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The use of R code for modeling and simulation of 2-D contaminant migration through a soil for the pulse source

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Abstract: In this study, based on an existing analytical solution for the two-dimensional transport of contaminants in a saturated soil layer, for the pulse source, the R program code was developed. The simulation is used to obtain the profiles of contaminant concentration, for a steady groundwater velocity, as a function of distance from the source and time. The problem is analytically solved by leveraging the similarity between the Gaussian (normal) distribution and contaminant concentration distribution, the development of the analytical model (i.e., solution of partial differential equation) by using this similarity is explained step by step since it may be of interest to researchers. Contaminant propagation is modeled using R software, which helps to understand how contaminants migrate through a saturated soil layer. This approach aids in comprehending the mechanisms and spatial dynamics of contaminant dispersion, facilitating the prediction and management of soil and groundwater contamination. The provided R code can be altered for different parameters and time intervals.

Keywords: computer program; contaminant migration; modeling; simulation; soil

1. Introduction

The transport of contaminants in groundwater has been extensively studied due to its critical importance in environmental engineering and public health. Early foundational work (e.g., Bear [1], Freeze and Cherry [2]) provided comprehensive frameworks for understanding groundwater flow and contaminant transport mechanisms.

Hazardous contaminants can enter the ground unintentionally through leaks in tanks (pulse sources). For instance, underground storage tanks (USTs) containing gasoline and other petroleum products can develop leaks over time, resulting in the release of hydrocarbons into the soil. Likewise, industrial sites with large chemical storage tanks may experience accidental spills or leaks, introducing solvents, heavy metals, and other toxic substances into the subsurface. Additionally, agricultural storage of pesticides and fertilizers can lead to localized contamination from leaks or spills. These pulse sources pose significant environmental risks, highlighting the need for effective modeling and simulation tools to predict contaminant transport and guide remediation efforts.

Bear and Verruijt [3] stated that when it is desired to model the real system mathematically, it is simplified by making some assumptions and a conceptual model is created.

Rushton [4] stated that the contaminant transport model should be as simple as possible. Contaminant transport models can be calibrated using field measurements. They can predict the future migration of contaminants. Better estimations can be made

by using site-specific data.

Brenner et al. [5] state that the use of modeling and simulation can be very beneficial in practice. Seeing a profile considerably contributes to the understanding of the processes involved. The solution to the differential equation can predict the contaminant migration profile within an acceptable accuracy.

Three main processes govern the transport of contaminants in groundwater: advection, dispersion, and retardation. Advection refers to the movement of contaminants with the groundwater flow. Dispersion, influenced by density and viscosity differences, can increase the spread and speed of contaminant movement. Retardation processes, on the other hand, slow down the contaminant's movement, typically due to interactions with the soil matrix, such as adsorption. Together, these processes determine the overall behavior and migration rate of contaminants in groundwater systems.

Analytical simulation models have developed for the contaminant transport through a saturated soil layer [6–9]. This process often relies on solving partial differential equations that accounts advection, dispersion, and retardation.

Sophisticated numerical models for simulating contaminant transport have been developed due to advancements in computational methods. For example, Zheng and Bennett [10] introduced the modular groundwater flow model, MODFLOW and three-dimensional multi-species mass transport model, MT3DMS, which are widely used for simulating groundwater flow and contaminant transport in three dimensions.

There are many other studies on the contaminant migration through soils such as: Ding and Feng [11] studied the contaminant migration due to two points pulse sources. Shu et al. [12] integrated the modeling of contaminant transport in unsaturated and saturated groundwater zones. Soraganvi et al. [13] studied the contaminant transport in heterogeneous unsaturated soils. Zheng et al. [14] studied the migration of light non-aqueous phase liquids (LNAPLs) in porous media. Behdad and Moradi [15] studied the contaminant migration of LNAPL in unsaturated soil. Rahhal et al. [16] studied the migration of contaminants from landfills. Feo and Celico [17] investigated the contaminant migration in homogeneous and heterogeneous aquifers with numerical simulations. Zhou et al. [18] studied the migration of chlorinated organic matter in groundwater of Yangtze delta region. You et al. [19] studied the contaminant migration between high- and low-permeability zones in groundwater systems. Filippini et al. [20] studied the migration of mixed organic contaminants of industrial origin, in multi-layered, alluvial aquifer-aquitard system. Chowdhury and Rahnuma [21] studied the contaminant transport by using MODFLOW and MT3DMS for a case in Rajshahi city. Pareta [22] developed a contaminant prediction model for total dissolved solids (TDS), nitrate, and fluoride for a case in Rajasthan.

In recent years, the integration of programming languages, such as R, into hydrological modeling has gained traction due to their flexibility and powerful data analysis capabilities. As other programming languages, such as Python, R programming language offers a comprehensive environment for statistical computing and graphics, making it an attractive choice for environmental modeling.

In this paper, modeling steps are explained and the application of modeling steps to the contaminant migration through saturated soil is introduced and computer software (R Code) is given for the analytical simulation model. Contaminant

concentration in soil layer $C(x, y, t)$ due to an instantaneous source will be estimated as shown in **Figure 1**.

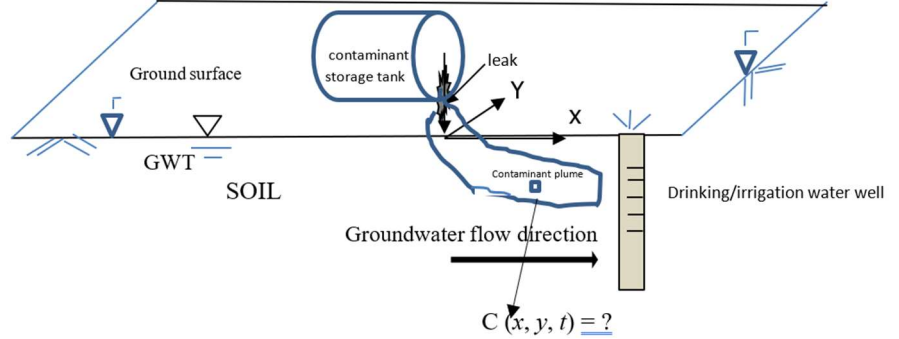


Figure 1. Conceptual representation of contaminant migration process.

2. Modeling of contaminant migration

a) Development of a conceptual model.

Contaminant Migration problem can be described by differential equations that are mathematical approximations of the physical reality as follows:

Change (increase in concentration) with time = [Net increase in mass of contaminant in a small volume of pore fluid due to advective-diffusive transport] – [Mass of contaminant removed from this pore fluid by “sorption” processes].

The concentration equation says, roughly, that Concentration at a given time and point $C = C(x, t)$ rises or falls at a rate $(\partial C/\partial t)$.

Experimentally, it is known that the advection is responsible for the displacement Δx proportional to the concentration gradient $(\partial C/\partial x)$. As the slug moves downstream with v_x in the x direction, it becomes $v_x (\partial C/\partial x)$.

Diffusion causes the dispersal of soluble substances in the groundwater flow. The accumulation is proportional to the diffusivity D_x [cm^2/s] and $(\partial/\partial x. (\partial C/\partial x))$, measures how far off the Concentration is from satisfying the mean value. $(\partial/\partial x. (\partial C/\partial x))$ is the concavity of the concentration profile $C(x, t)$ (or curvature of the concentration profile).

b) Development of a mathematical model.

The 1-D contaminant transport equation is given below [6]:

$$n \frac{\partial C}{\partial t} = \left[n \left(\frac{\partial}{\partial x} \left(D_x \frac{\partial C}{\partial x} \right) \right) - n \left(v_x \frac{\partial C}{\partial x} \right) \right] - \rho_b K_d \frac{\partial C}{\partial t} \quad (1)$$

where: n = the effective porosity,

C = contaminant concentration,

t = time,

D_x = longitudinal dispersion coefficient,

x = distance in longitudinal direction,

v_x = pore-water velocity,

ρ_b = the bulk mass density of the porous medium (M/L^3),

K_d = the distribution coefficient (a linear partition of a contaminant between the soil solution and the soil particles).

If $R = [1 + (\rho_b K_d/n)]$ = the retardation factor, Equation (1) can be rearranged as:

$$\frac{\partial C}{\partial t} = \frac{D_x}{R} \left(\frac{\partial^2 C}{\partial x^2} \right) - \left(\frac{v_x}{R} \right) \left(\frac{\partial C}{\partial x} \right) \quad (2)$$

The one-dimensional advection-dispersion equation for a reactive contaminant with first-order contaminant degradation is given below [23] and Equation (2) becomes:

$$\frac{\partial C}{\partial t} = \frac{D_x}{R} \left(\frac{\partial^2 C}{\partial x^2} \right) - \left(\frac{v_x}{R} \right) \left(\frac{\partial C}{\partial x} \right) - \left(\frac{k \cdot C}{R} \right) \quad (3)$$

k = first-order rate constant for contaminant degradation (day^{-1}) t = time (day).

In two dimensions, the governing partial differential equation (i.e. mathematical model) for a one-dimensional velocity becomes:

(D_y = transverse dispersion coefficient and y = distance in transverse direction)

$$\left[\frac{D_x}{R} \cdot \left(\frac{\partial^2 C}{\partial x^2} \right) + \frac{D_y}{R} \cdot \left(\frac{\partial^2 C}{\partial y^2} \right) \right] - \frac{v_x}{R} \cdot \left(\frac{\partial C}{\partial x} \right) = \frac{\partial C}{\partial t} \quad (4)$$

c) Development of an analytical model.

Above partial differential Equation (4) can be solved using different methods:

i) Exact Analytical Methods (a. Laplace transform, b. Fourier transform).

ii) Analytical methods (by using the similarity of concentration distribution curves) (a. Green's Function (and Dirac delta function), b. Gaussian (normal) distribution).

iii) Numerical Methods (a. Finite difference, b. Finite element).

De Long [24] derived a solution to this problem based on a statistical treatment of lateral and transverse dispersivities (method ii. b). Bear [1] later verified it experimentally. Watts [23] stated that, "analytical solutions are often somewhat limited in their potential to accurately predict contaminant concentrations downgradient as a result of simple boundary conditions that must be used to provide a closed form solution. However, Bedient et al. [6] emphasized that, "Their simplicity of use and understanding make them valuable and convenient tools. Equations that use more complex governing equations and boundary conditions must be approximated using numerical methods". By statistically treating the dispersivities, this solution accounts for the inherent variability and anisotropy in subsurface materials, thereby improving the predictive capabilities of groundwater contamination models. **Figure 2** shows the similarity between Gaussian (normal) distribution and the normal distribution of concentration for the instantaneous pulse source in one dimension. The bell-shaped curve with different centers and spreads depending on μ (mean) and σ (standard deviation). Changing μ shifts the curve to the right or left. Changing σ , increases or decreases the spread. Where the curvature changes at $(\mu - \sigma)$ and $(\mu + \sigma)$. See also Brownian motion for $\sigma_x = (2D_x t)^{1/2}$.

The derivation of Equation (7) (i.e., solution of partial differential Equation (3)) by using the similarity between the Gaussian (normal) distribution and contaminant concentration distribution is explained step by step since it may be of interest to researchers.

Equation (3) can be solved using different initial and boundary conditions. The following initial and boundary conditions are commonly applicable for pulse model:

$$C(x, y, 0) = 0; x, y \geq 0; \text{ Initial condition, } t = 0$$

$$C(0, 0, t) = C_0; \text{ Boundary condition, } t = 0$$

$$C(\alpha, \alpha, t) = 0; \text{ Boundary condition, } t \geq 0$$

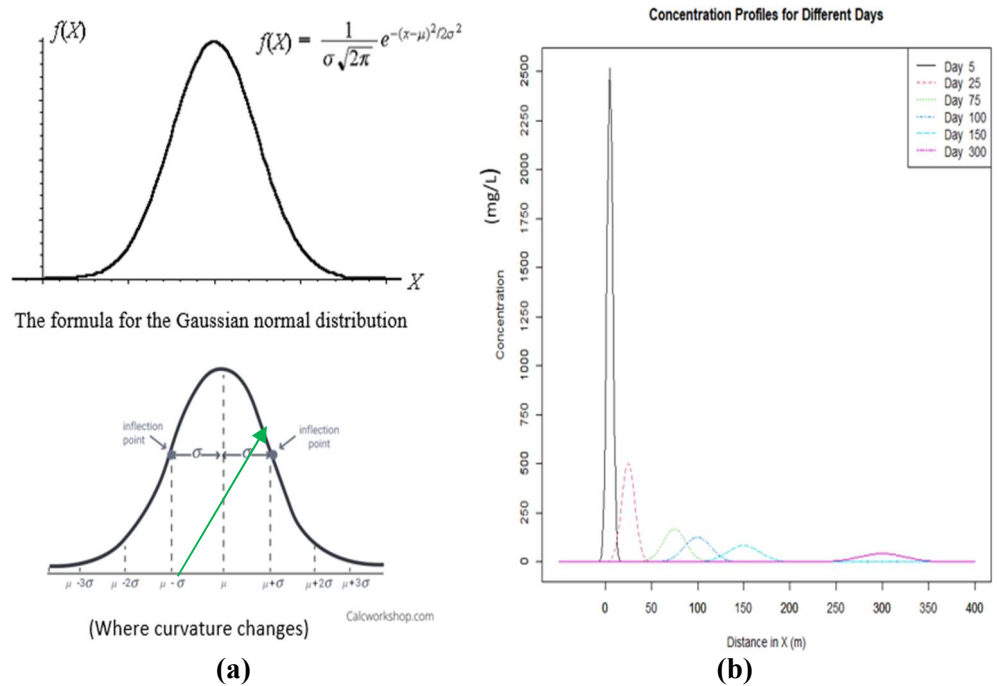


Figure 2. The similarity between (a) Gaussian normal distribution; and (b) Contaminant propagation in X direction (when Y = 0) (graph is taken from the example case 1 in this study).

Brownian motion refers to movement of small particles suspended in a fluid. This movement is caused by collisions between the particles and the molecules of the fluid. The concept is significant in physics and mathematics because it exemplifies a type of stochastic process, often modeled by Gaussian distributions. Similarity between the Gaussian (normal) distribution and Brownian motion of one particle and the particle’s mean squared displacement (msd) from its original position is used for the solution of pde for 1-D (Figure 3).

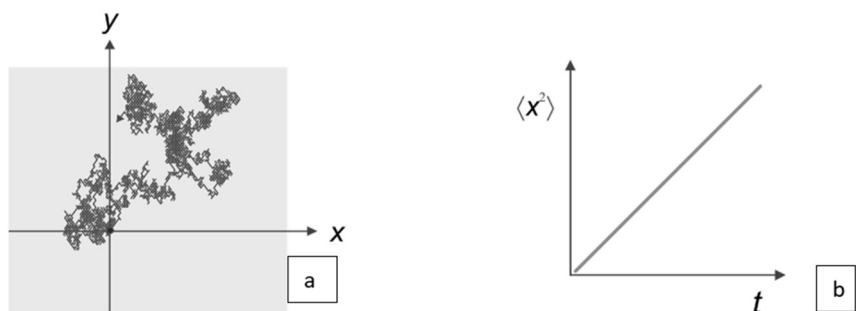


Figure 3. (a) The Brownian motion of a particle; and (b) the mean-squared displacement of a contaminant particle with time.

The proportionality factor between $\langle x^2 \rangle$ and t for diffusion in 1D, $\langle x^2 \rangle/t = 2 \cdot D_x$. The contaminant particle’s msd from its original position (x_0) is:

$$(x(t) - x_0)^2 = \sigma_x^2 = (2D_x t) \tag{5}$$

The square root of $(x(t) - x_0)^2$, is:

$$(x(t) - x_0) = \sigma_x = (2D_x t)^{1/2} \quad (6)$$

The corresponding analytical solution of partial differential Equation (2) can be derived if the instantaneous input is injected at $x = 0$ with a background concentration equal to zero in area $x, y > 0$ (Bedient et al. [6], after De Long [24]). If the contaminant moves downstream with v_x in the x direction, it spreads out according to Equation (6):

$\sigma_x = (2D_x t)^{1/2}$ can be substituted in Gaussian (normal) distribution formula given in below:

$$f(x) = \frac{1}{\sigma\sqrt{2\pi}} e^{-\frac{1}{2}\left(\frac{x-\mu}{\sigma}\right)^2} \quad (7)$$

Diffusion of contaminants can be explained by the Brownian motion of molecules within concentration gradients. It is observed that the mean-squared displacement (x^2) of a contaminant particle increases linearly with time (due to diffusion).

Solution of the pde for 1-D is: As the slug moves downstream with v_x, D_x and k' in the x direction, it spreads out according to the one-dimensional advection-dispersion equation for a reactive contaminant with first-order contaminant degradation [23] is given below:

$$C(x, t) = \left[\frac{C_0 A}{2(\pi t D_x)} \right]^{-1/2} \text{Exp} \left\{ -\left[\frac{(x - x_0) - v_x t}{4D_x t} \right]^2 \right\} e^{(-k' t)} \quad (8)$$

where $k' = k/R$, the first order loss coefficient (day^{-1});

The solution of the pde for 2-D (x, y) with first-order contaminant degradation is given as:

$$C(x, y, t) = \left[\frac{C_0 A}{4\pi\sqrt{D_x D_y}} \right] e^{-\left\{ \left[\frac{(x-x_0)-v_x t}{4D_x t} \right]^2 + \left[\frac{(y-y_0)^2}{(4D_y t)} \right] \right\}} e^{(-k' t)} \quad (9)$$

where $C_0 A$ is the injected mass per unit cross-sectional area at $t = 0$.

The maximum concentration occurs at the center of the Gaussian plume where $y = 0$, and $x = v_x t$.

$$C(x, y, t)_{\max} = \left[\frac{C_0 A}{(4\pi t(D_x D_y))^{1/2}} \right] e^{(-k' t)} \quad (10)$$

The dimensions of the plume (X, Y) are estimated by its longitudinal and transverse standard deviations, σ_x and σ_y respectively.

$$X = 3\sigma_x, \text{ where } \sigma_x = (2D_x t)^{1/2} \quad (11)$$

$$Y = 3\sigma_y, \text{ where } \sigma_y = (2D_y t)^{1/2} \quad (12)$$

3. Application of R code

Two example cases solved to demonstrate capability and illustrative power of the developed R code is explained.

3.1. Example case 1 (from Bedient et al. [6])

In this example case, a tank holding chloride at a concentration of $C_0 = 5000$ mg/L accidentally leaks over an area of $A = 10 \text{ m}^2$ into an aquifer (**Figure 1**). Assuming that chloride is a completely conservative tracer ($R = 1$), $D_x = 1 \text{ m}^2/\text{day}$, $D_y = 0.1 \text{ m}^2/\text{day}$ and the seepage velocity is $v_x = 1 \text{ m/day}$.

The Equation (8) can be used to describe the contaminant propagation, and this equation was handled by writing an R code [25]. This code is used to illustrate magnitude of a contaminant concentration over a 2-dimensional grid area with certain

time intervals (5, 25, 75, 100, 150 and 300 days) after initiation of leakage. A concentration boundary of approximately 0.1 mg/L was used due to the grid sensitivity of 1 m.

3.2. Example case 2-Pulse model with first-order contaminant degradation (modified from Watts [23])

In this example case, the trichloroethane (TCA) mass spilled into an aquifer is (M) 1740 g/m². The pore water velocity in the aquifer is (v_x) 5 m/day in the x-direction, and the porosity (n) of the soil layer is 0.40. The dispersion coefficient in the x-direction (D_x) is 0.8 m²/day, and the retardation factor (R) has been estimated as 8.0. The TCA degradation is described by a first order rate constant (k) of 0.0004 day⁻¹. Based on these data, TCA concentration C at the end of 365 days at distance of 200 m is estimated ($D_x = D_y$).

Equation (8) was assigned by R code [25]. This code is used to illustrate magnitude of a contaminant concentration over a 2-dimensional grid area with 365 days after initiation of leakage. A concentration boundary of approximately 0.1 mg/L was used due to the grid sensitivity of 1 m. Maximum concentration and concentration at 200 m distance from source was investigated.

4. Results and discussion

Example case given in section 3 executed for 5, 25, 75, 150 and 300 days after the leakage. **Figure 4** illustrates the maximum concentration at $t = 75$ days, which is found as 167.764 mg/L. **Figure 5** illustrates the contaminant plume dimensions in $t = 75$ days.

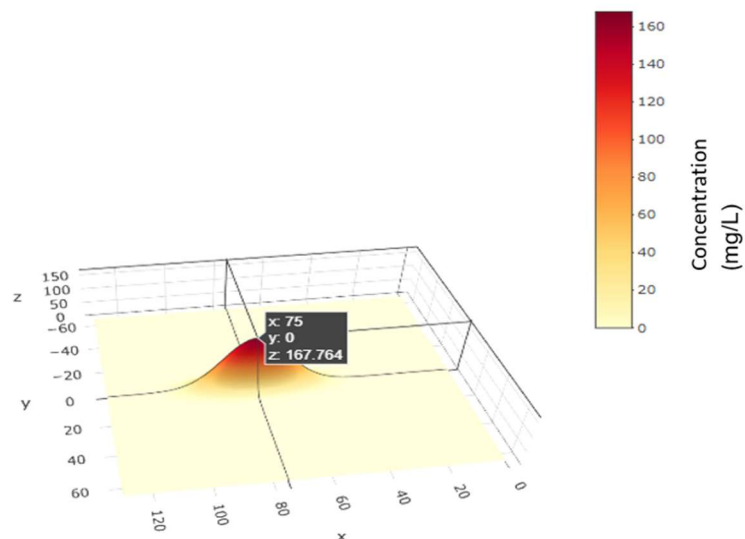


Figure 4. Plume location at $t = 75$ days in 3D graph.

R code is executed to derive the surface function of the contaminant plume for a given coordinate system. By this code, contaminant concentration amount at a random time can be estimated for different coordinates on a 2D-plane. To illustrate, graphical representation of the concentration function was drawn in terms of surface area with respect to time (**Figure 2**). Six different points representing different times (after 5,

25, 75, 100, 150 and 300 days) were selected to be used. In (Figures 4–7), the Z axis illustrates the magnitude of contaminant concentration with respect to spatial position.

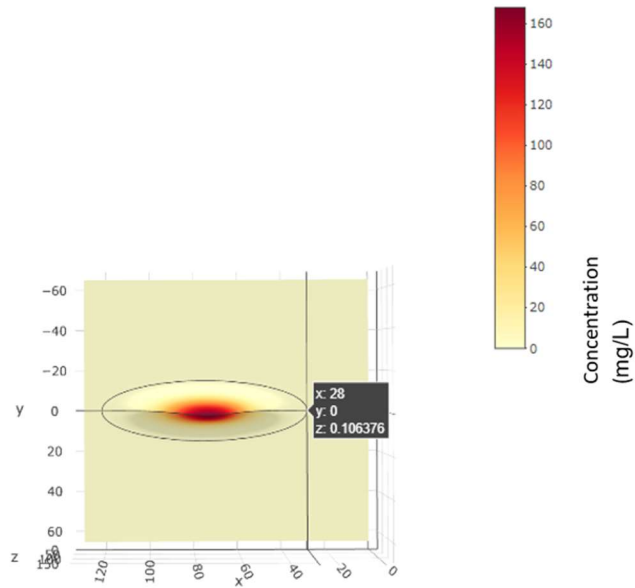


Figure 5. Contaminant plume dimensions in $t = 75$ days.

Figures 6 and 7 represents the location of the plume. Similar trends were observed with the numerical simulation of the problem [8], and this can be proof of the suitability of the solution to the contaminant transport problem by using the similarity between Gaussian normal distribution and contaminant concentration distribution.

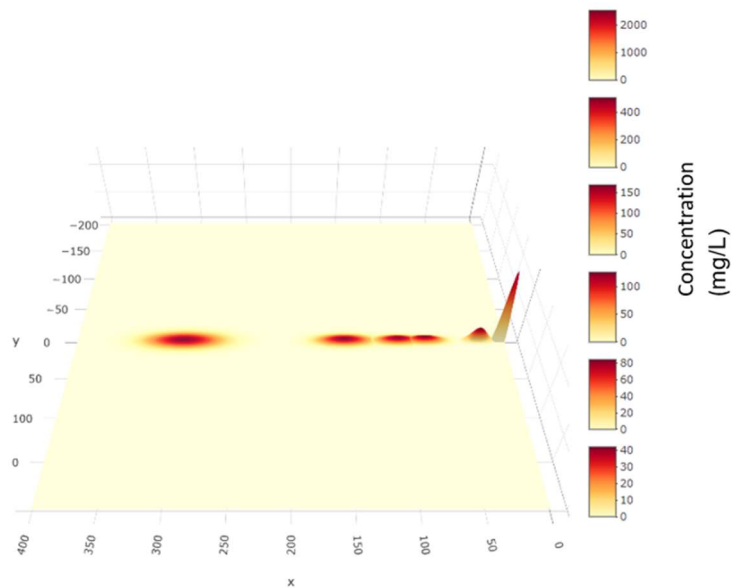


Figure 6. Contaminant plume with respect to time in 3D coordinate system.

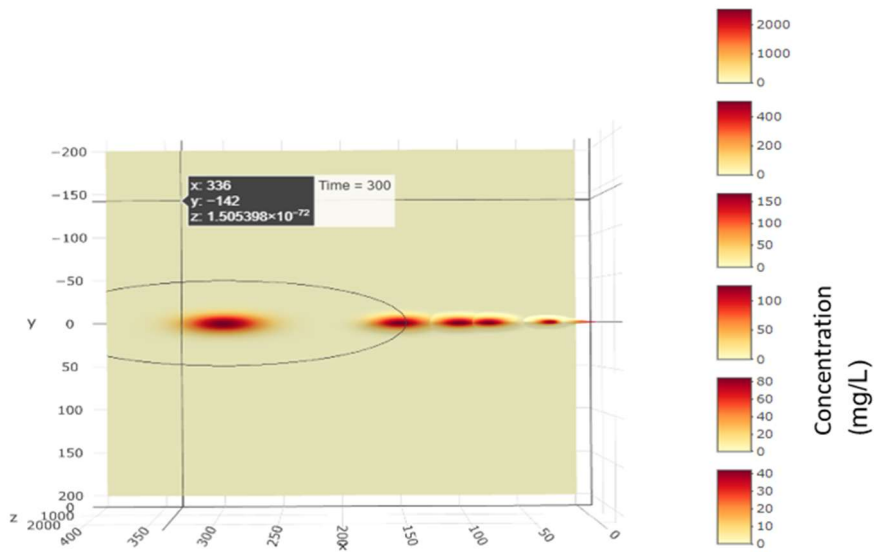


Figure 7. Overview of contaminant plume with respect to time.

The concentration of contaminant decreases as it is transported longitudinally away from the source. The decay effect was not considered in this example case, but it may decrease the pollution concentration of non-conservative contaminants with distance and time.

EPA recommends chloride levels ≤ 250 mg/L and at a distance of > 75 m from the source and after 75 days, the concentration is lower than 250 mg/L.

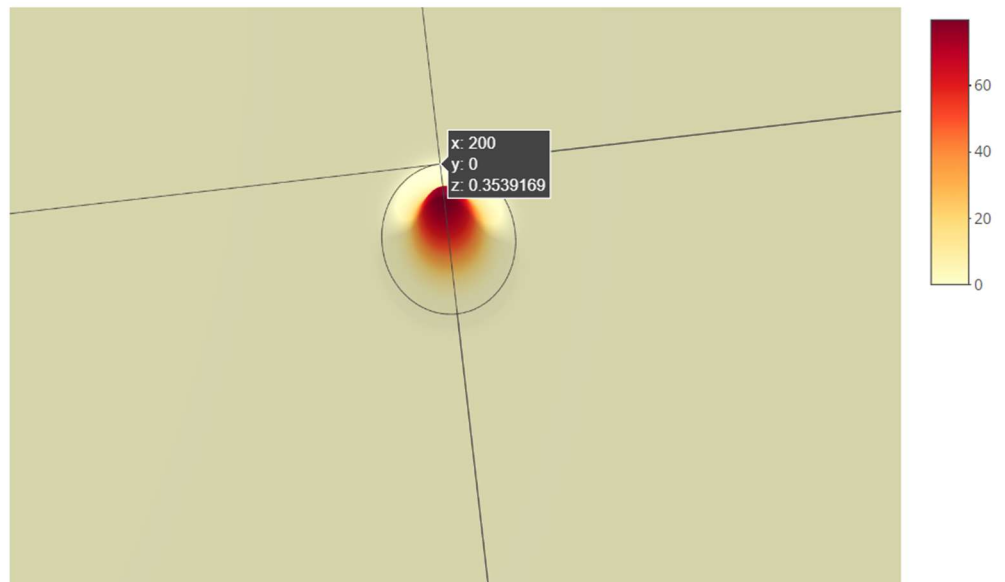


Figure 8. Plume concentration at coordinate (200, 0) after 365 days ($Z = 0.354$).

Example case 2 (from Watts [23]) was also solved through a 2D domain where it is assumed that dispersion coefficients at both sides were equal ($D_x = D_y$). In this case, first order degradation of organic contaminants and exchange of metals are also included the model. Assuming source of leakage is located at (0,0) coordinate, concentration of plume after 365 days at $x = 200$ m is found to be 0.354 g/m³ (**Figure 8**). Maximum concentration is observed to be 79.767 g/m³ at coordinate of (228, 0)

with respect to Cartesian coordinate system. Moreover, **Figure 9.** illustrates three-dimensional illustration of flume at 365 days, wherein **Figure 10.** Shows concentration curve over x -axis where $y = 0$.

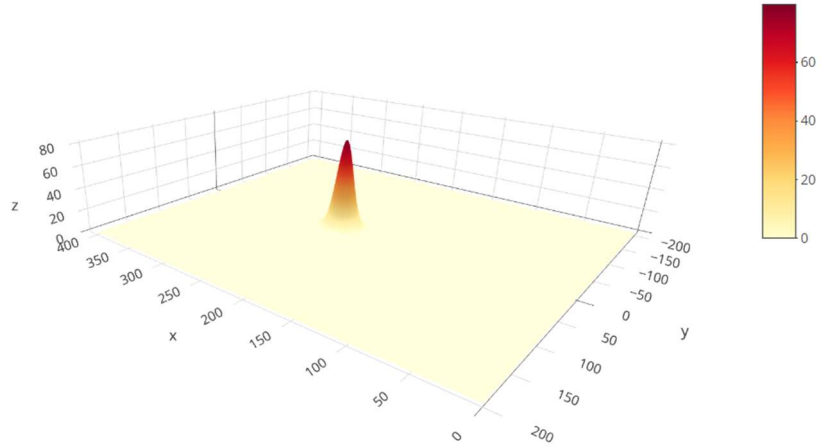


Figure 9. 3D illustration of flume concentration after 365 days.

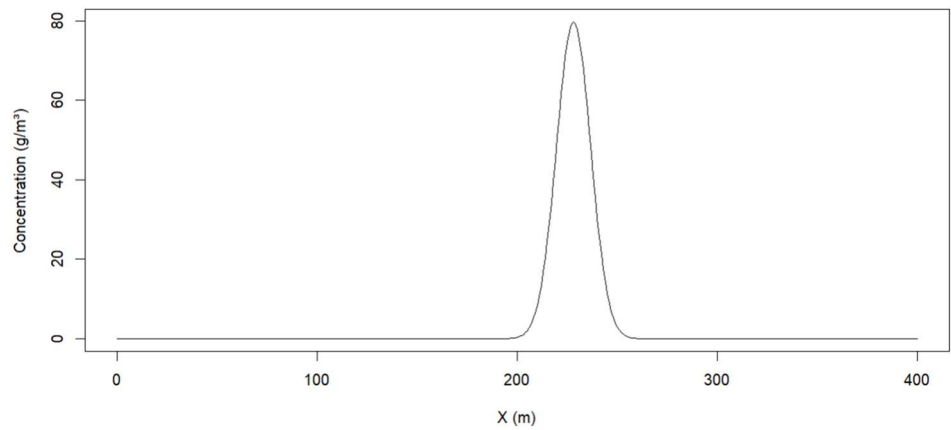


Figure 10. Contaminant concentration curve with respect to x -axis ($t = 365$ days, $y = 0$).

The provided R code (in Appendix) can be altered to be used in different parameters and different amount of time intervals. This code can be altered to find amount of contaminant concentration at any location by graphical interpretation by selecting a constant random time.

5. Conclusions

Since aquifer systems are complex, a conceptual model is developed as a simplified representation of contaminant migration through a saturated soil layer. Seeing a contaminant migration profile on a graph makes it easier to understand the processes.

A computer program using R language is prepared to predict 2D contaminant migration through a saturated soil layer. From the results and figures, it can be observed that the concentration decreases with increase of the time, and the x distance from the source and with increase of y distance away from the center of contaminant.

Solving the problem analytically by using the similarity between Gaussian

normal distribution and contaminant concentration distribution and drawing the contaminant propagation by R software may help us to understand how contaminants migrate through a saturated soil layer. It also allows users to illustrate the contaminant amount with 3-D graphic by checking coordinate in *X-Y* plane. This code may also be arranged to be used in different cases, different parameters (such as dissipations coefficients) and different resolution sizes by changing input values.

As a future research direction, the contaminant transport model can be calibrated using field observations and measurements by a site-specific data. After the model was constructed and calibrated, it can be used to predict the future migration of contaminants originating from the site. These simple calculations in this study can be compared with more complex calculations, the 3-D analysis can also be done based on the proposed approach.

Author contributions: Conceptualization, AOT and EC; methodology, AOT and EC; software, AOT; validation, AOT; formal analysis, AOT and EC; investigation, AOT and EC; writing—review and editing, AOT and EC; visualization, AOT; supervision, EC. All authors have read and agreed to the published version of the manuscript.

Conflict of interest: The authors declare no conflict of interest.

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Appendix (R Code)

For Case 1

```

# input (t in terms of day)
t <- c(5,25) # desired days
Dx <- 1
Dy <- 0.1 # dispersion
v <- 1 # seepage velocity
A <- 10 # area
C0 <- 5000 # mg/L
X_max <- 50
Y_max <- 25 # must be always Xmax/2 for grid purposes
grid_size <- 1
##Execution##
# grid form
X <- seq(0, X_max, grid_size)
Y <- seq(-Y_max, Y_max, grid_size)
# Corrected formula for c
c <- C0 * A / (4 * pi * t * sqrt(Dx * Dy) * 5)
C <- function(x, y, t) {
  result <- c * exp(-((x - v * t)^2 / (4 * Dx * t)) - (y^2 / (4 * Dy * t)))
  return(result)
}
# Initialize array for storing results
Z <- array(1, dim = c(length(X), length(Y), length(t)))
for (k in seq_along(t)) {
  for (j in seq_along(Y)) {
    for (i in seq_along(X)) {
      Z[i, j, k] <- C(X[i], Y[j], t[k])[1]
    }
  }
}
Z_f <- Z
K <- Z
i=1
for (i in seq_along(t)) { ##scale correction
  Z_f[,i] <- Z[,i] * c[i] / c[1]
  K[,i] <- t(Z_f[,i])
}
}
subplot_traces <- list()
# Create subplot traces for each time step
for (i in seq_along(t)) {
  subplot_trace <- plot_ly(x = Y+Y_max, y = X - X_max/2, z = K[,i], type = "surface", colors = "YlOrRd", opacity =
1, name = paste("Time =", t[i]))

```

```

subplot_traces[[i]] <- subplot_trace
}
# Create a subplot with multiple traces
subplot <- subplot(subplot_traces, nrows = length(t), margin = 0.05)
fig <- subplot %>% layout(
  scene = list(title = "Concentration Distribution Over Time",
    xaxis = list(nticks = 10),
    zaxis = list(nticks = 5),
    yaxis=list(ntick = 2),
    camera = list(eye = list(x = 0, y = 1, z = 1)),
    aspectratio = list(x = .9, y = .8, z = 0.2)))
fig

```

For Case 2

```

library(tidyverse)
library(plotly)
library(rgl)
grid <- expand.grid(x = X, y = Y)
grid$z <- with(grid, C(x, y))
##### pulse source#####
# input (t in terms of day)
t <- c(365) # desired days
Dx <- 0.8 # ( D/R for m2/day)
Dy <- 0.8 # dispersion
M<- 1740 #( weight per cross sectional area (g/m2))
n <- 0.4 # porosity
R <- 8 # retardation factor
k_ret <- 0.0004 #degradation coefficient ( day-1)
v <- 5 # seepage velocity (v/R for m/day)
X_max <- 400
Y_max <- 200 # must be always Xmax/2
grid_size <- 1
# grid form
X <- seq(0, X_max, grid_size)
Y <- seq(-Y_max, Y_max, grid_size)
# Corrected formula for c
#c <- C0 * A / (4 * pi * t * sqrt(Dx * Dy) )#
c_source <- M /sqrt(4*pi*t*(Dx/R))
C <- function(x, y, t) {
  result <- c_source * exp(-((x - v/R * t)2 / (4 * (Dx/R) * t)) - (y2 / (4 * (Dy/R) * t)))*exp(-k_ret*t/R)
  return(result)
}
# Initialize array for storing results
Z <- array(1, dim = c(length(X), length(Y), length(t)))
for (k in seq_along(t)) {

```

```

for (j in seq_along(Y)) {
  for (i in seq_along(X)) {
    Z[i, j, k] <- C(X[i], Y[j], t[k])[1]
  }
}
Z_f <- Z
K <- Z
i = 1
for (i in seq_along(t)) { ##scale correction
  Z_f[,i] <- Z[,i]*c[i]/c[1]
  K[,i] <- t(Z_f[,i])
}
P <- seq_along(t)
i = 1
for (i in seq_along(t)) {
  P[i] <- plot_ly(x = Y+200, y = X-200, z = K[,i], type = "surface", colors = "Blues", opacity = 1)
}
subplot_traces <- list()
# Create subplot traces for each time step
for (i in seq_along(t)) {
  subplot_trace <- plot_ly(x = Y+Y_max, y = X - X_max/2, z = K[,i], type = "surface", colors= "YlOrRd", opacity =
1, name = paste("Time =", t[i]))
  subplot_traces[[i]] <- subplot_trace
}
#1D plot over X#
plot(X,C(X,0,t),type = "l", xlab="X (m)", ylab = "Concentration (g/m³)")
# Create a subplot with multiple traces
subplot <- subplot(subplot_traces, nrows = length(t), margin = 0.05)
subplot
fig <- subplot %>% layout(
  scene = list(title = "Concentration Distribution Over Time",
  xaxis = list(nticks = 10),
  zaxis = list(nticks = 5),
  yaxis=list(ntick = 2),
  camera = list(eye = list(x = 0, y = 1, z = 1)),
  aspectratio = list(x = .9, y = .8, z = 0.2)))
fig

```