real-world processes and events, whose creation and use require many observation-based judgments. Simulations must be demonstrated under varieties of defined conditions and must incorporate scientific facts before the developed model can be considered reliable. Heavy metal pollutants, not being a new phenomenon especially, due to the industrial revolution, have also received numerous attentions, regarding models, both theoretical and experimental.

Many researchers in the various fields of environmental studies have used experimental models for many simulation purposes because it provides an element of reality that is enlightening and satisfying from an intuitive viewpoint. These models have been widely used in the field of environmental science, for the determination of the presence, types and the number of contaminants present in the environment. [9] used a non-reactive tracer test method, to monitor contaminant migration rates in the Niger Delta where hydrocarbon pollution had occurred. The results revealed that kerosene and diesel were the principal components of the soil matrix while the aquifer migrating tracer plume arrival time is $1.403 \times 10^{-3} \text{ms}^{-1}$ (121 m/day), with longitudinal and transverse dispersion coefficients of $2.459 \times 10^{-3} \text{m}^2 \text{s}^{-1}$ and $2.39 \times 10^{-3} \text{m}^2 \text{s}^{-1}$ and 1.78 and 1.64 m, respectively. [10] did a site investigation on the heavy-metal contaminated ground in Estareja, Portugal. High concentrations of toxic metals (As, Hg, Pb and Zn) were discovered in the soil of the industrial area, while very high concentrations were found in sediments of the water streams, several kilometres away from the industrial complex (the pollution source area). [11] studied mangrove Oyster, *Crassostrea agasari* from the lower Bonny estuary concerning lead (Pb). The results show that lead has a preferential accumulation in Oyster shells than in the tissues of the oysters. The values of tissue lead were greater than 0.5ppm indicating contamination of oyster tissues

in the study area. [12] determined the concentration of Zinc (Zn), Lead (Pb), Copper (Cu) and Cadmium (Cd) in the littoral gastropod (*Littorina Saxatilis*) and the algae (*Enteromorpha intestinalis*) from five sites, in the Isle of Man. The results show *L. Saxatilis* having the highest concentration of Zn, Pb and Cd.

2.2 Transport Modelling

Extensive modelling efforts have been channelled towards predicting the mass transport of contaminants in soils/aquifer over the past two decades. This has led to appropriate modifications of the flow and transport equations to show the intentions of the various researchers. [13] gave an equation is shown below for the three-dimensional flow of water in porous media.

$$\frac{\partial}{\partial x_i} \left[k_{ij} \frac{\partial}{\partial x_j} \right] (\Psi + x_3) = (c + \beta_s S_s) \frac{\delta \Psi}{\delta t} - q_s, \text{ in } \Omega \quad (3)$$

where x_i is the spatial coordinates ($i = 1, 2, 3$ with x being vertical); k_{ij} is the hydraulic conductivity tensor which is a function of moisture content or pressure under unsaturated conditions; β_s is the index for saturation and is 0 in the unsaturated zone ($\Psi < 0$) and 1 in saturated zone ($\Psi \geq 0$); S_s is the specific storage defined as the volume of water released from storage per unit volume of saturated soil due to unit decrease in the pressure head; t is the time; q is the source/sink term (positive for source) which represents the volume of water added/removed per unit time to/from a unit volume of soil, and Ω is the solution domain.

Similarly, the equation governing the transport of chemically reactive solute was given as

$$\frac{\partial}{\partial x_i} \left[D_{ij} \frac{\partial C}{\partial x_j} \right] - q_i \frac{\partial C}{\partial x_i} = \theta \frac{\partial C}{\partial t} + \frac{\partial}{\partial t} (\rho b C^*) + f k_2 \rho b C_k^* + q_s (C - C_s), \text{ in } \Omega \quad (4)$$

$$\text{With } \frac{\delta (\rho b C^*)}{\delta t} = k_1 \theta C - k_2 \rho b C_k^* + \frac{\partial}{\partial t} (\rho b C_e^*)$$

Where C is the solute concentration in the liquid (in unit of mass per unit volume), C^* is the adsorbed phase concentration (in unit of mass of adsorbed chemical per unit mass of porous media), C_k^* is the kinetic fraction of the adsorbed chemical, $C_e^* (= \frac{K_3 \theta C}{P_b})$ is the equilibrium fraction, k_1 is the forward (adsorption) rate constant, k_2 is the backward (desorption) rate constant, k_3 is the equilibrium constant, f is the loss coefficient for

the selective first-order removal, q_i is the specific discharge components, ρ_b is the bulk density, q_s is the injected/pumped fluid volume per unit aquifer volume,

C_s is the solute concentration in q_s , and

$$D_{ij} = (\alpha_L - \alpha_T) \frac{q_{iaj}}{q} + \alpha_T \delta_{ij} \quad (5)$$

In which α_L is the longitudinal dispersivity, α_T is the transverse dispersivity, $q (= \sqrt{q_i q_j})$ is the magnitude of the specific discharge while δ_{ij} is the Kronecker delta.

The above transport model is similar to the mobile-immobile physical partitioning model of [14] given as

$$\frac{\partial}{\partial x_i} \left[D_{ij} \frac{\partial C_m}{\partial x_j} \right] - q_i \frac{\partial C_m}{\partial x_i} = (\theta_m + \rho_b f * k) \frac{\partial C_m}{\partial t} + [\theta_{im} + (1 - f *) \rho_b k] \frac{\partial C_{im}}{\partial t} \quad (6)$$

$$\text{With } (\theta_{im} + (1 - f *) \rho_b k) \frac{\partial C_{im}}{\partial t} = \alpha_\tau (C_m - C_{im}) \quad (7)$$

θ_m and θ_{im} are the mobile and immobile phase water contents respectively, C_m and C_{im} are the mobile and immobile zone solute concentrations, f is the fraction of solid matrix in contact with the mobile zone, k is the distribution coefficient, α_τ is the first order rate constant.

Similar models have also been developed for the multiphase flow and transport of Non-aqueous phase liquid contaminants in porous media [15].

2.3 Conceptual Model

Descriptions of contaminant migration in soils or in aquifers are usually based on the equations

defining conservation of mass. Advanced engineering studies have made familiarisation with the use of systems having defined boundaries as in fluid mechanics, a possibility. However, considerations of individual chemical species within the fluid, movement of materials through chemical and biochemical reactions results in somewhat, more complicated expressions.

This research work considers the area as being represented by a two-dimensional plane with the x-axis being the horizontal expanse and the Z-axis representing the vertical direction. The horizontal direction has a length which is infinitely large, with the area, under consideration being represented by (b-a) as shown in the Fig (1) below. This area suffers from combined effects of pollutants from various sources in the area.

The z-direction is divided by the water table into the upper unsaturated zone and the lower saturated zone, with the distance of the unsaturated zone being represented by H. This work is based on a monthly recharge rate of 0.268 m, from available meteorological data records from the area, while the pollutant concentrations shall be simulated.

2.4 Assumptions

Coupling the mathematical representations of the effects of variations of density, hydraulic conductivity and the effect of various subsurface biogeochemical processes (sorption, ion complexation and precipitation) will result in a complete flow and mass transport equation. This work has considered and made the following assumptions.

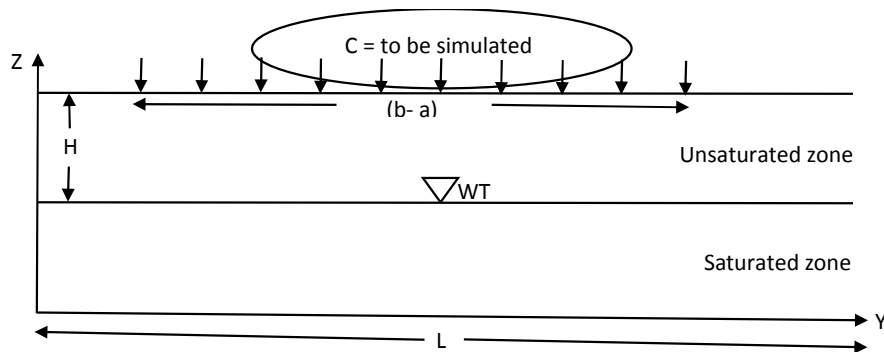


Fig. 1. The conceptual model

- That the contaminants under consideration, which are heavy metals, are conservative.
- The area under consideration is homogeneous and well stratified.
- The permeability and hydraulic conductivity are also taken to be constant throughout the strata.
- We have also assumed that there is a matching of density between that of the dissolved contaminants and the groundwater.

These assumptions are necessary to reduce the effects of variations in the porosity of the medium, as the porosity variation within each stratum may be considered constant throughout each stratum. Thus, the effects of density variations are ignored.

[16] undertook Spatial detection of the Presence of some Heavy Metal Pollutants in the study area heralding this phase of research which is aimed at determination of the temporal transport of these metals with time through the unsaturated sub-surface towards the water table in the area, using mathematical simulation models.

2.5 The Study Area

The area of study comprises host communities for the following industries: National Fertilizer Company of Nigeria Limited (NAFCON), Port Harcourt Refining Company (PHRC) and Eleme Petrochemicals Company Limited (EPCL) in Eleme Local Government Area, Rivers State, Nigeria.

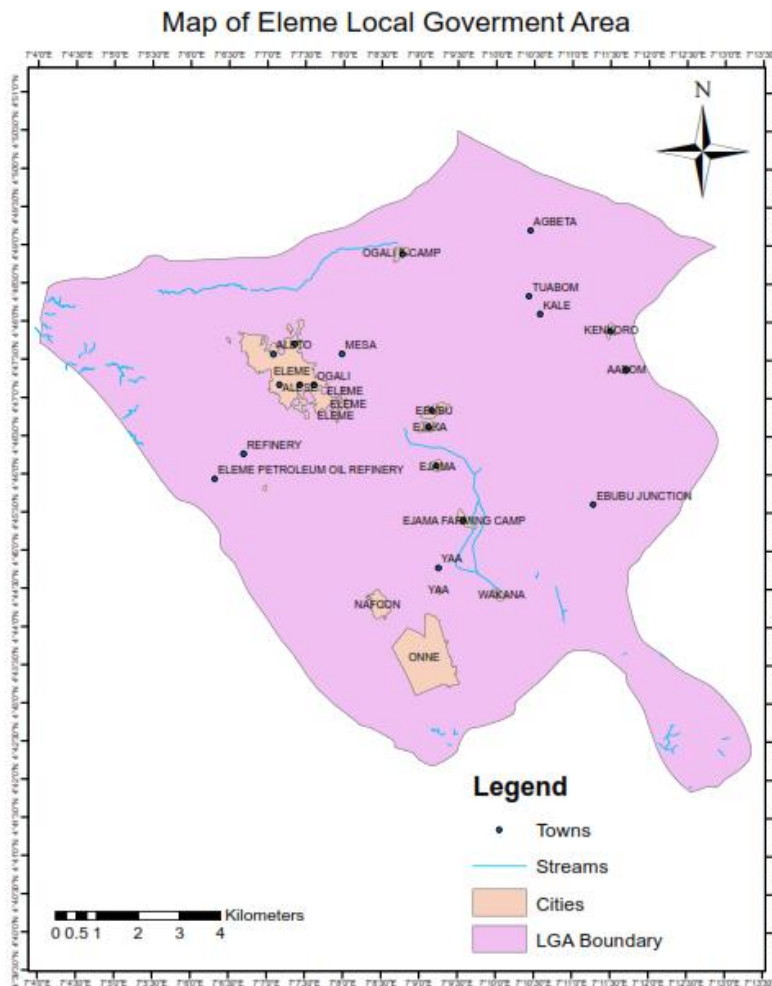


Fig. 2. The study area [16]

2.6 Formulation/Model Development

The Advection-Dispersion flow equation model was used to determine the temporal transport simulation of the heavy metal pollutants found to be in existence in the study area. The flow of groundwater is governed by the principles of conservation of mass and momentum. The mass conservation for the fluid is expressed as the equation of continuity, and the conservation of momentum is expressed as the Navier-stokes equation for the flow of viscous compressible fluid. However, these conservation equations obey Darcy's law, which is the governing equation for groundwater movements. Darcy's law is a macroscopic equation of motion for the flux of a unit mass of fluid flow relative to a formation under the fluid potential (mechanical energy per unit mass of fluid) and is expressed as

$$v = -k\nabla h \quad (8)$$

Where v is the flow per unit area, h is the hydraulic head above a datum, k is the hydraulic conductivity of the formation. The equation of continuity (conservation of mass) for the fluid was written by [17] as

$$\nabla(\nabla\rho) + \frac{\partial}{\partial t}(\rho\theta) + \rho q = 0 \quad (9)$$

t is the time, θ is the porosity ($0 \leq \theta \leq 1$), q is the source or sink of volumetric flow per-unit-volume ($\frac{1}{t}$). Eqn (9) applies either to a porous medium ($\theta < 1$) or fractures ($\theta = 1$) and describes the rate of accommodation of fluid mass within a given volume of the medium. It also accounts for transient effects from changes in storage due to the compressibility of both the rock matrix $\alpha(\frac{LT^2}{M})$ and the fluid, $\beta(\frac{LT^2}{M})$. The effect of the second term in (9) may be written as

$$\frac{s_s \delta h}{\delta t} \quad (10)$$

Where $s_s = \rho g (\alpha + \phi\beta)$ is the coefficient of specific storage ($\frac{1}{t}$) that describes the volume of fluid released from storage under a unit decline in hydraulic head. Expanding the terms in equation (9) and neglecting terms involving changes in density when compared to terms involving changes in velocity over the volume of spatial mesh element, yields

$$\nabla v = \frac{-\delta(\theta\rho)}{\delta t} - \rho \quad (11)$$

Substituting equation (10) into (11) for the first term on the right-hand side and introducing Darcy's law gives

$$-\nabla v = \nabla(k \cdot \nabla h) = S_s \frac{\delta h}{\delta t} + \rho \quad (12)$$

Eqn. (12) can be written in three dimensions as

$$-\nabla v = \frac{\delta}{\delta x} \left(K_x \frac{\delta h}{\delta x} \right) + \frac{\delta}{\delta y} \left(K_y \frac{\delta h}{\delta y} \right) + \frac{\delta}{\delta z} \left(K_z \frac{\delta h}{\delta z} \right) = S_s \frac{\delta h}{\delta t} + \rho \quad (13)$$

Equation (12) is the generalised diffusion equation describing the transient-flow of groundwater as a function of hydraulic head in the presence of sources or sinks in an anisotropic saturated medium.

For flow in the saturated media, the total head, h , is introduced as the sum of the suction head, Ψ , and the height, Z , above a datum as

$$h = \Psi + Z \quad (14)$$

Expressing Eqn (13) in terms of the total head, h , and introducing the specific water constant $\Gamma(\psi)$ to replace the storage terms gives

$$\frac{\delta}{\delta x} \{ K_x(\Psi) \frac{\delta \Psi}{\delta x} \} + \frac{\delta}{\delta y} \{ K_y(\Psi) \frac{\delta \Psi}{\delta y} \} + \frac{\delta}{\delta z} \{ K_z(\Psi) \frac{\delta \Psi}{\delta z} \} + 1 \} = \Gamma(\Psi) \frac{\delta \Psi}{\delta t} + \rho \quad (15)$$

The gradient terms in parenthesis are the respective velocities V_x , V_y and V_z for the x-, y- and z- directions respectively. Replacing these terms with their velocities changes equation (15) to

$$\frac{\delta}{\delta x} \{ K_x(\Psi) V_x \} + \frac{\delta}{\delta y} \{ K_y(\Psi) V_y \} + \frac{\delta}{\delta z} \{ K_z(\Psi) V_z \} + 1 \} = \Gamma(\Psi) \frac{\delta \Psi}{\delta t} + \rho \quad (16)$$

Assuming lateral isotropy in the flow equation (16) yields

$$\frac{\delta}{\delta x} \{ K_x(\Psi) V_x \} + \frac{\delta}{\delta z} \{ K_z(\Psi) V_z \} + 1 \} = \Gamma(\Psi) \frac{\delta \Psi}{\delta t} + \rho \quad (17)$$

The task before us here is to solve for the flow velocity functions from the highly hysteretic dependence of hydraulic conductivities on moisture contents and substitute these velocity functions into the advection-dispersion equation of solute transport to describe the displacement of the pollutants from the land surface with time.

2.7 Transport

The mass transport of constituents by advection and dispersion is dependent on the hydrologic and hydrodynamic characteristics of the particular environment. The well-known advection-dispersion equation is formulated based on the Fick's law of molecular diffusion and states that the rate of mass transport of a material through a unit cross-sectional area of fluid by molecular diffusion is proportional to the concentration gradient of the material in the fluid. That is

$$F = -D\nabla c \quad (18)$$

F is the mass flux through the cross-sectional area, D is the diffusion/Dispersion coefficient; C is the material concentration in the fluid and ∇ is the gradient operator.

The continuity equation for the guest article is written as

$$\frac{\delta C}{\delta t} + \nabla \cdot F = 0 \quad (19)$$

For a case of dispersion within a laminar flow situation with velocity V , which is independent of the position R , the flux will also have a component due to the velocity, V as the guest particles are moving within the flow, such that,

$$F = vC - D\nabla \cdot C \quad (20)$$

Using equations (20) and (18) and (19) yields

$$\left. \begin{aligned} y &= \alpha y \sqrt{\frac{k_{sz}}{k_{sy}}}, \text{ so that } L = \alpha L \sqrt{\frac{k_{sz}}{k_{sy}}} \\ \alpha &= \alpha z \sqrt{\frac{k_{sz}}{k_{sy}}}, \quad b = \alpha b \sqrt{\frac{K_{sz}}{K_{sy}}} \\ z &= \alpha z^*, \quad \text{so that } H = \alpha H^* \\ K &= \frac{k_{i^* x}}{K_{i^* sx}} \quad \frac{K_{i^* z}}{K_{i^* sz}} \\ q &= \frac{q^*}{K_{sz}} \end{aligned} \right\} \quad (24)$$

Where k_i^* are the hydraulic conductivities in the i -direction. α is the pore-size distribution parameter $\text{cm}^{-1} (\text{L}^{-1})$

$$D\nabla^2 C - \nabla(vC) = \frac{\delta C}{\delta t} \quad (21)$$

Equation (21) above is the well-known advection-dispersion equation for solute transport, which can be expressed in a more convenient form as

$$\frac{\delta C}{\delta t} + V_z \frac{\delta C}{\delta z} + V_x \frac{\delta C}{\delta x} = D_z \frac{\delta^2 C}{\delta z^2} + D_y \frac{\delta^2 C}{\delta y^2} - kC \quad (22)$$

Where k is a first-order decay constant.

2.8 Computational and Flow Model Techniques

Consider the two-dimensional flow model for flow in variably saturated media shown below (Fig. 3).

The actual variables are asterisked to distinguish them from their dimensionless forms. Exponential relations are assumed to exist between the pressure head and conductivity as well as pressure head and moisture content as follows:

$$\left. \begin{aligned} K^* y &= K_{sy} \exp(\alpha \Psi) \\ K^* z &= K_{sz} \exp(\alpha \Psi) \\ \theta &= \theta_r + (\theta_s - \theta_r) \exp(\alpha \Psi) \end{aligned} \right\} \quad (23)$$

Where θ_s = Saturated water content

θ_r = residual water content

K_{si} = saturated conductivities in i -direction

Dimensionless variables are defined as

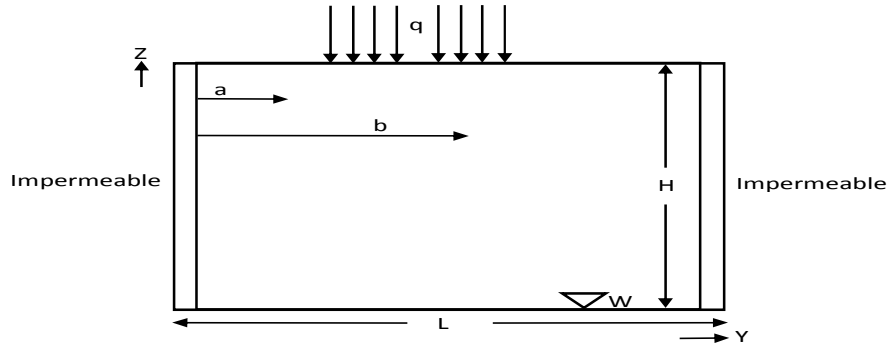


Fig. 3. 2-D flow model in variably saturated media

Taking the Laplace transform of the flow equation (17) gives a steady-state solution of the form

$$K = e^{-z} + \frac{q(b-a)}{L} \left(1 - e^{-z} \right) + \frac{2q}{L} e^{H-z/2} \sum_{n=1}^{\infty} \frac{\left\{ \sin(\lambda_n b) - \sin(\lambda_n a) \right\} \cos(\lambda_n y) \sin h(P_n z)}{\lambda_n \left\{ \frac{1}{2} \sin h(P_n H) + P_n \cosh(P_n H) \right\}} \lambda \quad (25)$$

Where λ_n and P_n are given values that enable the simulation to proceed to infinity. They are defined as

$$\lambda_n = \frac{\eta\pi}{L} \quad \text{and} \quad P_n = \sqrt{\frac{1}{4} + \lambda_n^2} \quad (26)$$

The dimensional Darcy velocity components in the y- and z-directions are then given as

$$v_y = \frac{v^* y}{\sqrt{K_{sy} K_{sz}}} = - \frac{\partial K}{\partial y} \quad (27)$$

$$v_z = \frac{v^* z}{K_{sz}} = - \left(\frac{\partial K}{\partial z} + K \right) \quad (28)$$

Applying equations (27) and (28) to the steady-state solution of the hydraulic conductivity equation (30) above results in.

$$v_y = - \frac{\partial K}{\partial y} = \frac{2q}{L} e^{H-z/2} \sum_{n=1}^{\infty} \frac{\left\{ \sin(\lambda_n b) - \sin(\lambda_n a) \right\} \cos(\lambda_n y) \sin h(P_n z)}{\lambda_n \left\{ \frac{1}{2} \sin h(P_n H) + P_n \cosh(P_n H) \right\}} \quad (29)$$

Similarly,

$$v_z = - \frac{q(b-a)}{L} - \frac{q}{L} e^{H-z/2} \sum_{n=1}^{\infty} \frac{\left\{ \sin(\lambda_n b) - \sin(\lambda_n a) \right\} \cos(\lambda_n y) \sin h(P_n z)}{\lambda_n \left\{ \frac{1}{2} \sin h(P_n H) + P_n \cosh(P_n H) \right\}} \times \left[\sinh(P_n z) + 2P_n \cosh(P_n z) \right] \quad (30)$$

2.9 Transport Model Techniques

The transport model for the Two-dimensional flow in the porous media considers a strip source with infinite width as shown below.

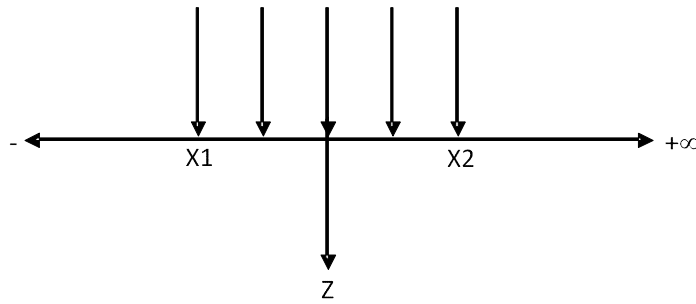


Fig. 4. A strip source (infinite width)

The governing equation is given as

$$\frac{\partial C}{\partial t} + V_z \frac{\partial C}{\partial z} + V_x \frac{\partial C}{\partial y} = D_z \frac{\partial^2 C}{\partial z^2} + D_y \frac{\partial^2 C}{\partial y^2} - KC \tag{31}$$

With the boundary conditions of

$$\begin{aligned} C &= C_0 e^{-\lambda z} \quad , \quad z=0 \quad \text{at } x_1 \leq x \leq x_2 \\ C &= 0 \quad z=0, \quad \text{for all other } x \\ \frac{\partial C}{\partial y} &\rightarrow 0 \quad , \quad y \rightarrow \pm \infty \\ \frac{\partial C}{\partial z} &\rightarrow 0 \quad , \quad z \rightarrow \pm \infty \\ C &= 0 \quad , \quad t = 0 \end{aligned}$$

Applying laplace's transform to the above, advection-dispersion equation and simplifying, result in a solution of the form

$$C(z, y, t) = \frac{C_0 z}{4\sqrt{\pi D_z}} \exp \left\{ \frac{V_z z}{2D_z} - rt \right\} \int_{\tau=0}^t \exp \left[- \frac{\left(K - r + \frac{V_z^2}{4D_x} \right) \tau - \frac{z^2}{4D_z \tau}}{\frac{3}{\tau^2}} X \right] \left\{ - \operatorname{erfc} \left(\frac{(\chi_2 - \chi)}{2\sqrt{D_y \tau}} + \frac{V_y}{2} \sqrt{\frac{\tau}{D_y}} \right) + \operatorname{erfc} \left(\frac{(\chi_1 - \chi)}{2\sqrt{D_y \tau}} + \frac{V_y}{2} \sqrt{\frac{\tau}{D_y}} \right) \right\} dy \tag{32}$$

Where

- D_i = dispersion coefficient in the i -direction
- K = the first order decay constant
- Y = distance in the y - direction
- C = contaminant concentration
- λ = contaminant decay constant
- t = time
- v_i = 1 – direction velocity

The equation above (i.e. the velocity equations, flow equations as well as the equation of transport) are computed using the two-

dimensional groundwater mass transport model analytic solution computer program, which takes in certain parameters from the study area to make it area- sensitive. These parameters are the height of the vadoze zone (i.e. the static water level), vadoze zone soil type, the effective grain size of the vadoze zone soils, permeability, porosity, moisture content and pressure head. Other sensitive parameters incorporated into the computer program from the study area are the dispersion coefficient, the rainfall rate and infiltration/percolation rate. Some of these data and their values are as shown in Table 1.

Table 1. Specific necessary parameters of the study area

Height of vadose zone	12.0 meters
Vadose zone soil type	Silty clay
Effective size of vadose zone soils	3.17µm
Rainfall rate	6.65x10 ⁻³ m/day
Infiltration rate, q	2.22z10 ⁻³ m/day

The above parameters and their values are uniform for the entire study area, as they are mainly averaged values. The variation of dispersion coefficient and other transport parameters in the soil with moisture contents is shown in the equation

$$\theta D = \alpha_L v \delta + (\alpha_L - \alpha_T) \frac{vV}{v} + \alpha_m \theta \tau \delta \quad (33)$$

θ is moisture content; d is the dispersion coefficient tensor (L^2/T); α_i is the longitudinal dispersion coefficient (L)

α_T = transverse dispersion coefficient (L)

α_m = molecular diffusion coefficient (L)

τ = tortuosity (L)

(tortuosity is a factor that account for the distances of a diffused ion around sand grains).

v = the magnitude of the Darcy velocity (L/T)

δ = Kronecker delta tensor.

The above equation (33) reveals that at a certain depth in the vadose, dispersion may no longer play a prominent role in the transport of the solute, hence diffusion will dominate. The Stokes-Einstein equation was found a little more useful. According to this equation, single phase diffusion coefficients may be related to molecular size and phase viscosity by

$$D_{\alpha\rho}^0 = \frac{RT}{6\eta_\rho r_\alpha} \quad (34)$$

Where R is the gas constant, T is absolute temperature, η_ρ is the phase viscosity, r_α is the molecular radius of the species. In porous media, the actual/effective diffusive flux is usually less because diffusion occurs only within the fraction of the pore spaces occupied by the solute and because diffusion paths are more circuitous owing to the presence of gases. Thus, we will then have that,

$$D_{\alpha\rho}^{diff} = \tau_\rho D_{\alpha\rho}^0 \quad (35)$$

Where $D_{\alpha\rho}^{diff}$ is the effective diffusion coefficient and τ_ρ is the phase tortuosity coefficient

A theoretical analysis suggests the latter to be of the form.

$$\tau_\rho = \theta^{\frac{1}{3}} S\rho^{\frac{7}{3}} \quad (36)$$

The water content is equal to the slope of the moisture content versus pressure head curve.

The generating curves are the [18] equation and that:

$$\theta_w = \phi S_w \quad (37)$$

And $\theta_{my} + \phi_{we} = \phi$

Where S_w is the saturated water content; ϕ is the porosity; θ_{my} is the specific yield and θ_{wr} is the specific water retention. Dividing through by ϕ gives

$$S_{wy} + S_{wr} = 1 \quad (38)$$

In the direction of flow,

$$D_L = \frac{V_L \lambda_L}{\phi S_L} \quad (39)$$

With D_L , being the longitudinal dispersion coefficient; λ_L , the longitudinal dispersivity; S_L is the longitudinal phase saturation. It should also be noted that:

- (a) $\lambda_L(\alpha_i)$ is the typically found in the range of 0.01-0.1 of the mean travel distance for distance <1km and diminishes to a smaller fraction for distance > 1km.
- (b) $\lambda_T(\alpha_T)$ is typically in the range of 0.1-0.3 times λ_L .
- (c) $\tau = \phi^{\frac{1}{3}} S\rho^{\frac{7}{3}} = \phi^{\frac{8}{3}} \theta_w^{\frac{7}{3}}$ (40) [15]

3. RESULTS

The results of the analytical solution to the unsaturated steady-state two-dimensional groundwater flow velocity field are shown in Fig. (5) for the vertical velocity field and Figs. (6 to 17) for horizontal flow

A plot of Vertical Flow Velocity field considering Vertical and Horizontal Distances

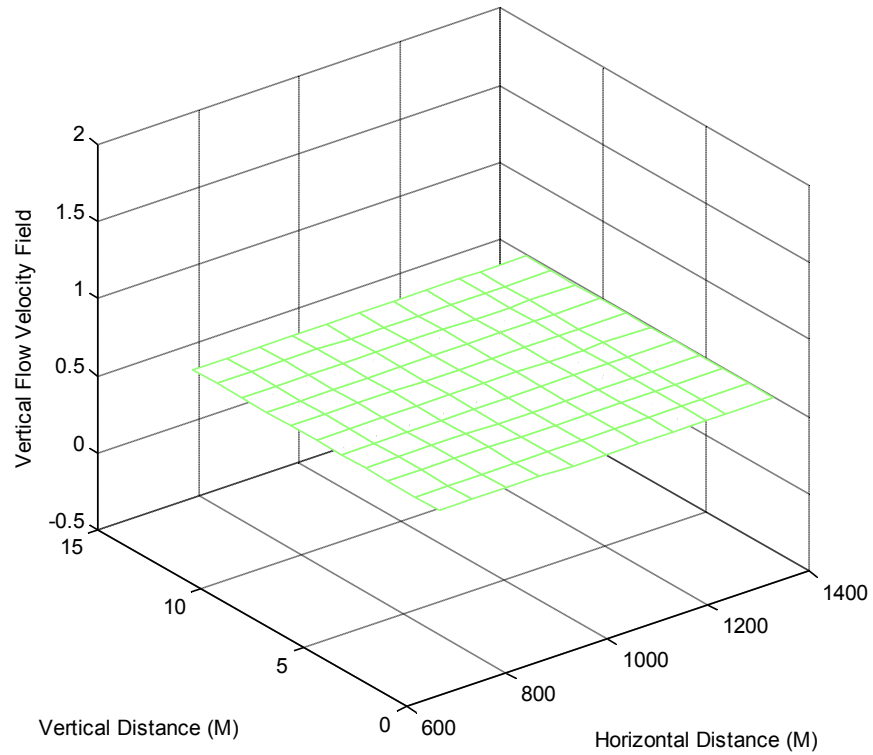


Fig. 5. Vertical flow velocity field

A plot of Horizontal Flow Velocity field considering Vertical and Horizontal Distances

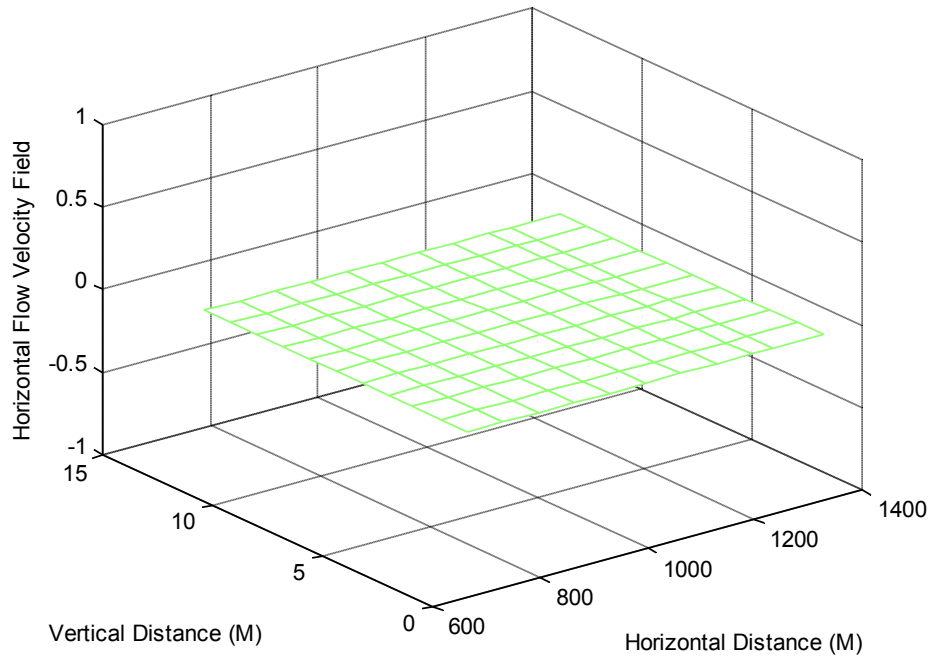


Fig. 6. Horizontal flow velocity field

A plot of Pollutant Horizontal Displacement after 1 day considering Vertical and Horizontal Distances

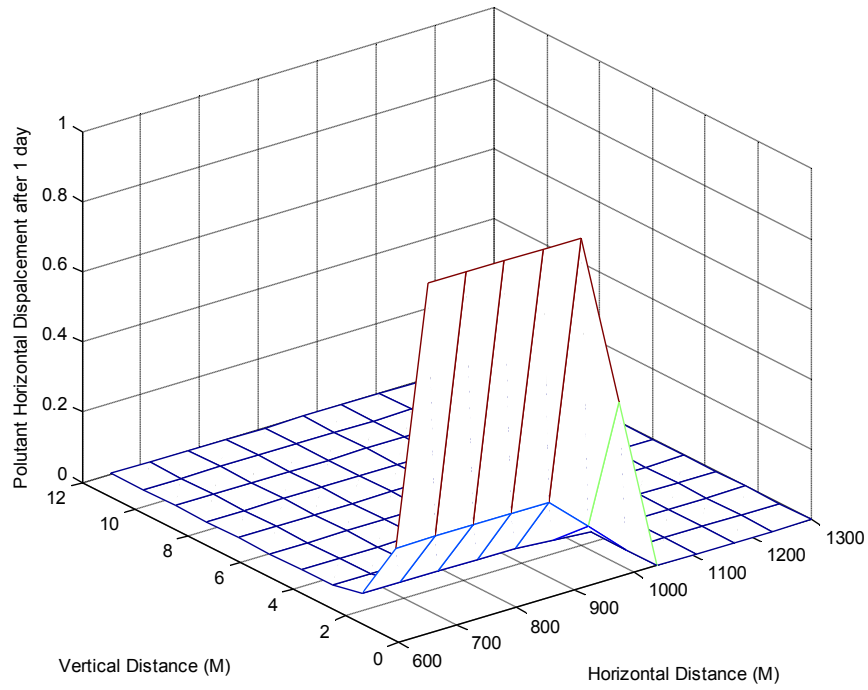


Fig. 7. Pollutant horizontal displacement after 1 day

A plot of Pollutant Horizontal Displacement after 3 days considering Vertical and Horizontal Distances

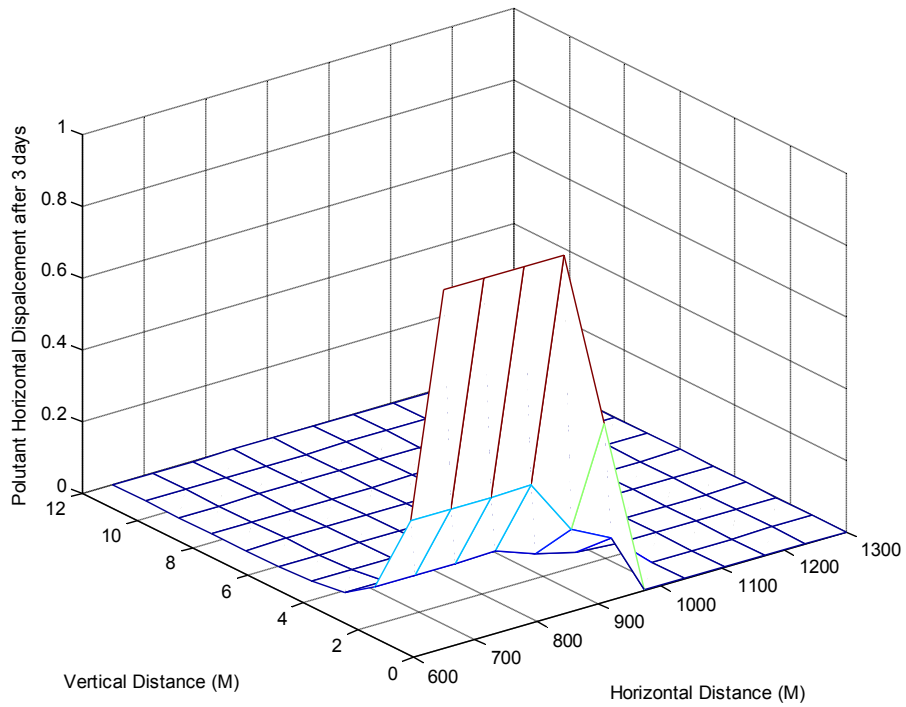


Fig. 8. Pollutant horizontal displacement after 3 days

A plot of Polutant Horizontal Dispalcement after 4 days cosidering Vertical and Horizontal Distances

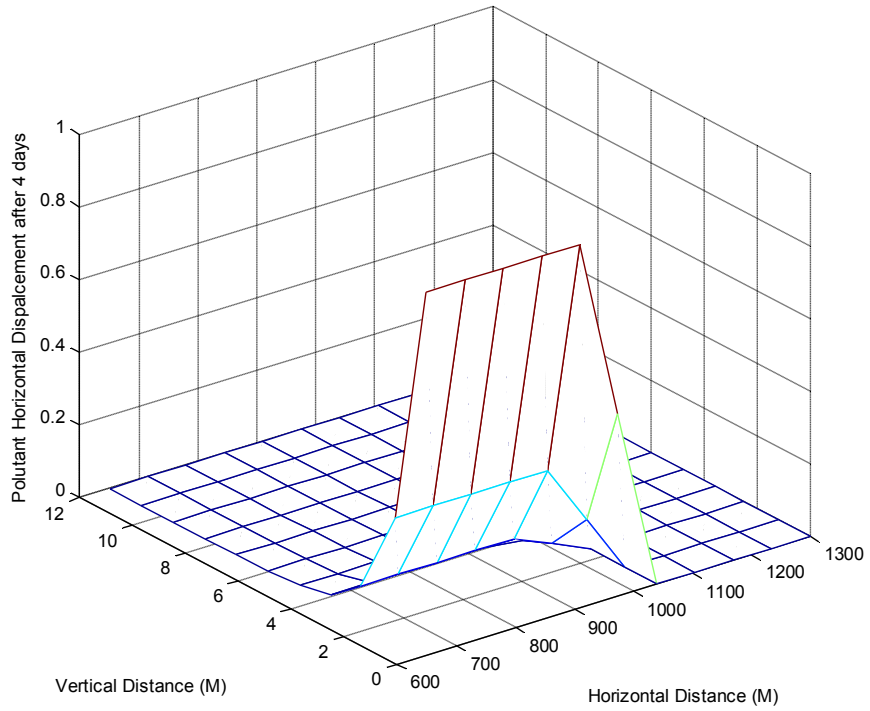


Fig. 9. Pollutant horizontal displacement after 4 days

A plot of Polutant Horizontal Dispalcement after 5 days cosidering Vertical and Horizontal Distances

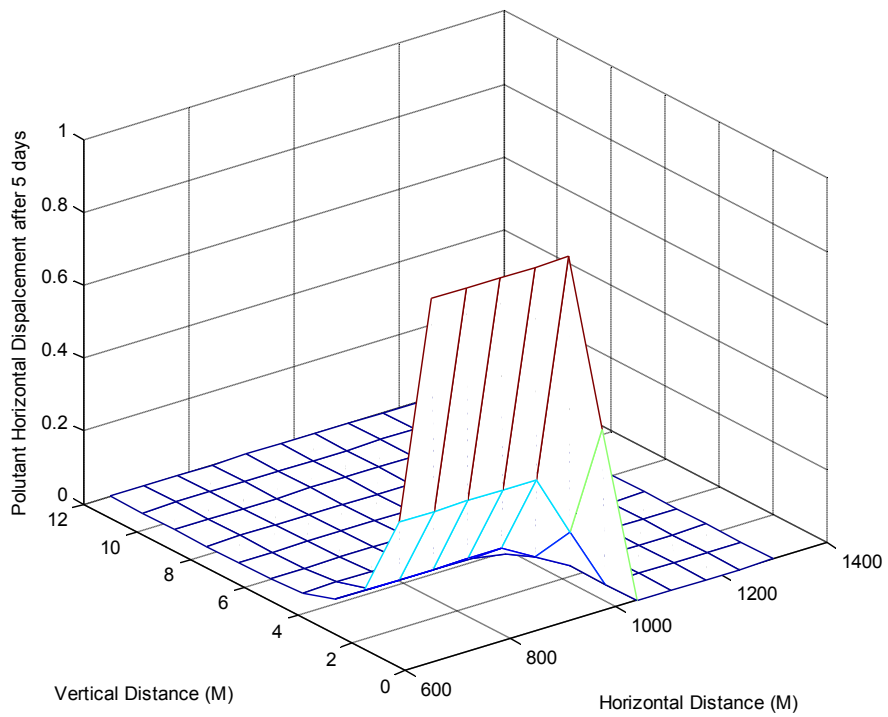


Fig. 10. Pollutant horizontal displacement after 5 days

A plot of Pollutant Horizontal Displacement after 10 days considering Vertical and Horizontal Distances

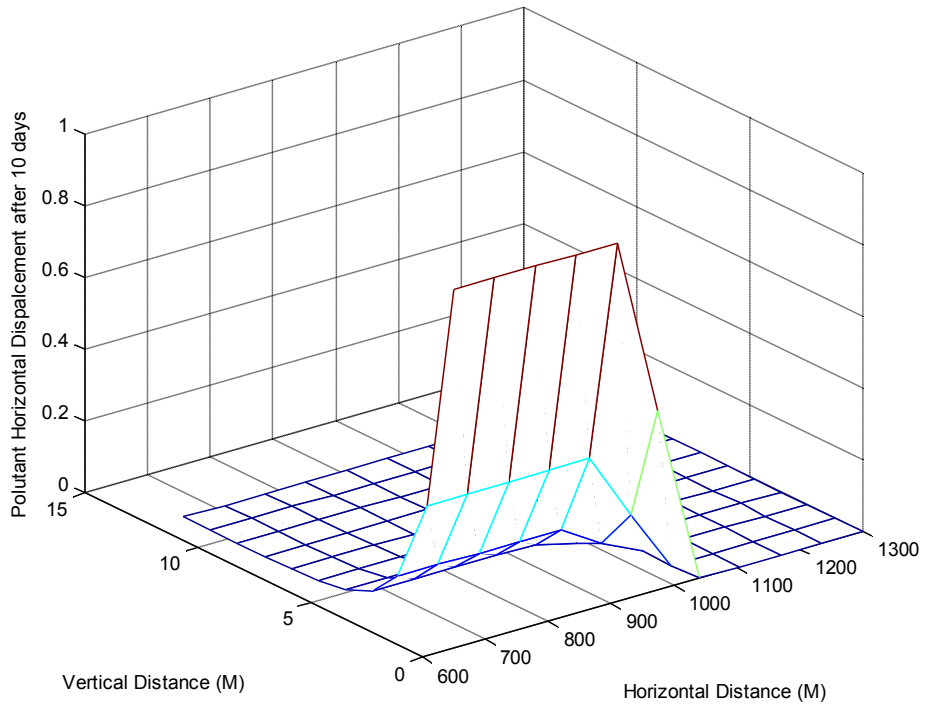


Fig. 11. Pollutant horizontal displacement after 10 days

A plot of Pollutant Horizontal Displacement after 20 days considering Vertical and Horizontal Distances

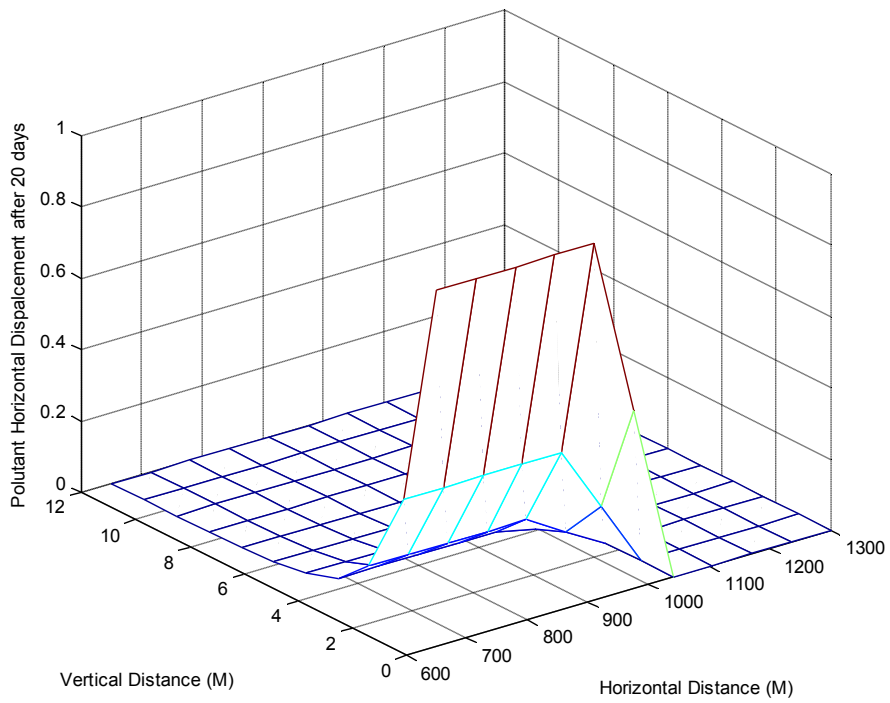


Fig. 12. Pollutant horizontal displacement after 20 days

A plot of Pollutant Horizontal Displacement after 30 days considering Vertical and Horizontal Distances

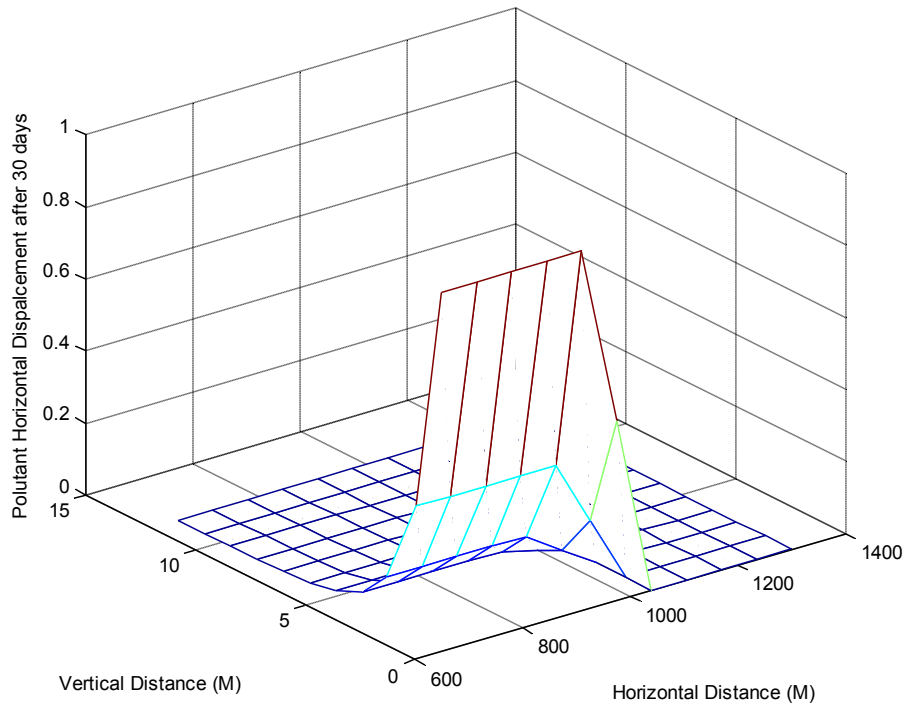


Fig. 13. Pollutant horizontal displacement after 30 days

A plot of Pollutant Horizontal Displacement after 1825 days considering Vertical and Horizontal Distances

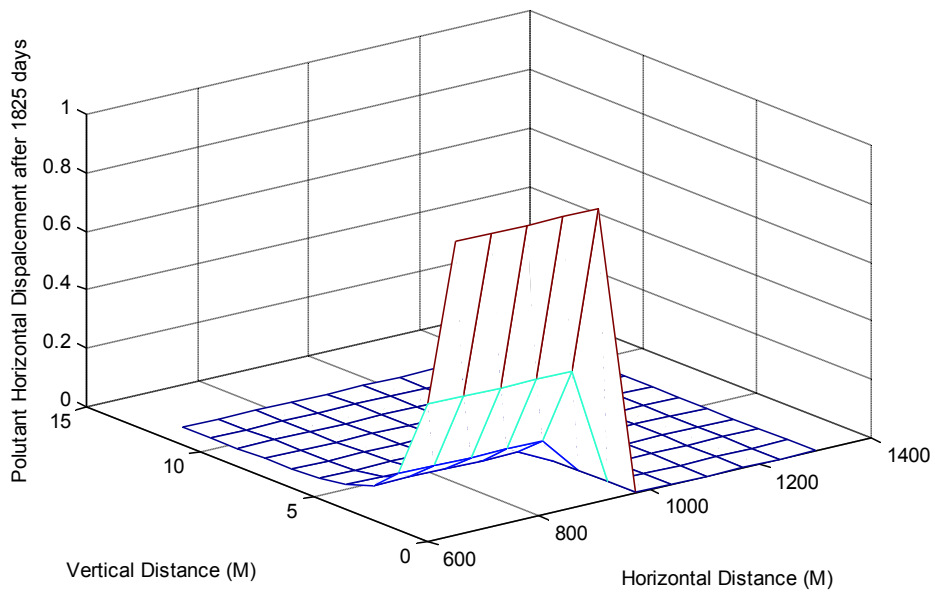


Fig. 14. Pollutant horizontal displacement after 1825 days

A plot of Pollutant Horizontal Displacement after 5875 days considering Vertical and Horizontal Distances

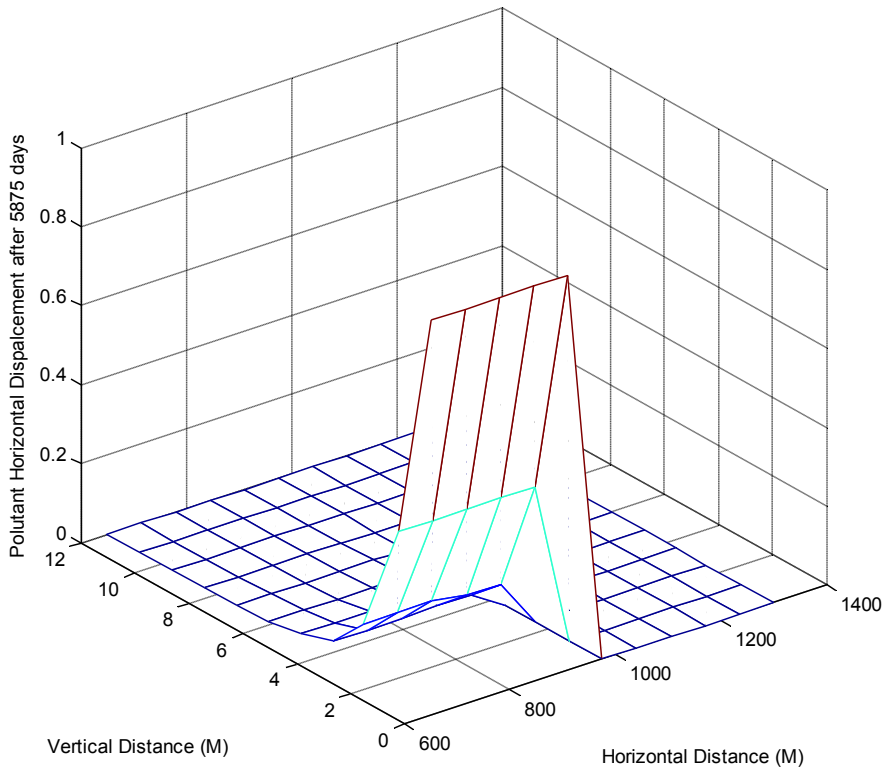


Fig. 15. Pollutant horizontal displacement after 5875 days

A plot of Pollutant Horizontal Displacement after 365 days considering Vertical and Horizontal Distances

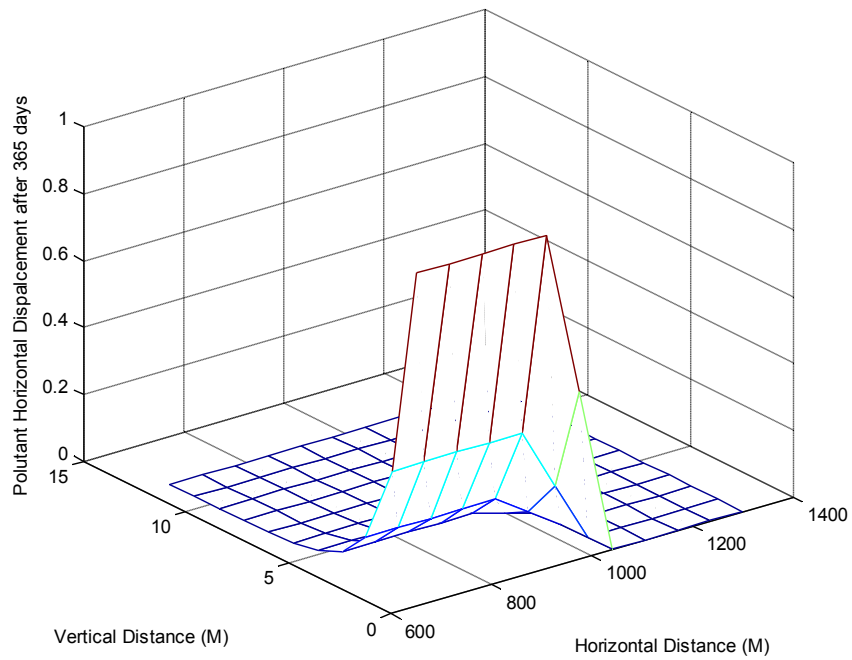


Fig. 16. Pollutant horizontal displacement after 365 days

A plot of Polutant Horizontal Dispalcement after 3650 days cosidering Vertical and Horizontal Distances

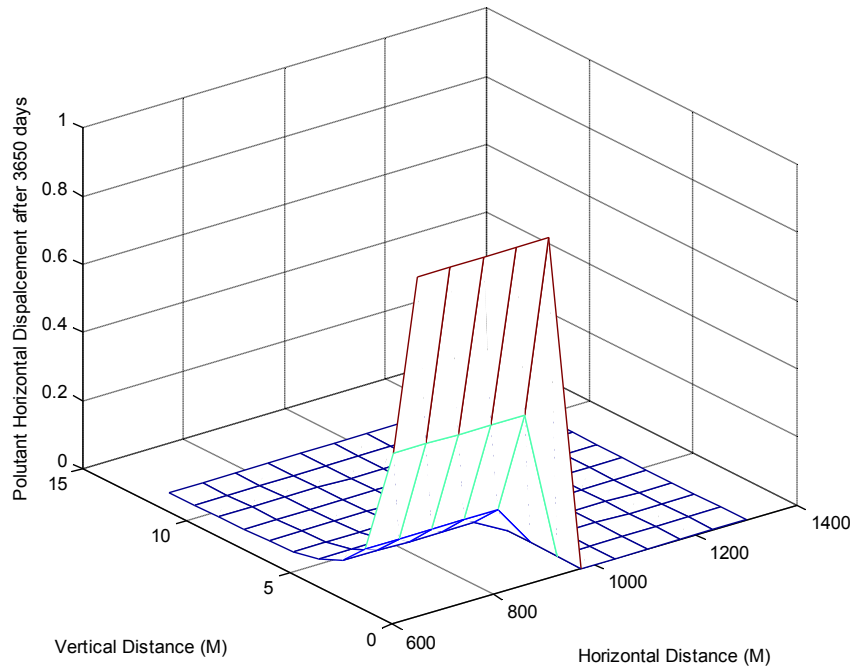


Fig. 17. Pollutant horizontal displacement after 3650 days

Table 2. Vadose parameter variation with head

Piezometric head	Effective porosity	Relative permeability	Moisture content
0.0	1.00000	1.00000	0.36000
1.2	0.96329	0.00628	0.34935
2.5	0.93437	0.00211	0.34097
3.6	0.91590	0.00113	0.33561
4.8	0.89970	0.00067	0.33091
6.0	0.88633	0.00044	0.32704
7.2	0.87499	0.00031	0.32375
8.4	0.86516	0.00023	0.32090
9.6	0.85650	0.00017	0.31838
10.8	0.84877	0.00014	0.31614
12.0	0.84180	0.00011	0.31412

The result of the variation of some necessary vadose zone parameters with pressure head is as shown Table 2.

4. DISCUSSION

The result of theoretical modelling and program simulations for this study are shown in Figs. 1 to 14. Figs. 2 and 3 display the analytical solution of the unsaturated steady state two-dimensional groundwater flow velocity in the vertical directions with Fig. 4 to 14 in the horizontal directions. The results show a vertical flow velocity of 0.7m/day and a horizontal velocity of zero. This is consistent with the assumption of

even discharge throughout the discharge length leaving no space for horizontal flow but allowing only the vertical velocity flow. Also, the results of the numerical solution to unsaturated unsteady state two-dimensional groundwater pollution problems are shown in Figure 4 to 14 for the 1, 3, 4, 5, 10, 20, 30, 365, 1825, 3650, and 5475 days period. After 1 day, the pollutant decayed vertically to 20% of its original value within 1.2m from the land surface and 1.9% within 2.5m from the surface and stops with a value 0.1% at 3.6m from the surface (Fig. 4). It also shows a horizontal spread of its original value within 520m and a horizontal decay to 50% of this value in the next 65m.

After 3 days, the pollutants extend to 6.0m from the surface with 0.1% its original value at this point while still maintaining its horizontal spread (Fig. 5). On the 4th day, the vertical and horizontal spread remains the same with a concentration build-up of 0.2% at 6.0m from the surface (Fig. 6). After the 5th day, the pollutants had extended vertically to 7.2m from the surface, while at the 20th day, the pollutants have spread (Fig. 7). After the 10th day, the pollutant has extended to 8.4m from the surface (Fig. 8) while at the 20th day, the pollutants have spread to 9.6m from the land surface (Fig. 9). The various vertical and horizontal spread of the pollutants after 365, 1925, 3650 and 5475 days are shown in Figs. 10, 11, 12, 13 & 14 respectively.

It should be noted that the vertical spread of the pollutants as a function of variation of many of the vadose zone soil parameters with the pressure head. These parameters comprise the effective porosity, relative permeability and particularly the moisture content of this zone. While dispersion was mainly responsible for the vertical spread of the pollutants up to the level the available soil water and/or moisture could allow it. This means that, as the soil gets drier, molecular diffusion should come to play a more prominent role, and this has been the problem because we could not think of the right diffusion model for the spread of the pollutants beyond the region of hydrodynamic dispersion.

5. CONCLUSION

With the detected concentration of the metals on the land surface [16], Advection-Dispersion mathematical equations and a computer program were used to determine the possible displacement of these metals laterally and transversely with time towards the water table. The result of the displacement shows that the various metals travel as much as 9.6 meters out of the static water level of 12.0 meters towards the water table while having a lateral (horizontal) extension up to 75 percent of the discharge of these industrial settings.

COMPETING INTERESTS

Authors have declared that no competing interests exist.

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