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Numerical Reconstruction and Remediation of Soil Acidity on a One Dimensional Flow Domain Where the Diffusion Coefficient and Advection Velocity are Exponentially Dependent on Time

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Abstract

A one dimensional mass transport equation in porous medium whose solution is ill-posed is considered. Appropriate flow parameters that are consistent to flow of solutes are determined. Solutes diffusion coefficient and advection velocity are taken to be exponentially changing with time. Flow domain is assumed semi infinitely deep and homogeneous. Finite volume and finite difference methods are used spatial and temporal discretization of the governing PDE. Solutions for possible combinations of time dependent flow parameters at different soil depths and time intervals are compared with help of graphs. It is observed that the concentration levels of ions with depth and time can be detected early when the two parameters are negative exponential functions of time before further pollution takes place in the underground environment.

Keywords: Inverse prolems, Finite Volume Method, Advection, Diffusion, Reconstruction, Remediation

INTRODUCTION

Movement of pollutants from a ground surface of soil through the vadose zone to the Ground-water is a major pollution to the hydrological environment in the subsurface. This phenomenon has negatively impacted on human life, livestock who depend heavily on groundwater in addition to degradation of flora and fauna on the terrestrial and aquatic environment. The uncontrolled and excess use of chemical fertilizers are known to be major cause of this pollution.This is because chemicals under investigation in this study which include high nitrogen synthetic fertilizers percolate in soil over time thus becoming responsible for soil acidification. Some of the studies conducted on soil acidification include [1] who defined soil acidification as the decrease in acid neutralization capacity of the soil. It is one of the factors limiting crop production in many parts of the world. Although soil acidification is a natural process, it has recently been accelerated by human practices on the farm lands which causes gradual accumulation of hydrogen ions in the soil. These practices include addition of agricultural synthetic fertilizers and pesticides, inorganic matter and minerals that break down in the soil over time. Some of the industrial effluent causes great concern because they hardly break down, are carcinogenic and their extraction is extremely expensive. In addition and to large extent, it has been documented that chemical fertilizer on excess percolation into the soil contribute immensely to acidification when they stay and break down over time.

In this paper,we intend to develop a mathematical understanding of the initial root causes and levels of acidification in priori, by solving mathematical backward problem which translates to inverse problem as opposed to solving a forward problem, whose solution is ill- posed in such a way that the infinitesimal error always magnifies un-proportionally in final solution hence requiring regularization schemes. This is what is being referred to as reconstruction of acidity. Remediation in this context is the reversibility of intensively acidified arable land to traditional health and fertile land. This should be a priority for land conservation.

To model this processes mathematically, we invoke a mathematical thinking by developing mathematical models from Navier-Stokes Equations to simulate advection and diffusion process of solute transport in homogeneous soil structures which are an exceptionally rare case of soil structure as much as the plant root zone can be considered to be almost homogeneous or weakly heterogeneous.

In this work we have solved an inverse problem modelled from the advection diffusion equation, numerically by adopting a hybrid of Finite volume method and Finite difference schemes for spatial and temporal discretization respectively with some fundamental assumptions utilized. The process of acidification is complex indeed expressible in terms of non linear PDEs. Thus determination of analytic solution involves a lot of assumptions thus making the results unrealistic.

Flow of contaminated fluids from the soil surface in to the ground water has been studied by many researchers in the past like [2] , [3] among others.

When fertilizers are applied on a wet ground they dissolve easily to form a solute because of their characteristic nature of been highly miscible with water, volatile and hygroscopic. Thereafter the solute will be transported through advection also referred to as convection, deep into the soil due to the bulk fluid motion after an irrigation or even a heavy downfall. However when advection slows down due to soil saturation, the level of wetness attained will vary from the surface soil downwards. As this infiltration process occurs, the solute simply disperses away from the source in a diffusive manner and thus the flow of the chemicals can be described using the Advection- diffusive equation (ADE). The classical Advection and Dispersion equation has commonly been used to characterize the transport of non-reactive solutes through homogeneous porous media consisting of impermeable grains, see [4] and [5]. There are also other processes that are responsible for movement of solutes , see [6], [7] and [8]. Various approaches that have previously been employed to solve the Advection Dispersion equations include analytical, experimental, Case studies and Numerical studies applied to the transport of chemicals through saturated and unsaturated porous media. , see [9], [10], [11]Harmon and Wiley [2011], [12], [13], [14], [15], [16], [17], [18] among others.

This study is intended to determine appropriate diffusion coefficient and advection velocities in the advection diffusion equation. Identification of the unknown diffusion coefficient in a linear parabolic equation via semi group approach was performed by [19]. Identification of coefficients for a parabolic equation where the unknown coefficient depends on an over specified datum is presented by [20]. Identification of a Robin Coefficient on a non- accessible part of the boundary from available data on the other part is reported by [21]. Coefficients problems are used to estimate values of parameters in a governing equation. Previously, techniques used for remediation of polluted soil and groundwater included pump- and -treat, using a combination of the optimization methods and simulation models as proposed by [22], Hot water flushing [23], [24], air sparging [25], Cosolvent flushing [23], the use of surfactants [26], In situ bio-remediation [27].The effectiveness of the remediation may be substantially improved if the location and extent of the contaminants source are known.

ONE DIMENSIONAL ADVECTION DIFFUSION MODEL

Let the domain of flow $\Omega = [0, z]$ represent the semi- infinite flow domain given that $0 \le z \le \infty$ and time t varies from 0 to final time T . The general non-linear form of one dimensional advection diffusion equation describing solute flow in Cartesian system given by equation (1)

$$\frac{\partial C}{\partial t} = \frac{\partial}{\partial z}\left[D_z(z,t)\frac{\partial C}{\partial z} - w(z,t)C \right] + S_0 \qquad (1)$$

Where $C(z,t)$ is the function representing concentration of the substance to be transported at depth z of the domain at time t taking z axis as the direction of flow, $D_z(z,t)$is the diffusion coefficient which can represent molecular diffusion while $w(z,t)$is the advection velocity.

The last term on the right hand side is taken to be the source or sink term for production or loss of solutes within the system. Since we are concerned with solutes flow in agricultural land the source term S_0 is taken to represent fertilizer application and other human related activities that can lead to in-equilibrium in soil PH. It is assumed that in this paper, soil is of semi –infinite depth and the soil properties like the permeability and porosity are uniform along the z axis.

We need to analyze the situation where the source term is zero. In the present case, we need to reconstruct the initial condition $C(z,t) = f(z), t = 0$ and the flow parameters $D_z(z,t)$ and $w(z,t)$ exponentially varied with time. We shall determine a suitable function $f(t)$ for boundary condition $C(0,t)$ on one side of the domain taking $C(z,t) = 0, z = z_\infty$ on the other side of the domain.

TIME VARIATION OF ADVECTION VELOCITY $w(z,t)$ AND DIFFUSION COEFFICIENT $D_z(z,t)$ IN THE ABSENCE OF SOURCE TERM

When the diffusivity coefficient $D_z(z,t) = D_z(t)$ and the advection velocity $w(z,t) = w(t)$, we

obtain a particular case to the problem in the equation (1) given by equation (2)

$$\frac{\partial C}{\partial t} = D_z(t)\frac{\partial^2 C}{\partial z^2} - w(t)\frac{\partial C}{\partial z} \tag{2}$$

$$\text{for } \Omega \times t \in (0,T]$$

In the current problem we shall consider varying the parameter values of $w(z,t)$ as :

(i) advection velocity exponentially decreasing with time $w(z,t) = w_0 \exp(-at)$

(ii) advection velocity exponentially increasing with time $w(z,t) = w_0 \exp(at)$

where a is the rate at which the flow velocity is varying with time

Similarly we shall also consider varying the diffusion coefficient $D_z(z,t)$ as

(iii) Diffusion coefficient exponentially decreasing with of time $D_z(z,t) = D_0 \exp(-at)$

(iv) Diffusion coefficient exponentially increasing with time $D_z(z,t) = D_0 \exp(at)$

where a is the rate at which solutes diffusion is varying with time.

SPATIAL AND TEMPORAL DISCRETIZATION IN THE FLOW DOMAIN

The flow domain is subdivided into infinitesimal volumes called control volumes and the differential equations represented in integral form using Finite volume method. The integral form of each conservation law is written separately for each control volume. Discretization process of time is then carried out for each control volume by finite difference scheme. Higher order terms are reduced into weak form which are then solved numerically by inversion. The components of the discretised equation are used to approximate the discrete values at the centre of the domain after implementing the prescribed initial and boundary conditions.

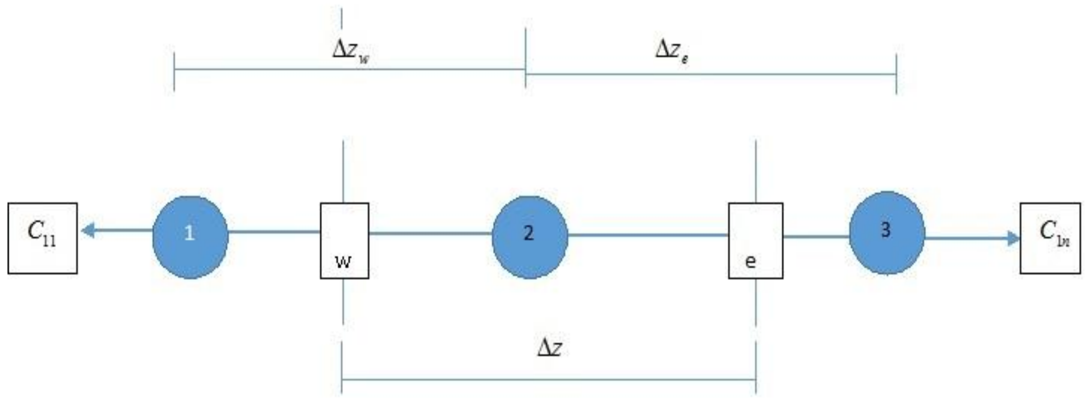

Figure 1: Discretized one dimensional domain into control volumes of width Δz

Taking the discretized flow domain illustrated in figure 1, in which node 2 serves as the centre node of the control volumes $\Delta x \Delta y \Delta z$ with unit thickness and nodes 1 and 3 and are the centres of the neighbouring control volumes, w and e are the western and eastern boundaries of the control volume respectively. Since the control volume is taken to be one dimensional, th thickness $\Delta x = \Delta y = 1$ thus the control volume reduces to Δz. C_{11} and C_{1n} are the conditions at the western and eastern boundaries of the control volume respectively that can be assumed to be known. When C_{11} and C_{1n} are known, the problem becomes a forward problem and it can easily be solved using the standard techniques available. However whenever they aren't known the problem is ill posed and thus calls for the techniques of solving inverse problems to be employed.

With no loss of generality this study focus on flow of soluble pollutants like fertilizers represented by smooth function $C(z,t)$in porous medium assumed to have uniform structure in the solution domain.

DISCRETISATION OF GOVERNING EQUATION WHEN FLOW PARAMETERS ARE DECREASING EXPONENTIALLY WITH TIME

The diffusivity and fluid velocity are taken to be $D(z,t) = D_0 \exp(-at)$ and $w(z,t) = w_0 \exp(-at)$.

Here both parameters are exponentially decreasing in time such that at start i.e. $t = 0$, both

$D(z,t)$ and $w(z,t)$ assume a value equal to D_0 and w_0 respectively. As time increases, their values decreases. We need to determine the solute concentration for varying values of

$D(z,t)$ and $w(z,t)$ at varied time and depth. $w(z,t)$ dominates the flow although at a decreasing rate. The one dimensional advection diffusion equation ((2) becomes

$$\frac{\partial C}{\partial t} = D_0 \exp(-at)\frac{\partial^2 C}{\partial z^2} - w_0 \exp(-at)\frac{\partial C}{\partial z} \tag{3}$$

Integrating over the control volume and with respect to time, we obtain the generalized discretised equation

$$\Delta z\left[C_P - C_{i,j-1}\right] = -\frac{D_0}{a}\left[\exp(-at_j) - \exp(-at_{j-1})\right]\left[\frac{dC}{dz}_e - \frac{dC}{dz}_w\right] +$$

$$\frac{w_0}{a}\left[\exp(-at_j) - \exp(-at_{j-1})\right]\left[C_e - C_w\right] \tag{4}$$

At the first control volume, where C_w is assumed to be known, the discretised equation becomes

$$\left[\left(\frac{3D_0}{a\Delta z} + \frac{w_0}{2a}\right)\left(\exp(-at_j) - \exp(-at_{j-1})\right) - \Delta z\right]C_{i,j}$$

$$+\left(\frac{-D_0}{a\Delta z} + \frac{w_0}{2a}\right)\left(\exp(-at_j) - \exp(-at_{j-1})\right)C_{i+1,j}$$

$$= \left(\frac{2D_0}{a\Delta z} + \frac{2w_0}{2a}\right)\left(\exp(-at_j) - \exp(-at_{j-1})\right)C_{i-\frac{1}{2},j} - \Delta z C_{i,j-1} \tag{5}$$

The discretised equation for the $2nd$ to the $(N-1)th$ control volumes will be

$$\left[\left(-\frac{D_0}{a\Delta z} - \frac{w_0}{2a}\right)\left(\exp(-at_j) - \exp(-at_{j-1})\right) - \Delta z\right]C_{i-1,j}$$

$$\left[\frac{2D_0}{a\Delta z}\left(\exp(-at_j) - \exp(-at_{j-1})\right) - \Delta z\right]C_{i,j} +$$

$$\left(\frac{-D_0}{a\Delta z} + \frac{w_0}{2a}\right)\left(\exp(-at_j) - \exp(-at_{j-1})\right)C_{i+1,j} = -\Delta z C_{i,j-1} \tag{6}$$

The Nth control volume, where C_e is assumed to be known, precisely representing the boundary condition at that control volume, the following discretised equation is obtained

$$\left[\left(-\frac{D_0}{a\Delta z}-\frac{w_0}{2a}\right)\left(\exp\left(-at_j\right)-\exp\left(-at_{j-1}\right)\right)-\Delta z\right]C_{i-1,j}$$

$$\left[\left(\frac{3D_0}{a\Delta z}-\frac{w_0}{2a}\right)\left(\exp\left(-at_j\right)-\exp\left(-at_{j-1}\right)\right)-\Delta z\right]C_{i,j}$$

$$=\left(\frac{2D_0}{a\Delta z}-\frac{2w_0}{2a}\right)\left(\exp\left(-at_j\right)-\exp\left(-at_{j-1}\right)\right)C_{i+\frac{1}{2},j}-\Delta zC_{i,j-1} \quad (7)$$

DISCRETISATION OF GOVERNING EQUATION WHEN FLOW PARAMETERS ARE INCREASING EXPONENTIALLY WITH TIME

Here we consider $D(z,t)=D_0\exp(at)$ and $w(z,t)=w_0\exp(at)$. This case demonstrates a situation where at time $t=0$, both flow parameters are equal to D_0 and w_0 and as time increases, the $D(z,t)$ and $w(z,t)$ increase exponentially with time. $w(z,t)$ dominates the flow at an increasing rate. Equation (2) becomes

$$\frac{\partial C}{\partial t}=D_0\exp(at)\frac{\partial^2 C}{\partial z^2}-w_0\exp(at)\frac{\partial C}{\partial z} \quad (8)$$

Integrating over the control volume and from time t_{j-1} to t_j, we obtain the generalized equation for this case.

$$\Delta z\left[C_P-C_{i,j-1}\right]=\frac{D_0}{a}\left[\exp\left(at_j\right)-\exp\left(at_{j-1}\right)\right]\left[\frac{dC}{dz}_e-\frac{dC}{dz}_w\right]$$
$$-\frac{w_0}{a}\left[\exp\left(at_j\right)-\exp\left(at_{j-1}\right)\right]\left[C_e-C_w\right] \quad (9)$$

At the first control volume, where C_w is assumed to be known, we obtain

$$\left[-\left(\frac{3D_0}{a\Delta z}+\frac{w_0}{2a}\right)\left(\exp\left(at_j\right)-\exp\left(at_{j-1}\right)\right)-\Delta z\right]C_{i,j}+\left(\frac{D_0}{a\Delta z}-\frac{w_0}{2a}\right)\left(\exp\left(at_j\right)-\exp\left(at_{j-1}\right)\right)C_{i+1,j}$$

$$=-\left(\frac{2D_0}{a\Delta z}+\frac{2w_0}{2a}\right)\left(\exp\left(at_j\right)-\exp\left(at_{j-1}\right)\right)C_{i-\frac{1}{2},j}-\Delta zC_{i,j-1} \quad (10)$$

For the $2nd$ through the $(N-1)th$ control volumes we have the following discretized equation

$$\left[\left(\frac{D_0}{a\Delta z}+\frac{w_0}{2a}\right)\left(\exp\left(at_j\right)-\exp\left(at_{j-1}\right)\right)\right]C_{i-1,j}-\left[\frac{2D_0}{a\Delta z}\left(\exp\left(at_j\right)-\exp\left(at_{j-1}\right)\right)+\Delta z\right]C_{i,j}$$
$$+\left(\frac{D_0}{a\Delta z}-\frac{w_0}{2a}\right)\left(\exp\left(at_j\right)-\exp\left(at_{j-1}\right)\right)C_{i+1,j}=-\Delta z C_{i,j-1} \qquad (11)$$

Finally at the Nth control volume, the discretized equation will be

$$\left[\left(\frac{D_0}{a\Delta z}+\frac{w_0}{2a}\right)\left(\exp\left(at_j\right)-\exp\left(at_{j-1}\right)\right)\right]C_{i-1,j}+\left[\left(-\frac{3D_0}{a\Delta z}+\frac{w_0}{2a}\right)\left(\exp\left(at_j\right)-\exp\left(at_{j-1}\right)\right)-\Delta z\right]C_{i,j}$$
$$=\left(-\frac{2D_0}{a\Delta z}+\frac{2w_0}{2a}\right)\left(\exp\left(at_j\right)-\exp\left(at_{j-1}\right)\right)C_{i+\frac{1}{2},j}-\Delta z C_{i,j-1} \qquad (12)$$

RESULTS AND DISCUSSIONS

A non linear mass transport equations is used to determine flow characteristics of pollutants in soils. A one dimensional ADE is considered in which the coefficients are exponentially dependent on time. The $D(z,t)$ and $w(z,t)$ are first decreasing with time and secondly increasing with time at varied depths in the soil.

Advection and diffusion processes are playing a key role in determination of the concentration at different levels in soils at different times although advection is dominant.

The results are presented in form of graphs and the discussions for each are made here under. The flow domain is divided into zones of uniform width. In Figure 2, Saturation in zone $z=0.25$ takes place at time $t=0.45$. The concentration level attained is 0.35. The same level of pollution is reached at time $t=0.35$ in Figure 3. It took longer for zone $z=0.5$ to become saturated in figure 2 than in figure 3. The flow parameters are increasing with time in figure 3 while in figure 2, they are decreasing and this explains the reason why more pollutants are able to reach zones deep down in the soil in figure 3 unlike in figure 2 where very little or no pollutants reach these zones. It is important to notice that the concentration is higher in figure 3 for zone $z=0.75$ than in figure 2.

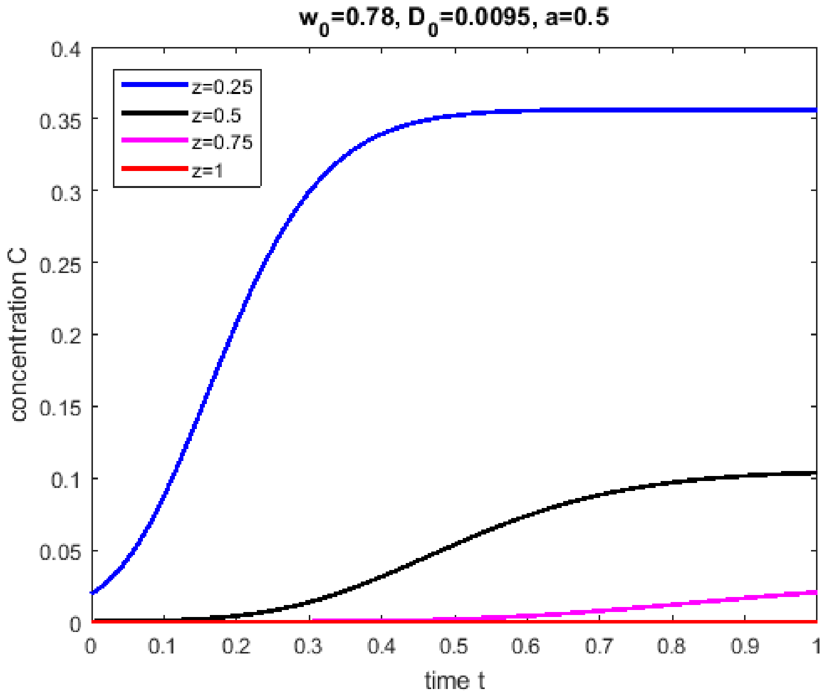

Figure 2: Non dimensional concentration C against time t at varied depth z when D(z,t) and w(z,t) are negatively decreasing in time

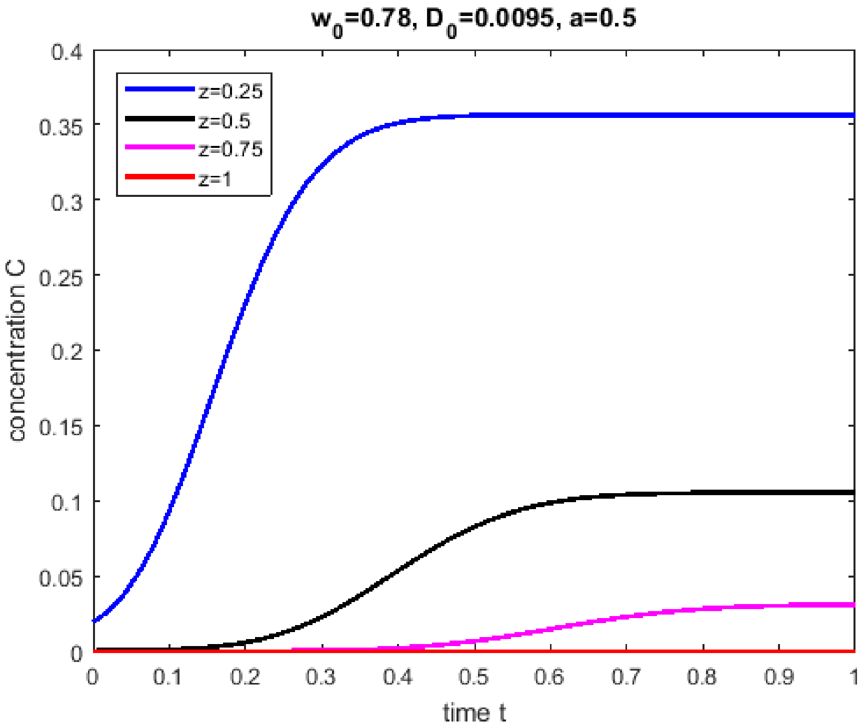

Figure 3: Non dimensional concentration C against time t at different depths z when D(z,t) and w(z,t) are positively increasing in time

In figures 4 and 5, Pollution is notable at a depth of $z = 0.5$ within the first time level $t = 0.25$.

Pollutants penetrate deeper in figure 5 than in figure 4 during the time level $t = 0.5$. Because of reducing advection and diffusion, little pollution is able to penetrate to a depth of $z = 0.8$ to $z = 1.0$ in figure 4 during time level $t = 0.75$ and $t = 1.0$. In figure 5, chemicals are able to percolate to unreachable zones (outside the domain under consideration). This is noted during time level $t = 0.75$ and $t = 1.0$ where the curves overlap. This is as a result of increasing $D(z,t)$ and $w(z,t)$.

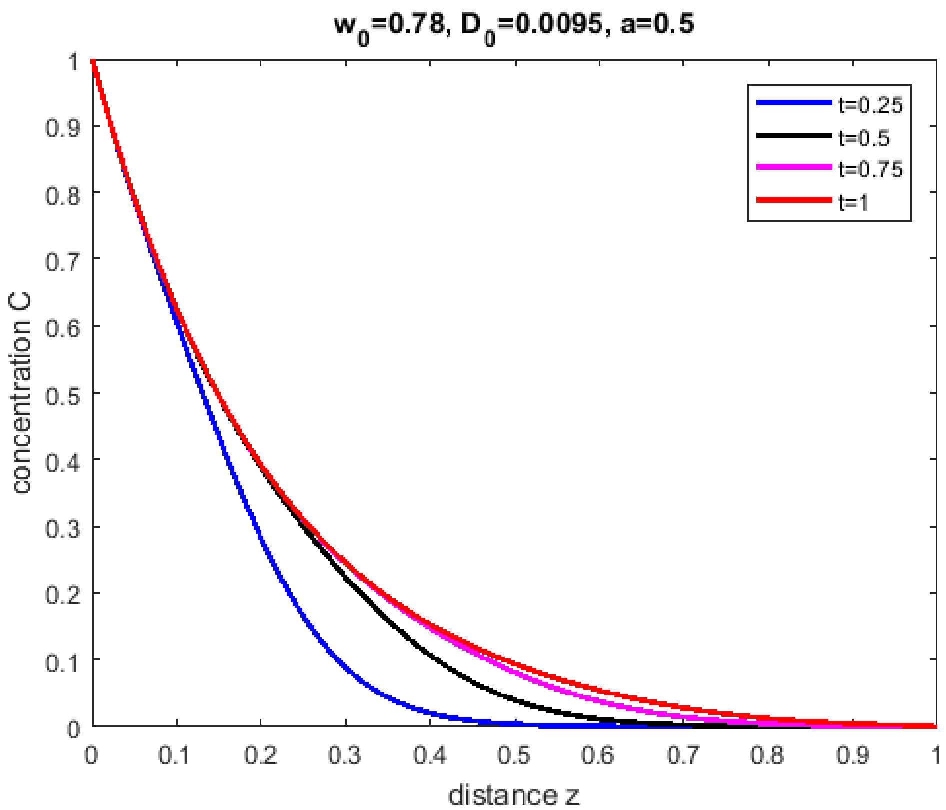

Figure 4: Non dimensional concentration C against depth z at different time t when D(z,t) and w(z,t) are exponentially decreasing in time.

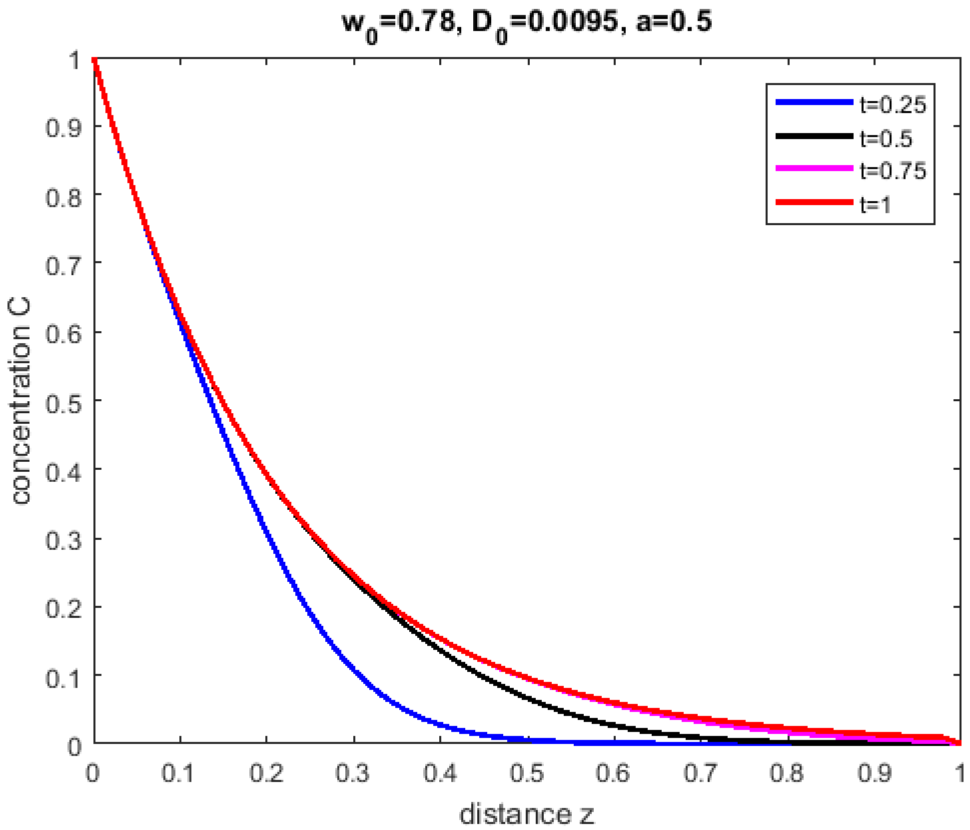

Figure 5: Non dimensional concentration C against depth z at different time t when D(z,t)and w(z,t) are exponentially increasing in time

CONCLUSION AND RECOMMENTATIONS

CONCLUSION

In this work we considered a mathematical model that shows chemicals being transported in a homogeneous soil structure where reaction was negligible. The model helped to predict the flow characteristics of pollutants in soils. The model was anchored on the classical mass transport equation with appropriate initial and boundary conditions which were numerically tested for their applicability. A one dimensional flow domain was considered where the flow parameters being investigated were negative exponential and positive exponential functions of time.

Since the parameters $D(z,t)$ and $w(z,t)$ are exponentially increasing in time in figure 3 and 5, it is expected that the concentration deep down the soil are higher than zero. This is only possible if the soil particles deep down allow faster penetration of chemicals and fluids. Using the assumption that the soil structure under consideration is homogenous, the opposite is expected which is not the case here. This does not represent a physical situation. However, mitigation of the noted pollution can be performed in cases where $D(z,t)$ and $w(z,t)$ are decreasing with time exponentially.

This can be done by introducing a parameter that tries to reduce the values of $D(z,t)$ and $w(z,t)$ at every time interval.

RECOMMENDATIONS

More research can be carried out on this present work by considering the following

i) Introduce a parameter that can reduce the values of $D(z,t)$ and $w(z,t)$

ii) Analysis of flow parameters which are depended on depth

It is our intention to carry our further research in one or more areas cited above though other researchers are encouraged to come on board.

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