Numerical Reconstruction and Remediation of Soil Acidity on a One Dimensional Flow Domain with Constant and Linear Temporally Dependent Flow Parameters

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Authors' contributions

This work was carried out in collaboration between all authors. Author CMM designed the study, performed the numerical analysis, wrote the protocol, and wrote the first draft of the manuscript. Authors TTMO and CM provided the necessary guidance for publication. All authors read and approved the final manuscript.

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ABSTRACT

A mathematical backward problem which involves solving a mathematical model based on a one dimensional advection - diffusion process of solute transport in a homogeneous soil structure is considered. The diffusion coefficient and advection velocity in the governing unsteady non-linear partial differential equation (PDE) are varied from constant to linearly dependent on time. This is done to develop a mathematical understanding of the initial root causes and levels of acidification in priori because determination of analytic solution involves a lot of assumptions making the results unrealistic as opposed to the our numerical experiment approach which is cost effective and more reliable results are obtained. Flow domain is assumed semi infinitely deep and homogeneous and it

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is subdivided into small units called control volumes of uniform dimension. A hybrid of Finite volume and Finite difference methods are used to discretize space and time respectively in the governing PDE. Discretized equations are inverted to obtain the concentrations at various nodes of the control volumes by using mathematical codes developed in Mat-lab and the results presented using graphs at different soil depths and time to determine the parameters that can help detect the contamination levels before disastrous levels are reached and with ease.

From the results it is observed and concluded that the concentration levels of ions with depth and time can easily be detected when diffusion coefficient and advection velocities are linearly depended on time and mitigation strategies can easily be employed.

1. INTRODUCTION

Movement of pollutants from a ground surface of soil through plant root zone to the groundwater is a major pollution to the hydrological environment in the subsurface. This phenomenon has negative impact 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, pesticides, salts and minerals that percolate in soil over time are becoming responsible for soil acidification. Some of the studies conducted on soil acidification include [1] who started off by defining 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. Crop production in the high rainfall areas like in Kenya is constrained by soil acidity and soil fertility depletion as suggested by Kanyanjua et al. [2]. 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. These practices have caused great concern to environmentalists, hydrologists, civil engineers as well as mathematicians.

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. Homogeneous soils are an exceptionally rare case of soil structure as much as the plant root zone can be considered to be almost homogeneous. This is expected in a farmland where the soil columns are often disturbed during land preparation and planting which lead to mixing of different soil layers leaving the transport behaviour to be uniform all through. Homogeneous soils are not only ideal for pure studies but also for developing models that can predict the transport of both organic and inorganic materials when the soil is 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. Hence numerical experiment is a cost effective avenue for obtaining better and reliable results for the PDEs and more so methods based on control volumes.

Flow of contaminated fluids from the soil surface in to the ground water has been studied by many researchers in the past all taking different view point. Myron [3] quoted that water flow in the unsaturated zone is complicated due to the fact that the soil permeability to water depends on its water saturation. Ueoka et al. [4] in their paper cited that fertilizers, pesticides and industrial waste may be small in quantity but highly toxic and can be transported to ground water to remain there for hundreds of years. A chemical becomes a pollutant if its concentration exceed some prescribed water quality standard or soil attains an un-allowable PH after chemicals have been applied. This impairment of beneficial water and soil use has been known to be induced by natural processes and human activities. Specifically, 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 solutes through homogeneous porous media. It has also been modified to incorporate the effects of adsorption, desorption and hysteresis.Various approaches have previously been employed to solve the Advection Dispersion Equations applied to the transport of chemicals through saturated and unsaturated porous media. They include analytical solutions, numerical studies included [5-10] among others.

We need to solve the unsteady advection diffusion equation in which the coefficients are unknown. Researches that have been conducted to identify the unknown coefficients include

studies like identification of the unknown diffusion coefficient in a linear parabolic equation via semi group approach was performed by Demir et al. [11], Identification of coefficients for a parabolic equation where the unknown coefficient depends on an over-specified datum is presented by Trong and Ang [12], Identification of a Robin Coefficient on a non-accessible part of the boundary from available data on the other part is reported by Boulakia et al. [13]. Others include [14,15,16,17]. Coefficients problems are used to estimate values of parameters in a governing equation.

Techniques for remediation of polluted soil and groundwater previously applied include pump-and -treat, using a combination of the optimization methods and simulation models as proposed by Gorelick et al. [18], Hot water flushing [19,20], air sparging [21] Cosolvent flushing [19], the use of surfactants [22], In situ bio-remediation [23]. The effectiveness of the remediation may be substantially improved if the location and extent of the contaminants source are known.

2. 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 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)

$$\frac{\partial C}{\partial t} = \frac{\partial}{\partial z}\left[D_z(z,t)\frac{\partial C}{\partial z} - W(z,t)C \right] + S_o \quad (1)$$

where $C(z,t)$ is the function representing concentration 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 average pore water 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 S_o is the source term 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 analyse the situation where the source term is zero and when the source term is present is left out for further research. In the present case, we need to reconstruct the initial condition $C(z,t) = f(z)$, $t = t_0$ and the flow parameters $D_z(z,t)$ and $W(z,t)$. 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.

3. WELL-POSEDNESS OF THE PROBLEM

Problems expressible in terms of PDE given by equation (1) subject to relevant boundary or initial condition(s) is well posed if a solution exists, the solution is unique and it continuously depends on the data given. We consider the continuous problem above for $0 \leq z \leq 1$, $D_z \geq 0$. The problem is strongly well-posed if the solution is bounded in terms of all the data i.e. the terms are known explicitly. However we can demonstrate the well-posedness by considering the source term and the boundaries on either sides of the domain to be zero using the Energy method.

Take a one dimensional A-D model in equation (1), initial condition $C(z, t_0) = f(z)$ and boundary conditions $C(0,t) = f(t)$ and $C(1,t) = 0$.

Multiply the differential equation by $2C$ for constant $D_z(z,t)$, $W(z,t)$ and $S_0 = 0$ to get

$$2C\frac{\partial C}{\partial t} = 2CD\frac{\partial^2 C}{\partial z^2} - 2CW\frac{\partial C}{\partial z} \qquad (2)$$

Integrating equation (2) over the spatial domain $0 \leq z \leq 1$,

$$\int_0^1 2C\frac{\partial C}{\partial t}dz = \int_0^1 2CD\frac{\partial^2 C}{\partial z^2}dz - \int_0^1 2CW\frac{\partial C}{\partial z}dz \quad (3)$$

$$\frac{d}{dt}\|C\|^2 = 2D\{-C(0,t)C_z(0,z) + C(1,t)C_z(1,t)\}$$
$$+ WC(0,t)^2 - WC(1,t)^2 - \|C_z\|^2$$

Where $\|C^2\| = \int_0^1 C^2 dz$

Given $D = 0$, the differential equation is hyperbolic and we need only one boundary condition. If $W > 0$, $C(0,t) = f(t)$ has to be given; if $W < 0$, $C(1,z) = 0$ has to be given instead. If $W > 0$ and $f(t) = 0$ then

$$\frac{d}{dt}\|C\|^2 = -WC(1,t)^2$$

Assuming a parabolic case where $D \neq 0$ and that we have to give data at both boundaries, inserting the zero boundary data yields,

$$\frac{d}{dt}\|C\|^2 = -2D\|C_z\|^2$$

Time integration of the above two results gives that the original differential equation is well posed in the classical sense assuming that the correct number of boundary condition is used.

4. TIME VARIATION OF ADVECTION VELOCITY $W(z,t)$ AND DIFFUSION COEFFICIENT $D(z,t)$ IN THE ABSENCE OF SOURCE TERM

When the diffusivity $D_z(z,t) = D(t)$ and the flow velocity $W(z,t) = W(t)$ we obtain a particular case to the problem in the equation (1) given by equation (4)

$$\frac{\partial C}{\partial t} = D_z(t)\frac{\partial^2 C}{\partial z^2} - W(t)\frac{\partial C}{\partial z} \qquad (4)$$

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

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

(i) Constant advection velocity $W(z,t) = W_0$
(ii) Advection velocity is a linear function of time $W(z,t) = W_0(at + b)$

where a is the rate at which the flow velocity is varying with time and b is the initial velocity at time $t = 0$

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

(iii) Constant Diffusion coefficient $D(z,t) = D_0$
(iv) Diffusion coefficient is a linear function of time $D(z,t) = D_0(at + b)$

where a is the rate at which solutes diffusion is varying with time and b is the initial solutes diffusion at time $t = 0$ and W_0 and D_0 are constant values.

5. DISCRETIZATION OF THE GIVEN SPACE AND TEMPORAL DOMAIN

Finite volume method developed by Pantanker and Spalding in 1972 involves subdivision of the flow domain into infinitesimal volumes called control volumes and representation of the differential equations in integral form. 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 discretized equation. Discrete values are estimated at the centre of the control volume of the domain after implementing the prescribed initial and boundary conditions.

Taking the discretized flow domain illustrated in Fig. 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 dimension, the thickness $\Delta x = \Delta y = 1$ thus the control volume reduces to Δz. C_A and C_B are the conditions at the western and eastern boundaries of the control volume respectively that can be assumed to be known or unknown and thus need to be determined. When C_A and C_B 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. Specifically C_A is condition prevailing at the surface of the soil and C_B is representing the condition deep down in the flow domain. This study will test the validity of chosen functions C_A and C_B numerically.
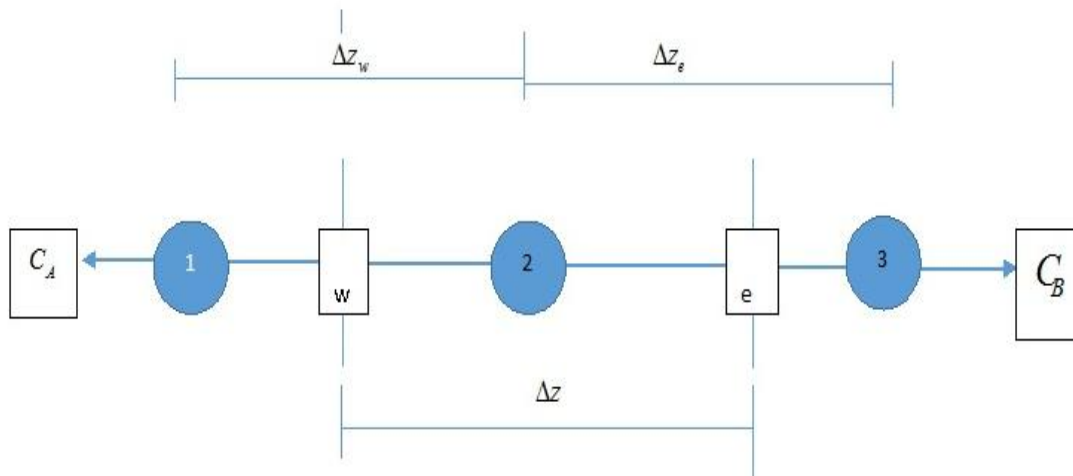

Fig. 1. Discretised one dimensional domain into control volumes of width Δz

With no loss of generality we focus on flow of fertilizer represented by smooth function $C(z,t)$ in porous medium assumed to have uniform structure in the solution domain.

6. DISCRETISATION OF GOVERNING EQUATION WHEN FLOWPARAMETERS $W(z,t) = W_0$ AND $D(z,t) = D_0$ ARE CONSTANT

The conservation law applies to each domain and equation (4) integrated over the ith control volume over the time interval from t_{j-1} to t_j and assuming the dimensions of the control volume Δx and Δy are unity, the following procedure is observed

$$\int_{cv}\left\{\int_{t_{j-1}}^{t_j} \frac{\partial C}{\partial t} dt\right\}dz = \int_{t_{j-1}}^{t_j}\left\{\int_{cv}\left[D_z \frac{\partial^2 C}{\partial z^2} - W \frac{\partial C}{\partial z}\right]dz\right\}dt \tag{5}$$

The discretized equation for the central control volumes is

$$\left(\frac{D_z}{\Delta z} + \frac{W}{2}\right)C_{i-1,j} + \left(-2\frac{D_z}{\Delta z} - \frac{\Delta z}{\Delta t}\right)C_{i,j} + \left(\frac{D_z}{\Delta z} - \frac{W}{2}\right)C_{i+1,j} = -\frac{\Delta z}{\Delta t}C_{i,j-1} \tag{9}$$

Using the notations $B = \frac{D_z}{\Delta z} - \frac{w}{2}$, $E = \frac{D_z}{\Delta z} + \frac{w}{2}$, $G = \frac{D_z}{\Delta z}$, $HH = \frac{\Delta z}{\Delta t}$ in equation (9),we obtain

$$EC_{i-1,j} + (-2G - HH)C_{i,j} + BC_{i+1,j} = -HHC_{i,j-1} \tag{10}$$

In order to guarantee that the numerical scheme is stable, we have to make sure that the matrix is symmetric, diagonally dominant and real, with non- negative diagonal entries then the matrix is positive definite.

7. LINEAR VARIATION IN $w(z,t) = w_0(at + b)$ AND $D(z,t) = D_0(at + b)$ WITH TIME

Here we consider a case where the diffusivity and advection velocity are linear functions of time as $w(z,t) = w_0(at + b)$ and $D(z,t) = D_0(at + b)$, a and b are constants. The a in the linear function above is used to denote the rate at which the advection velocity and solutes diffusion are varying with time whereas b defines the initial velocity and diffusion coefficient at time $t = 0$.

Integrating over the control volume and over the time interval from t_{j-1} to t_j we see that equation (4) will give

The velocity field must satisfy the mass conservation law and the continuity equation becomes

$$\frac{dW}{dz} = 0 \tag{6}$$

Equation (5) becomes

$$\Delta z \int_{t_{j-1}}^{t_j} \frac{dC}{dt}dt = \left\{\left[D_z \frac{dC}{dz}\right]_e - \left[D_z \frac{dC}{dz}\right]_w - (WC)_e + (WC)_w\right\}dt \tag{7}$$

From this result we have the first order and zeroth order derivatives for the diffusion and advection terms respectively in the conservation law. This reduction of the order of the derivative is important in dealing with situations which change so rapidly in space that the spatial derivative does not exist. The diffusion coefficient and advection velocity are taken to be uniform on either sides of the control volume thus equation 5 reduces to

$$\frac{\Delta z}{\Delta t}[C(z_p,t_j) - C(z_p,t_{j-1})] = D_z\left[\frac{dC}{dz}_e - \frac{dC}{dz}_w\right] - w(C_e - C_w) \tag{8}$$

$$\Delta z \left[C_{i,j} - C_{i,j-1} \right] = \left[\frac{D_0}{2} \left(t_j^2 - t_{j-1}^2 \right) + D_0 b \left(t_j - t_{j-1} \right) \right] \left(\frac{dC}{dz}_e - \frac{dC}{dz}_w \right) - \left[\frac{w_0}{2} a \left(t_j^2 - t_{j-1}^2 \right) + w_0 b \left(t_j - t_{j-1} \right) \right] \left(C_e - C_w \right)$$

This reduces to

$$\Delta z \left[C_{i,j} - C_{i,j-1} \right] = \left[\frac{D_0}{2} a \Delta t \left(t_j + t_{j-1} \right) + D_0 b \Delta t \right] \left(\frac{dC}{dz}_e - \frac{dC}{dz}_w \right) - \left[\frac{w_0}{2} a \Delta t \left(t_j + t_{j-1} \right) + w_0 b \Delta t \right] \left(C_e - C_w \right)$$

(11)

which represents the general discretised equation in this case. The central nodes give

$$\left[\frac{D_0 \Delta t}{\Delta z} - \frac{w_0 \Delta t}{2} \right] \left[\frac{a}{2} \left(t_j + t_{j-1} \right) + b \right] C_{i-1,j} - \left[2 \frac{D_0 \Delta t}{\Delta z} \left[\frac{a}{2} \left(t_j + t_{j-1} \right) + b \right] + \Delta z \right] C_{i,j}$$

$$+ \left[\frac{D_0 \Delta t}{\Delta z} - \frac{w_0 \Delta t}{2} \right] \left[\frac{a}{2} \left(t_j + t_{j-1} \right) + b \right] C_{i+1,j} = -\Delta z C_{i,j-1}$$

(12)

8. RESULTS AND DISCUSSION

Both linear and non- linear mass transport equation are used to determine flow characteristics of pollutants in soils.

A one dimensional ADE is considered in which the coefficients were first taken constant. A variation was also made whereby both parameters are time dependent. The argument here is that as time increases then the $D_z(z,t)$ and $w(z,t)$ are also changing at varied depths in the soil until a point of saturation is reached. Advection and diffusion processes are playing a key role in determination of the concentration at different levels in soils at different times. Here we have considered advection effect higher than diffusion. This is because fluids percolate deep into soil due to their bulk motion after irrigation or a downfall and slows down due to soil saturation. The level of wetness varies from surface soil downwards. Now when solutes are applied in form of fertilizers, upon dissolving, they move away from the point of application to points of low concentration in a diffusive manner. To the contrary when $D_z(z,t)$ dominates the flow, it means that the solutes are being applied to already water logged soils and advection velocity is negligible. We are referring to nitrogenous fertilizers highly responsible for soil acidification and are applied to growing plants thus diffusion here is taking place where advection is present.

The results are presented in form of graphs and discussions are made here under.

In the Fig. 2 below flow parameters $D_z(z,t)$ and $w(z,t)$ are taken constant from time to time. This means even as time or depth changes, the two parameters remain unchanged, with advection playing a significant role in the transport of solutes as opposed to diffusion which takes a less value. The curve for z = 0.25 in Figs. 2 and 3 represents the first level in the flow domain. It is steep at the beginning then starts levelling near the concentration levels of 0.35. It means that this level is closer to the surface where application of fertilizers and other human activities are taking place. This level receives solutions containing pollutants first and attains saturation first and faster as opposed to other levels in the domain. It takes longer to attain saturation level for Fig. 3 compared to Fig. 2. Here $w(z,t) = w_0(at+b)$ and $D(z,t) = D_0(at+b)$ are increasing at a constant rate though less than when $W(z,t) = W_0$ and $D(z,t) = D_0$ are constants.

The zone z=0.5 is midway the depth of the semi - infinite flow domain. As advection continues to take place, less pollutants reach this zone and consequently takes longer to reach saturation level. Less pollutants reach the level z = 0.75. There is minimal pollution at the level z = 1.0 because the flow domain is assumed to be semi-infinite, thus this is the zone of semi- infinite depth it may take longer than the considered time.

In Figs. 4 and 5, concentration is taken to be a function of space/ depth. At time t = 0, the concentration is taking a maximum value of 1. As time increases by one step, pollution downwards decreases. It reduced to a non-dimensional depth of 0.4 in Fig. 5 and 0.5 in Fig. 4. Diffusion and advection are higher in Fig. 4 than in Fig. 5. Fig. 4 can be linked to soils with bigger pore spaces than those demonstrated by Fig. 5. A similar behaviour is noted in the other time levels where higher levels concentration variation with depth are notable in Fig. 4 than in Fig. 5. This shows that early control of pollution can easily be carried out before it sinks deep in to unreachable levels in situations where the flow parameters are linearly depended on time.
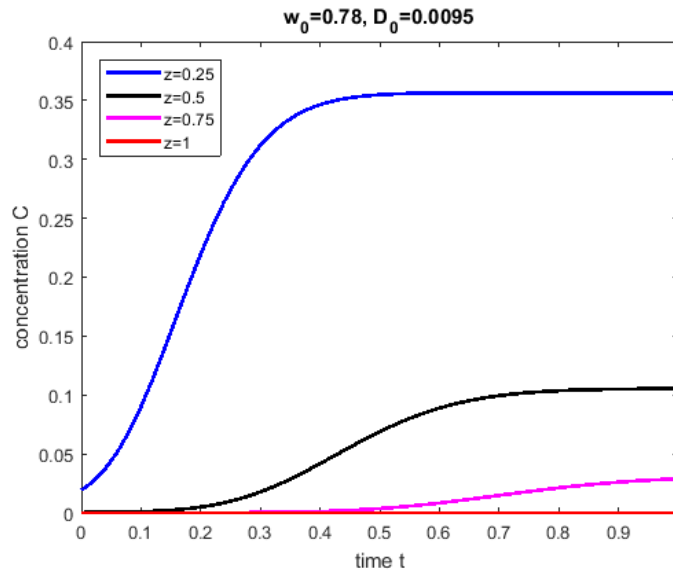

Fig. 2. Non- dimensional concentration C against time t at different depths when W (z,t) and D(z ,t) are constants
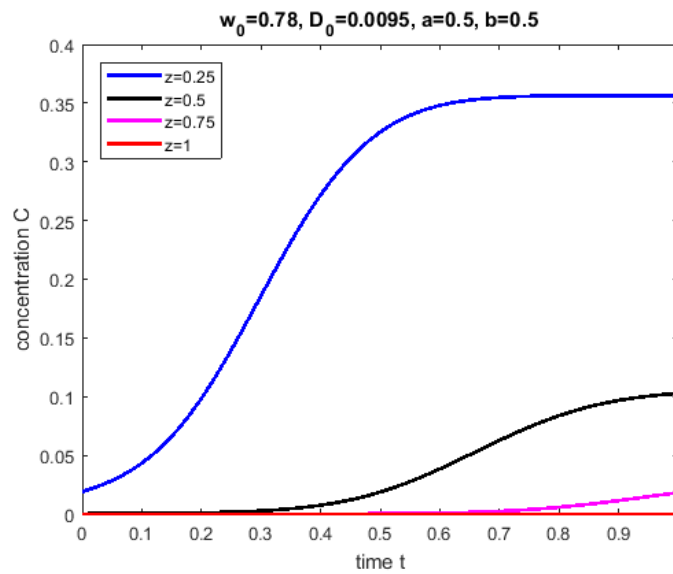

Fig. 3. Non-dimensional concentartion C against time t at varied depths z when D(z,t) and W(z,t) are linear functions of time
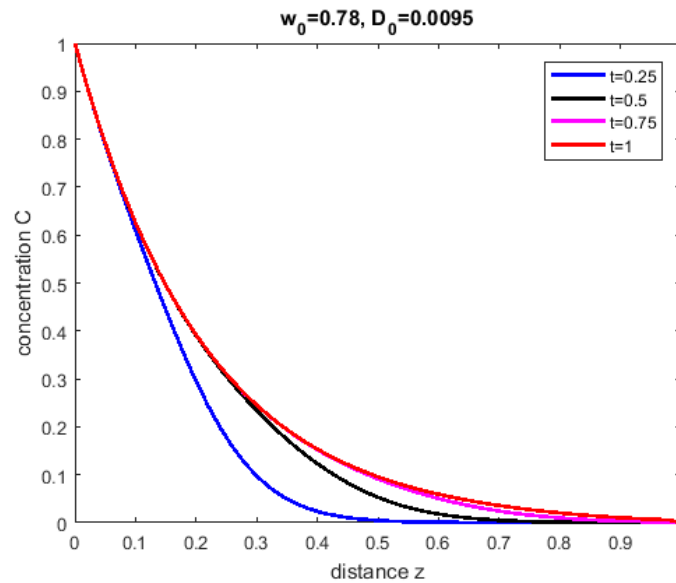
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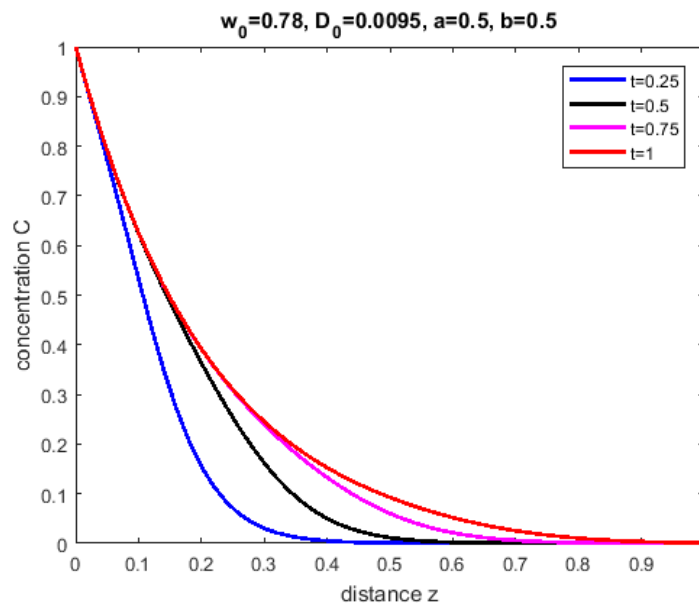**Fig. 4. Non dimensional C against depth z when D (z, t) and W (z,t) are constants**

Fig. 5. Non dimensional Concentration C against depth z for varied time when D(z,t) and W(z,t) are linear functions of time

9. CONCLUSION AND RECOMMENDA-TIONS

In this paper we considered a mathematical transport model 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 analysed constants and linear functions of time. A comparison was also made for concentration with respect to depth and also time for varied diffusion coefficients and advection velocity in order to provide advice to all with interest on

remediation strategies. Diffusion coefficient and advection velocity were varied with respect to time. Analysis performed with the help of graphs to determine how they will influence the transport of acids from the soil surface to unreachable levels in the ground. It was noted that for soils that allow pollutants to diffuse linearly with time take more time to reach saturation at the surface of the soil thus mitigation strategies can be employed to reduce on the rate of flow of more chemicals deep in to the soil. It is important to note that neutralization or extraction of pollutants can easily be performed in regions near the surface unlike when the pollutants have penetrated deep down to lower levels even though in small quantities. As a matter of policy, measures should be taken when fertilizers are been used in order to determine these two important flow parameters for the specific soil structures. This will help identify the best position to place the pollutants detectors as well as neutralizers. This can also help determine how to change the flow parameters for specific soils.

A lot more can be extended on the present work by considering the following:

i) Analysis of the flow parameters which are exponentially depended on time
ii) Experimental determination of the flow parameters for one dimensional domain.
iii) Analysis of the flow parameters when the soil structure is heterogeneous.

It is our intention to carry our further research in one or more areas cited above though other researchers are encouraged to carry out investigations on the same.

COMPETING INTERESTS

Authors have declared that no competing interests exist.

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