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# Migration of Contaminant through a Soil due to an Instantaneous Source

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***ABSTRACT—*** *Analytical and numerical simulation models help Civil and Geotechnical engineering to understand the physical and chemical processes that influence contaminant transport through a saturated soil layer, including advective and dispersive transport as well as sorption. The basic principles for simulation of contaminant migration through a saturated soil were introduced. Using the spreadsheet program MS Excel, based on existing analytical solution for two-dimensional transport of contaminants in a saturated soil layer, concentrations at several coordinates at several times were calculated. A MATLAB code was developed using finite difference approach for numerical solution. The programming steps followed for analytical and numerical solutions were explained. The analytical and numerical solution was compared. An example of the simulation models for the contaminant transport through a saturated soil layer is given. The study shows that the analytical solution and the numerical solution, for the given problem, match in an acceptable range.*

**Keywords— advection; contaminant migration; dispersion; soil; sorption.**

## 1, INTRODUCTION

In order to protect the environment from contamination by pollutants, waste materials are usually placed in engineered landfills. Modelling of contaminant migration through landfill liners and natural soil deposits in geoenvironmental engineering is an important task, as the landfills have to contain the waste till their design life. To demonstrate the likelihood of compliance with regulations, environmental engineers now make routine recourse to mathematical models of the proposed landfill. One outstanding feature of the modelling approach is the capacity for predictions to be made well into the future, thereby demonstrating the likely impacts of current practice on the environment and future generations (Fityus et al. 1999). The validity of predictions based on mathematical modelling of contaminant transport has been investigated and shown to be good for time periods measured in decades (Quigley and Rowe 1986) and even for time periods of thousands of years (Quigley et al. 1983). Impressive arrays of analytical and numerical models are available, both for instantaneous pluses and for continuous sources in the literature. Whatever model is contemplated, one of the more formidable problems in contaminant transport is the difficulty in assessing the important parameters and coefficients, including source concentration and dimensions, seepage velocity, time since the contaminant first entered the groundwater and upto three dispersivities for a three dimensional problem (Bear 1979; Domenico and Robbins 1985). The use of numerical models in problems of contaminant transport is rapidly increasing in response to the need to measure, monitor and apply predictive approaches to contaminant plumes of various size and shape. The available analytical solutions of the transport equation consider one or two governing processes, usually in a simple flow domain with uniform transport parameters. In contrast, numerical simulation of contaminant transport offers a vehicle that can integrate, in some approximate way, the effects of several controlling processes; and it is the only method of calculation which can accommodate geometries and parameter distributions.

Many hazardous materials have entered the ground unintentionally through leakage in tanks, releasing large quantities of contaminants (e.g., instantaneous source), in Figure 1 plan view of plume developed from an instantaneous point source at three different times is given (P.B. Bedient 1994) (i.e., a real-world, physical problem). The transport mechanisms and governing transport equations and the solutions of governing partial differential equations are given for instantaneous sources [1_5]. The use of these relatively simple analytical equations has a number of applications such as a simple check to more complicate models that require numerical solutions. More importantly, calculations using simple analytical equations provide a powerful conceptual knowledge of the effects of sorption, transformation, advection, and dispersion on the rate of subsurface transport. The migration and fate of contaminants dissolved in ground water are studied by using the spreadsheet program MS Excel for analytical solution; the approach considers the advective and dispersive transport of solutes dissolved in ground water, which may undergo linear sorption (i.e., retardation). In this study, a MATLAB code is developed using finite difference approach for numerical solution. Engineers should never rely on a single solution, because errors can be disastrous and expensive, and the results should be checked in as many ways as possible (analytical methods and numerical methods). The analytical and numerical solutions of a two-dimensional (2D) contaminant migration through a soil layer due to an instantaneous (pulse) source were compared in this study.

## 2, MODELING OF CONTAMINANT MIGRATION THROUGH A SOIL LAYER DUE TO AN INSTANTANEOUS SOURCE

### Working (Physical) Model

The main transport processes of concern in ground water include advection, diffusion, dispersion, and sorption (C.D.Shackelford 1993). Advection is the movement of contaminants along with flowing ground water at the seepage velocity in porous media in response to hydraulic gradient. Advection carries the contaminant at an average rate as a plug. However, in actual situations, the solute is seen to spread out from the flow path. This spreading or mixing phenomenon is called dispersion. Due to this phenomenon, solute will not move as a plug, but will spread out. Dispersion causes sharp fronts to spread out and results in the dilution of the solute at the advancing edge of the contaminant front.

Diffusive transport of solutes, which is due to concentration gradient, can result in significantly reduced transit times relative to those based solely on advective transport.
When contaminated water passes through a soil, the contaminant is usually attenuated. Some waste chemicals form coatings around soil particles through a process called adsorption, or soaked into the soil particles through absorption. In the field, it is difficult to distinguish which of these two is occurring, or in what proportions they occur, so we use the term sorption to describe their collective action (e.g., inorganic fix to clay minerals). Sorption, the partitioning of contaminants from the soluble phase onto the soil matrix, results in retarded fronts, thus producing plumes that move more slowly and have higher concentrations that would otherwise occur. When the partitioning of the contaminant can be described with a linear isotherm, the retardation factor, R, represents the relative rate of fluid flow to the transport rate of a reactive solute. The advection_diffusion equation can be modified to allow for loss of contaminant to solids.

**Mathematical Formulation for Contaminant Migration**

Derivation of one dimensional contaminant transport is given below;

$$n\frac{\partial C}{\partial t}=\left[nDx\left(\frac{\partial^2 C}{\partial x^2}\right)-nv_x\left(\frac{\partial C}{\partial x}\right)\right]-\rho_b K_d\frac{\partial C}{\partial t} \quad (1)$$

$$(n+\rho_b K_d)\frac{\partial C}{\partial t}=\left[nDx\left(\frac{\partial^2 C}{\partial x^2}\right)-nv_x\left(\frac{\partial C}{\partial x}\right)\right] \quad (2)$$

Dividing Eqn. (2) by 'n'

$$\left[\frac{1+\rho_b K_d}{n}\right]\frac{\partial C}{\partial t}=\left[Dx\left(\frac{\partial^2 C}{\partial x^2}\right)-v_x\left(\frac{\partial C}{\partial x}\right)\right] \quad (3)$$

$$R=\left[1+\left(\frac{\rho_b K_d}{n}\right)\right]=\text{Retardation Factor} \quad (4)$$

In two dimensions, the governing differential equation for a 1D velocity becomes

$$\frac{\partial C}{\partial t}=\left[\frac{Dx}{R}\left(\frac{\partial^2 C}{\partial x^2}\right)+\frac{Dy}{R}\left(\frac{\partial^2 C}{\partial y^2}\right)-\frac{v_x}{R}\left(\frac{\partial C}{\partial x}\right)\right] \quad (5)$$

where $D_x$ is the longitudinal dispersion coefficient ($L^2/T$), $D_y$ the transverse dispersion coefficient ($L^2/T$), C the contaminant concentration in the aqueous phase ($M/L^3$; mg/L), x, y the distance (within the soil layer in transverse and longitudinal directions, respectively), (L), $\rho_b$ the bulk mass density of the porous medium ($M/L^3$), $K_d$ the distribution coefficient, n the effective porosity, $v_x$ pore-water velocity (m/day) (seepage velocity) (L/T), and t the time (day) (T).

## 3, ANALYTICAL SOLUTION OF GOVERNING DIFFERENTIAL EQUATIONS

One of the first 2D analytical models was that developed by Wilson and Miller [1]. It is one of the simplest model to use and can account for lateral and transverse dispersion, and adsorption. Concentration C at any point in the x, y plane can be predicted by solving Equation (5) for an instantaneous spike source. Velocity in the y direction is assumed to be 0, and the x-axis is oriented in the direction of flow. Contaminants are assumed to be injected uniformly throughout the vertical axis. The flow velocity must be obtained from a flow model or from detailed field monitoring. If $C_0$ is injected over an area A at a point ($x_0$, $y_0$), the concentration at any point x, y at time t after the injection is given by the following equation:

$$C(x,y,t)=\left[\frac{C_0 A}{4\pi t(D_x D_y)^{1/2}}\right]\exp\left\{-\left[\frac{\left((x-x_0)-v_x t\right)^2}{4D_x t}\right]-\left[\frac{(y-y_0)^2}{4D_x t}\right]\right\} \quad (6)$$

## 4, NUMERICAL SOLUTION OF PROBLEM

Numerical Solution of Problem. For the numerical solution of Equation (5), a MATLAB code was developed, using finite difference approach. For the left-hand side of Equation (5), central difference equations are going to be used.
Inserting the finite difference formulation into Equation (5), the following equation can be derived for a single nodal element;

$$D_x\frac{C_{i+1,j,k}-2C_{i,j,k}+C_{i-1,j,k}}{\Delta x^2}+D_y\frac{C_{i,j+1,k}-2C_{i,j,k}+C_{i,j-1,k}}{\Delta y^2}-V_x\frac{C_{i+1,j,k}-C_{i-1,j,k}}{2\Delta x}=\frac{C_{i,j,k+1}-C_{i,j,k}}{\Delta t} \quad (7)$$

In Equation (7), Unknown is $C_{i,j,k+1}$ which represents concentration at time *t=k+1*, In Order to find this value Equation (7) is solved for $C_{i,j,k+1}$, The Resulting Equation is,

$$C_{i,j,k+1}=C_{i,j,k}\left[1-\frac{2D_x\Delta t}{\Delta x^2}-\frac{2D_y\Delta t}{\Delta y^2}\right]+C_{i+1,j,k}\left[\frac{D_x\Delta t}{\Delta x^2}-\frac{V_x\Delta t}{2\Delta x}\right]+C_{i-1,j,k}\left[\frac{D_x\Delta t}{\Delta x^2}+\frac{V_x\Delta t}{2\Delta x}\right]+C_{i,j+1,k}\left[\frac{D_y\Delta t}{\Delta y^2}\right]+C_{i,j-1,k}\left[\frac{D_y\Delta t}{\Delta y^2}\right] \quad (8)$$

To simplify the given expression, constant coefficients are called as M, N, P, and R as stated below (again both general and given data-specific solutions are given in following equations):

$$M=\left[1-\frac{2\Delta t}{\Delta x^2}-\frac{0.1(2)\Delta t}{\Delta y^2}\right] \text{.... (8A);} \qquad N=\left[\frac{\Delta t}{\Delta x^2}-\frac{\Delta t}{2\Delta x}\right] \text{.....(8B);}$$

$$P=\left[\frac{\Delta t}{\Delta x^2}+\frac{\Delta t}{2\Delta x}\right] \text{.....(8C);} \qquad R=\left[\frac{0.1\Delta t}{\Delta y^2}\right] \text{.....(8D);}$$

Now Equation (8) can be simplified as,

$$C_{i,j,k+1}=C_{i,j,k}[M]+C_{i+1,j,k}[N]+C_{i-1,j,k}[P]+C_{i,j+1,k}[R]+C_{i,j-1,k}[R] \quad (9)$$

## V. RESULTS AND CONCLUSIONS

### COMPARISION OF NUMERICAL AND ANALYTICAL SOLUTIONS

In order to see, how good the result of numerical solution matches with the analytical solution, following plots are prepared and results are interpreted:

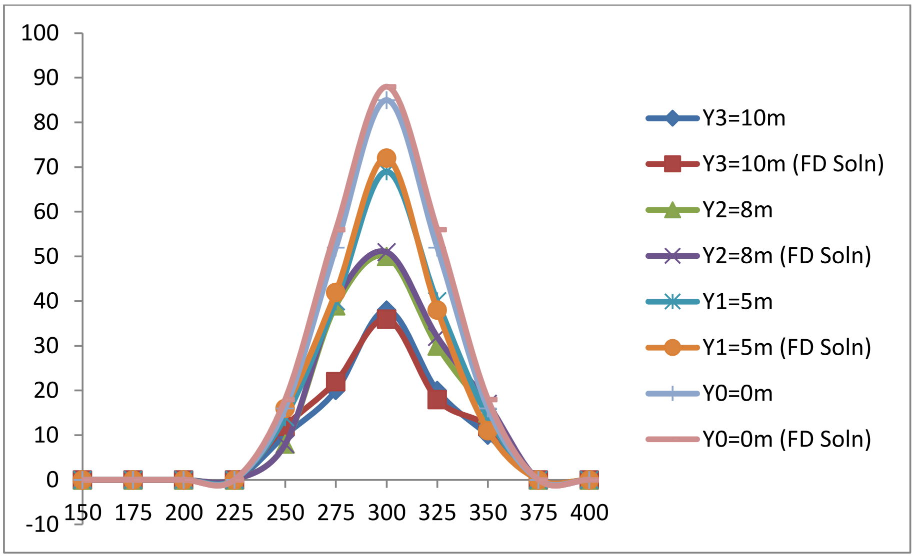


Figure 1. Concentration (C) versus distance (X) for different Y values (time=300 days)

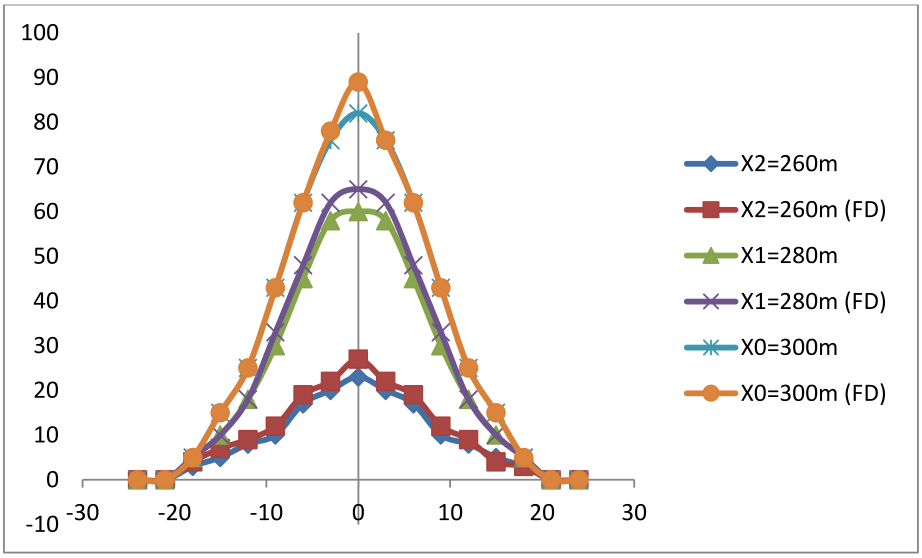


Figure 2. Concentration (C) versus distance (Y) for different X values (time=300 days)

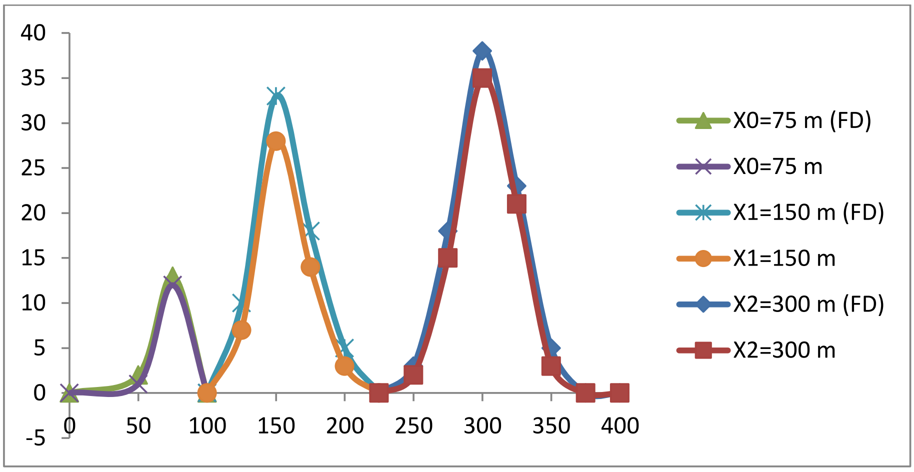


Figure 3. Concentration (C) versus time (T) for different X values (Y=10 m)

**The following conclusions can be drawn from this study:**

1. Concentration decrease with time when y=0. Otherwise the relationship depends on the relative concentrations at the studied points to the concentration at the plume centre. As seen in the graphs above, the contaminant travels in the direction of Vx with time and it is dispersed and expanded to the area with decreasing concentrations from the centre of the plume to the edges.
2. The plume is moving away from the origin with time by the steady seepage flow of water.
3. The dimensions of the plume are increased as it has been transported away from its origin.
4. The centre of mass is advected at the average linear velocity.
5. The study shows that the numerical solution and the analytical solution, for the given problem, match in an acceptable range.
6. Analytical and numerical simulation models can be used by instructors to effectively present contaminant transport through a saturated soil layer.

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