Mathematical Modelling of Groundwater Contaminants at Various Depth

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ABSTRACT

A deviant model is sought to the work "Mathematical Modelling of Groundwater Contamination with Varying Velocity Field" by Pintus Das, *et al*., in which analytical solutions are obtained using Laplace Integral Transform Technique (LITT) to measure impact of dispersion and diffusion coefficients in the solution of Advection-Dispersion Equation (ADE) subject to transient (time-dependent) boundary condition. However, the limit or extent to which solute/contaminant of fluid can be transported far down beneath the earth surface was not explored.

From a source point, this work employs similar Computational Fluid Dynamic (CFD) technique to analyze the limitation of water movement with respect to pores and soil composition in the bowels of the earth, thereby finding the longitudinal distance from the source point in which the concentration of the contaminant solute becomes zero.

(Keywords: longitudinal dispersion, diffusion, groundwater, contaminant, Computational Fluid Dynamics, CFD)

INTRODUCTION

Groundwater is an important source of getting adequate water supply into homes for human use. In recent times there have been a lot of concerns on how activities of man and his industries impact this underground flow in massive water body. Computational Fluid Dynamics (CFD) has been useful in studying the aquifer flow direction through heterogeneous medium, the movement of which is both transverse and longitudinal. The latter is responsible for the percolation of contaminants while the latter diffuses such within different layers of flows. The spreading is due to the heterogeneity of the medium, such as a distribution of pore sizes and shapes. (Pintu Das, *et al.*, 2017).

The nature of contaminant, the seepage velocity, the porosity of various media and the dispersion coefficient have been experimentally observed and developed into the generalized dispersion theory. (Scheidegger, 1961). A time-dependent input concentration model for longitudinal flow through beds of packed porous solids with seasonal patterns in tropical region using Laplace Transformation Technique (LTT) obtained an analytical solution for Ebach and White (1958) "Mixing of fluids flowing through beds of packed solids" with graphical representation made through MATLAB. (Mritunjay Kumar Singh, *et al.*, 2009).

The packed solid itself being composed of various chemical compounds, reacts with contaminant to sometimes produce fluidic material entirely different from the two reactants and thus made the observatory works complex to track. Aral and Liao (1996) worked on similar time-dependent models with dispersion coefficient for contaminant transport, while Basha and El-Habel (1993) gave analytical solutions with one-dimensional linear, asymptotic and exponential dispersivities in infinite domain. A closed form solution to solute transport in a semi-infinite domain with an arbitrarily time-dependent dispersion coefficient and arbitrary initial and boundary flux conditions by variable transformation shows that there is limitation to the depth a concentrated solute can attain. (Barry and Sposito, 1989).

Dispersion coefficient has also been ranked by various previous works. Ghosh and Sharma, (2006) found the dispersion coefficient to be directly proportional to seepage velocity within a boundary of 1 and 1.2. Freeze and Cherry, (1979) in its generalized dispersion theory ranked its coefficient between 1 to 2. Dispersion coefficients are usually much greater than diffusion coefficients and cause much more rapid mixing than would ever be possible from molecular motion alone (Cussler, 1977). The scale dependency of the hydrodynamic dispersion coefficient is an outcome of the associated Fickian assumptions that the mass of any dispersing/diffusing compound is conserved through the porous medium upon which is dependent. (Don Kulasiri and Wynand Verwoerd, 2002).

A stochastic component of dispersion is ignored here, and the variant of advection-dispersion equation is entirely deterministic. Axial dispersion coefficient is modified into an idealized linear dispersion in a longitudinal motion. The uncertainty of the geological formation at respective locations and variation in chemical concentration make coefficient of dispersion into a differentiable parameter with variable order in which there is a functional property that allows the value of the chemical concentration to recall its route through which it migrated through geological formation with time as retardation occurs with respect to the initial location where the contaminant was injected. (Abdon Atangana, 2018). The slowing down of the seepage velocity indicates that there will exist a longitudinal distance where the concentration of the transported solute/fluid becomes zero. In this work, we also consider the effect of addition of a solvent of volume V which when added reduced the concentration of the contaminant solute but increases its longitudinal distance.

MATHEMATICAL FORMULATION OF THE PROBLEM

Consider the geological formations to be in layer of finite beds B_i in longitudinal direction, the topmost layer being B_0 with each layer having the same porosity and composing of the same soil material. The dispersion velocity $v(B_i, \mu)$ changes with each layer and decreases as i increases and is of its greatest value when $i = 0$.

We assume that the effects of dispersion are constant and are in longitudinal direction only with solute/contaminant fluid being conserved and though could be reactive with other materials in the soil the effect of new compound formed is regarded as being one and the same as the original solute/contaminant fluid. With these assumptions the conservation of mass yields the constant parameter advection-dispersion equation (ADE):

$$\frac{\partial V}{\partial B} + \frac{1-n}{n}\frac{\partial F}{\partial B} = \frac{\partial}{\partial x}\left(D\frac{\partial V}{\partial x} - uB_i\right) - \mu B_i \qquad \textbf{(1)}$$

Where $V[L^3]$ is the volume of neutralizing solvent, $F[ML^{-3}]$ is the volume averaged dispersing solute/contaminant fluid, $D[L^2T^{-1}]$ is the longitudinal dispersion coefficient, $u[LT^{-1}]$ is the unsteady uniform downward pore seepage velocity, $x[L]$ is the length in longitudinal direction of flow, $\mu[T^{-1}]$ is the first order decay rate coefficient for solute/contaminant fluid production and n is the maximum number of beds of soil layers.

A linear absorption coefficient for the solute/contaminant fluid is considered as:

$$F = K_d V \qquad \textbf{(2)}$$

Where K_d is the distribution coefficient.

Combining Equations (1) and (2), gives:

$$R\frac{\partial V}{\partial B} = \frac{\partial}{\partial x}\left(D\frac{\partial V}{\partial x} - uB_i\right) - \mu B_i \qquad \textbf{(3)}$$

Where,

$$R = 1 + \tfrac{1-n}{n}K_d \qquad \textbf{(4)}$$

is the retarding factor.

The retardation occurs in two different ways: the dilution of the concentration of the solute/contaminating fluid F by the solvent V and the slowing down of the longitudinal movement of the same. The solvent, however, aids the travel of F further down the layers of soil after diluting it. Hence, we solve Equation (1) subject to the boundary condition:

$$\frac{\partial F}{\partial x} = 0, \quad x \to \infty\,. \tag{5}$$

ANALYTICAL SOLUTION OF ONE-DIMENSIONAL DISPERSION WITH DILUTING SOLVENT

Let $u = u_0 f(m)$, $D = D_0 f(m)$, $\mu = \mu_0 f(m)$, $\gamma = \gamma_0 f(m)$ and $B = B_0$ where $f(m)$ is non-dimensional and $m\,[T^{-1}]$ is the flow resistance coefficient, $D_0[L^2T^{-1}]$ is the initial longitudinal dispersion coefficient, $u_0[LT^{-1}]$ is the initial seepage velocity, $\mu_0[T^{-1}]$ is the initial first order decay term, $\gamma_0[ML^{-3}T^{-1}]$ is the initial zero-order production term and B_0 is the topmost soil layer in which the source F_n is poured.

Thus, we write Equation (3) as:

$$\frac{R}{f(m)}\frac{\partial V}{\partial B} = \frac{\partial}{\partial x}\left(D_0\frac{\partial V}{\partial x} - \mu_0 B_0\right) - \mu_0 B_0 \tag{6}$$

The impact of diffusion is not considered here as we are only interested in the longitudinal movement.

Now, we expressed the initial and boundary conditions in terms of non-dimensional parameters as:

$$F(X,0) = \frac{F_i}{F_0} + \gamma_1 X, \quad X > 0, \qquad V = 0 \tag{7}$$

$$F(0,V) = \frac{F_i}{F_0} + 1 - \frac{D_0}{{u_0}^2}V\,, \quad X = 0, \qquad V > 0 \tag{8}$$

$$\frac{\partial F}{\partial x} = 0\,, \qquad X \to \infty, \quad V \geq 0 \tag{9}$$

Using the transformation:

$$F(X,V) = K(X,V)exp\left[\frac{\alpha_0}{2D_1} - \frac{1}{R}\left(\frac{{\alpha_0}^2}{4D_1} + \mu_1\right)V\right] \tag{10}$$

where α_0 is the asymptotic dispersity at the initial layer and $K(X,V)$ is another dependent factor, the analytical solution subject to initial and boundary conditions given in Equations (7) – (9) by applying Laplace transform technique is:

where,

$$F(X,V) = \left[\left(\frac{F_1}{F_0} + 1\right)G(X,V) - \frac{D_0}{{u_0}^2}H(X,V) - \frac{F_1}{F_0}I(X,V) + \frac{\gamma_1\alpha_0}{R}J(X,V) + \left(\frac{F_1}{F_0} + \gamma_1 X - \frac{\gamma_1\alpha_0}{R}V\right)e^{-\left(\frac{\alpha_0}{2D_1}X - \frac{{\alpha_0}^2}{4D_1R}V\right)}\right]exp\left[\frac{\alpha_0}{2D_1} - \frac{1}{R}\left(\frac{{\alpha_0}^2}{4D_1} + \mu_1\right)V\right] \tag{11}$$

$$G(X,V) = \frac{1}{2}\left[exp\left(BV - \sqrt{\frac{BR}{D_1}}X\right)erfc\left(\frac{1}{2}\sqrt{\frac{R}{D_1V}}X - \sqrt{BV}\right) + exp\left(BV + \sqrt{\frac{BR}{D_1}}X\right)erfc\left(\frac{1}{2}\sqrt{\frac{R}{D_1V}}X + \sqrt{BV}\right)\right] \quad \textbf{(13a)}$$

$$H(X,V) = \frac{1}{4\sqrt{B}}\left[2\sqrt{BV} - \sqrt{\frac{R}{D_1}}X\right]exp\left(BV - \sqrt{\frac{BR}{D_1}}X\right)erfc\left(\frac{1}{2}\sqrt{\frac{R}{D_1V}}X\right) + \frac{1}{4\sqrt{B}}\left[2\sqrt{BV} + \sqrt{\frac{R}{D_1}}X\right]exp\left(BV + \sqrt{\frac{BR}{D_1}}X\right)erfc\left(\frac{1}{2}\sqrt{\frac{R}{D_1V}}X + \sqrt{BV}\right) \quad \textbf{(13b)}$$

$$I(X,V) = \frac{1}{2}\left[exp\left(\frac{\alpha_0^2}{4D_1R}V - \frac{\alpha_0}{2D_1}X\right)erfc\left(\frac{1}{2}\sqrt{\frac{R}{D_1V}}X - \frac{\alpha_0}{2}\sqrt{\frac{V}{D_1R}}\right) + exp\left(\frac{\alpha_0^2}{4D_1R}V + \frac{\alpha_0}{2D_1}X\right)erfc\left(\frac{1}{2}\sqrt{\frac{R}{D_1V}}X + \frac{\alpha_0}{2}\sqrt{\frac{V}{D_1R}}\right)\right] \quad \textbf{(13c)}$$

The four factors G, H, I and J determine the level of transportation of the solute and thus:

$$max{:}\,G(X,V);\ \ max{:}\,H(X,V);\ \ max{:}\,I(X,V);\ \ max{:}\,J(X,V)$$

subject to minimizing the error function (erfc) in each of them give the maximum longitudinal value to which the contaminant can travel in the aquifer.

CONCLUSION

The analytical model is to be compared with numerical models that would be obtained from data collected. However, this analytical solution serves as a preliminary predictive tool in ground water resource and management. Further studies would increase the variables in a multi-dimensional direction. This study will be found very useful in the clean-up of areas affected by spillage of oil during exploration and transportation in the downstream sector of crude oil production.

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SUGGESTED CITATION

Adeosun, T.A. and O. Onifade. 2025. "Mathematical Modelling of Groundwater Contaminants at Various Depth". *Pacific Journal of Science and Technology*. 26(2): 205-209.

Pacific Journal of Science and Technology