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Contaminant transportation modelling with time dependent dispersion

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Abstract

A mathematical modeling of contaminate transportation has been presented in the current paper. The time-dependent dispersion has been considered in the transportation of contaminant in a finite homogeneous porous medium. The study of contaminants concentration has been presented for the uniform unsteady flow of groundwater. Instead of a constant dispersion, in order to consider the effect of groundwater velocity on contaminant transportation, dispersion has been considered as a groundwater velocity-dependent quantity. As found in the many practical aspects, a linear increase in concentration at a source point with time has been assumed for the present modeling. The spread of the initial contaminant concentration has been considered linearly decreasing along the direction of one-dimensional flow. The contaminant transport equation for the above-mentioned conditions and environment has been solved. The Laplace transform variation iteration method (LVIM) has been adopted to obtain a solution. Spatial and temporal variations of concentration for a developed model have been presented graphically by varying dispersion. The LVIM has been found suitable for the present study of contaminant transport modeling. The MATHEMATICA package has been used for the present study.

Keywords. Contaminant transport, Correlation function, Laplace transform variational iteration method.

2010 Mathematics Subject Classification. 35G16, 35A15, 35C05, 44A10.

1. Introduction

The quality of groundwater has become a serious concern in the last few decades due to pollution. The very less availability of fresh water draws additional attention to the necessary measures those to be taken to deal with the said issue. The current scenario suggests that rigorous actions must be taken in order to prevent panic conditions regarding the quality of groundwater. Scientific research, including theoretical study, may provide a way out of a current situation of the global ecological problem. The mathematical modeling representing the phenomenon of contaminant transport can be a part of such a study. It can throw light on many aspects of groundwater study. A carefully designed mathematical model for contaminant transport can predict the futuristic condition of the groundwater. The analysis of such a model can be helpful for deciding preventive measures in advance. A large number of efforts have already been made for the study of groundwater quality [1, 4, 22, 23].

The study of problems arising in single-phase and multi-phase flow through porous media has been given by Narendrasinh Desai [2]. Mitesh Joshi *et. al.* [13] have obtained a solution of Burger's equation using the group theoretical method. Authors [13] have considered a longitudinal dispersion in miscible phase flow through porous media. Leo *et. al.* [16] have provided an analysis of contaminant migration in homogeneous medium. A boundary element method has been used by the authors [16] for solving the advection dispersion equation in their study. A numerical method for solving variable-order solute transport models has been given by Uddin *et. al.* [30]. The solution of fractional variable-order solute transport type models using radial basis function has been obtained in the study. The Volterra

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integro-differential equation of convolution type has been studied by Uddin *et. al.* [26]. Laplace transform and Quadrature rule with high order accuracy have been adopted by authors [26] to obtain the results. Uddin *et. al.* [31] have given the Laplace-transformed-based local meshless method for time fractional diffusion equation. Laplace transform together with the local kernel method has been proposed in their research. Computational study on the dynamics of fractional order differential equations with applications has been provided by Shah *et. al.* [27]. In their research, they have included existence theory stability and numerical analysis for fractional order systems. Shah *et. al.* [25] have given a numerical solution of variable order partial differential equation using a spectral method. The algebraic equations have been obtained from proposed equations using concepts of operational matrices. Two-dimensional coupled partial differential equations have been converted into a system of non-linear ordinary differential equations using a group theoretical method by Ali *et. al.* [26]. The Haar wavelets method has been used in the study.

Contaminant transport in fractured and non-fractured porous medium has been explained by Leo and Booker [17]. They obtained the solution using the boundary element technique. An analytic solution and sensitivity study of contaminant transport in fractured media has been given by David Ching Fang Shih *et. al.* [28]. Authors[28] have considered pulse, Dirac delta, and sinusoidal input sources. A numerical study of the effects of soil heterogeneity on contaminant transport in unsaturated soil has been given by Mousavi *et. al.* [20]. In their research, they described the mathematical framework and numerical implementation of the model. Ching and Shih [28] have derived the semi-analytic solution of one-dimensional contaminate transport equation using the Laplace transform and its numerical inverse. Their work is focused on radioactive nuclides with three-member decay chains in a single fracture for pulse and Heaviside input sources. Using variation's theory Ji-Huan He [5–9, 11] developed a Variation iteration method (VIM) for solving linear and non-linear differential equations. A study on a general numerical algorithm for non-linear differential equations by the variational iteration method presented by Ji-Huan He *et. al.* [10] proves the effectiveness of the method. The convergence results have also been provided with proof in the research. A study on the convergence of the variational iteration method has been given by Odibat [21]. The convergence of the VIM has been studied by the researcher in his research for non-linear differential equations. The convergence results are presented as well as verified by illustrating various problems to prove the efficiency of the method. Variation iteration method along with Laplace transform made VIM easier. Laplace transform variation iteration method (LVIM) is applied by many researchers [14, 15, 29, 34] in many fields of science and engineering and it showed the efficiency of LVIM. Matinfar *et. al.* [18] presented a paper on the combined Laplace-Variational Iteration Method for partial differential equations. Authors obtained approximate analytic solutions of linear and non-linear partial differential equations and also studied the convergence of the LVIM.

In the present research, the behavior of the contaminant transport in groundwater through porous media has been studied. The porosity of the medium is not change with space variables i.e., the medium is homogeneous. The concentration of the contaminant is predicted for a finite medium. The flow of the groundwater is considered as uniform and unsteady. As the medium is homogeneous, dispersion is not varying with the space variable. The variation in dispersion is considered as temporal. Initially, the medium is not solute free. The concentration exponentially decreases with a space variable at the initial time. At the source point concentration is linearly increasing with time. The mathematical formulation of the problem is given in section 2. Section 3 gave the brief idea of the adapted method and an analytic solution of contaminate transport equation with the said condition derived using LVIM is given in section 4. A graphical representation of the obtained solution is given in section 5 with a conclusion in section 6.

2. Mathematical formulation

Advection is a process by which the dissolved solids are transported with the flowing groundwater. The amount of solute transported by the advection process is a function of the quantity of groundwater flowing and the concentration of solute in the groundwater.
The mathematical formulation of the flow of a liquid through a sample volume element is provided by Freeze and Cherry [3]. To provide a better understanding to the readers of the present article it is included in the following section. Figure 1 [3] shows the elementary volume through which the solute is transported. The fluid flow through mass flux

(F_x) due to advection will be $F_x = ucn$ [3] where, u, c and n are the average linear velocity of water in a porous matrix, the concentration of contaminant in groundwater and effective porosity of the porous matrix respectively. The solute

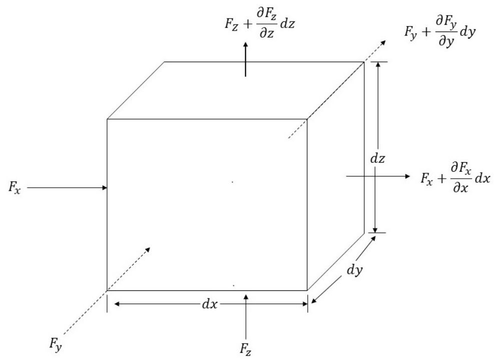

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FIGURE 1. Fluid flow through volume element.

entering into the control volume ($dxdydz$) in x-direction due to advection is $u_x ncdydz$ [3]. While the solute entering to the control volume in x-direction due to dispersion is $nD_x \frac{\partial c}{\partial x} dydz$ [3].
Now, total mass of solute transported per unit cross sectional area by advection and dispersion in x, y and z direction can be written as [3],

$$F_x = u_x nc - nD_x \frac{\partial c}{\partial x},$$
$$F_y = u_y nc - nD_y \frac{\partial c}{\partial y},$$
$$F_z = u_z nc - nD_z \frac{\partial c}{\partial z}.$$

Total mass of solute entering the representative elementary volume ($dxdydz$) in x-direction is $F_x dydz$ [3].
Total mass of solute leaving the representative elementary volume ($dxdydz$) in x-direction is $\left(F_x + \frac{\partial F_x}{\partial x} dx\right) dydz$ [3].
Net solute mass flux in x, y and z direction become $-\frac{\partial F_x}{\partial x} dxdydz$, $-\frac{\partial F_y}{\partial y} dxdydz$ and $-\frac{\partial F_z}{\partial z} dxdydz$ [3].
Hence, the total net flux of the representative elementary volume ($dxdydz$) is $n\frac{\partial c}{\partial t} dxdydz$ [3].
As per the law of conservation of mass, net mass flux is equal to the rate of change in mass stored in control volume in time dt is [3],

$$n\frac{\partial c}{\partial t} = -\left(\frac{\partial F_x}{\partial x} + \frac{\partial F_y}{\partial y} + \frac{\partial F_z}{\partial z}\right).$$

Replacing the values of F_x, F_y, F_z and considering n as constant, obtained equation is

$$\frac{\partial c}{\partial t} = \frac{\partial}{\partial x}\left(D_x \frac{\partial c}{\partial x}\right) + \frac{\partial}{\partial y}\left(D_y \frac{\partial c}{\partial y}\right) + \frac{\partial}{\partial z}\left(D_z \frac{\partial c}{\partial z}\right) - \frac{\partial}{\partial x}(u_x c) - \frac{\partial}{\partial y}(u_y c) - \frac{\partial}{\partial z}(u_z c). \tag{2.1}$$

Which is the contaminant transport equation for conservative solute transport in porous media. Where D_x, D_y and D_z are dispersion coefficients along x, y and z directions respectively. u_x, u_y and u_z are the velocities of the flow along x, y and z directions respectively and c is the solute concentration.
The one-dimensional solute transport equation with a variable coefficient and initial concentration is linearly decreasing with space variable is developed. As the containment dumped at a source point gradually disperse through the porous media, a concentration is highest at the source point at the initial time. This means that the concentration decreases with a distance from the source point at the initial time. Due to the dumping of domestic or other waste at the source point, the contaminant concentration entering into the groundwater at a source point continuously increases.

Therefore, it is required to incorporate such an increase in the model. The contaminant concentration in the porous medium at any time t[T] is denoted by $c(x,t)$ with dimension $[ML^{-3}]$. The solute particles are also transported along with groundwater. The velocity of groundwater is $u[LT^{-1}]$ in the porous medium and $D[L^2T^{-1}]$ is the solute dispersion.
Mathematical formulation of the proposed model is written as,

$$\frac{\partial c}{\partial t} = \frac{\partial}{\partial x}\left(D\frac{\partial c}{\partial x}\right) - \frac{\partial}{\partial x}(uc), \tag{2.2}$$

with initial and boundary conditions,

$$c(x,0) = c_0(1-mx), \quad x \geq 0, \tag{2.3}$$

$$c(0,t) = c_0(1+bt), \quad t \geq 0, \tag{2.4}$$

$$\frac{\partial c(x,t)}{\partial x} = -m, \quad t > 0, \tag{2.5}$$

where $m[L^{-1}]$ is a constant parameter and $c_0[M/L^3]$ is an initial constant concentration. Parameter $b[T^{-1}]$ is a coefficient that decides linearly increasing rate which is fixed.
Due to the equally spaced alignment of the pores in a homogeneous medium, the velocity of the flow remains constant along the space variable. Further, the unsteady flow of the groundwater is considered. In other words, the flow velocity (u) is considered time-dependent. In a present study, the flow velocity u is assumed as follows

$$u(x,t) = u_0(1-at),$$

where u_0 is the initial velocity and a show the rate at which the flow velocity decreases with time (t) and $a < 1$. The flow velocity can affect the dispersion of the contaminant. The dispersion coefficient (D) is directly proportional to the flow velocity (u) [24, 33] and so the dispersion coefficient changes with flow velocity (u) where (u) is linearly decreasing with the time as given below

$$D(x,t) \propto u(x,t), \tag{2.6}$$
$$D(x,t) = ku_0(1-at), \tag{2.7}$$
$$D(x,t) = D_0(1-at), \tag{2.8}$$

where $D_0 = ku_0$ and k is the longitudinal dispersivity. Equation (2.2) can be written as

$$\frac{\partial c}{\partial t} = \frac{\partial}{\partial x}\left(D(x,t)\frac{\partial c}{\partial x}\right) - \frac{\partial}{\partial x}(u(x,t)c),$$

$$\frac{\partial c}{\partial t} = D_0(1-at)\frac{\partial^2 c}{\partial x^2} - u_0(1-at)\frac{\partial c}{\partial x}. \tag{2.9}$$

Using dimensionless variables,

$$T = \frac{u_0^2 t}{D_0}, \quad X = \frac{u_0 x}{D_0}, \quad C = \frac{c}{c_0},$$
$$A = \frac{aD_0}{u_0^2}, \quad M = \frac{mD_0}{u_0}, \quad B = \frac{bD_0}{u_0^2}. \tag{2.10}$$

Using equation(2.10) into equation (2.9) and using chain rule to partial derivatives, equation (2.9) can be written into dimensionless form as

$$\frac{u_0^2 c_0}{D_0}\frac{\partial C}{\partial T} = D_0(1-AT)\frac{u_0^2 c_0}{D_0^2}\frac{\partial^2 C}{\partial X^2} - u_0(1-AT)\frac{u_0 c_0}{D_0}\frac{\partial C}{\partial X},$$

$$\frac{\partial C}{\partial T} = (1 - AT)\frac{\partial^2 C}{\partial X^2} - (1 - AT)\frac{\partial C}{\partial X}. \tag{2.11}$$

Initial condition (equation (2.3)) and boundary conditions (equations (2.4) and (2.5)) can be rewritten as,

$$C(X, 0) = 1 - MX, \quad X \geq 0, \tag{2.12}$$

$$C(0, T) = 1 + BT, \quad T \geq 0, \tag{2.13}$$

$$\frac{\partial C(X, T)}{\partial X} = -M, \quad T > 0. \tag{2.14}$$

Laplace transform has been used by Jaiswal*et. al.* [12] to give an analytic solution of a one-dimensional advection-dispersion equation in a semi-infinite medium. In their research, it is assumed that dispersion is proportional to the square of velocity and velocity is increased with space variable. The independent variable is reduced by one from governing equation using transformation and then the analytic solution is obtained by Laplace transform. In their research, the solute concentration is obtained at different distances from the source point. The results clearly show that the solute concentration is decreasing with the space variable ($0 < x < 1$) and increases with time. AJ Mohamad-Jawad *et. al.* [19] have solved linear and non-linear partial differential equations using VIM. The closed form of the exact solution of a non-linear homogeneous gas dynamic equation is obtained. A non-linear Burgers equation and the linear one-dimensional heat transfer equation are also analyzed using VIM. The graphical representations are included in the form of the results of the study. The successful applicability of VIM has been proved through the results for gas dynamic, Burgers and heat transfer equations under some conditions. The exact solution of the Cauchy problem, transport equation, non-homogeneous Cauchy problem, and inviscid Burgers equation is given by XW Zhou *et. al.* [35]. The authors concluded the above equations can provide an insight into different mathematical problems that include partial differential equations. Hence, looking at the above results of different researchers, the VIM together with the Laplace transform encourage us to apply it for the present research as it provides a less complicated way of study and has a scope to generate more precise results.

3. Methodology

Consider a non-linear differential equation

$$lu(x, t) + Nu(x, t) = f(x, t), \tag{3.1}$$

where l is a linear operator, N is a non-linear operator and $f(x, t)$ is a known analytical function. According to the variational iteration method, a correction functional constructed as,

$$u_{n+1}(x, t) = u_n(x, t) + \int_0^t \bar{\lambda}(x, \xi)[lu_n(x, \xi) + N\bar{u_n}(\xi) - f(x, \xi)]d\xi, \tag{3.2}$$

where λ is a general Lagrange multiplier, which can be identified optimally via the variational theory. The subscript n denotes the n^{th} approximation and $\bar{u_n}$ is a restricted variation $\delta\bar{u_n} = 0$.

Operating with Laplace transform on both sides of equation (3.2) the correction functional will be constructed in the following manner:

$$L[u_{n+1}(x, t)] = L[u_n(x, t)] + L[\int_0^t \bar{\lambda}(x, t - \xi)[lu_n(x, \xi), \quad n = 0, 1, 2, 3, ... \tag{3.3}$$

Using convolution theorem,

$$L[u_{n+1}(x, t)] = L[u_n(x, t)] + L[\bar{\lambda}(x, t)]L\left[lu_n(x, t) + N\bar{u_n}(x, t) - f(x, t)\right]. \tag{3.4}$$

Take the variation with respect to $u_n(x, t)$ and hence upon applying the variation this simplifies to

$$L[\delta u_{n+1}(x, t)] = L[\delta u_n(x, t)] + \delta[L[\bar{\lambda}(x, t)]L[u_n(x, t)]]. \tag{3.5}$$

Applying the inverse Laplace transform to equation (3.5) and using variational theory, the value of Lagrange multiplier is obtained.

4. Analytic solution using LVIM

The Laplace variational iteration correction functional of equation (2.11) will be constructed as,

$$\begin{aligned} L[C_{n+1}(X,T)] &= L[C_n(X,T)] + L[\int_0^T \bar{\lambda}(X,T-\xi)[(C_n)_T(X,\xi) - (1-AT)((\bar{C_n}))_{XX}(X,\xi) \\ &\quad +(1-AT)[(\bar{C_n})_X(X,\xi)]]d\xi, \end{aligned} \tag{4.1}$$

$$\begin{aligned} L[C_{n+1}(X,T)] &= L[C_n(X,T)] + L[\bar{\lambda}(X,T)]L[(C_n)_T(X,T) - (1-AT)((\bar{C_n}))_{XX}(X,T) \\ &\quad +(1-AT)[(\bar{C_n})_X(X,T)]. \end{aligned} \tag{4.2}$$

Taking the variation with respect to $C_n(X,T)$ of equation (4.2), and use the extreme condition $\delta C_{n+1}(X,T) = 0$ obtain result is,

$$\bar{\lambda}(X,T) = -1. \tag{4.3}$$

Using equations (4.2) and (4.3) obtained result is,

$$\begin{aligned} L[C_{n+1}(X,T)] &= L[C_n(X,T)] + L[(-1)]L[(C_n)_T(X,T) - (1-AT)(C_n)_{XX}(X,T) \\ &\quad +(1-AT)(C_n)_X(X,T)] \end{aligned} \tag{4.4}$$

Let the initial approximation is,

$$C_0(X,T) = C(X,0) = 1 - MX. \tag{4.5}$$

Using equation (4.4) ,

$$L[C_1(X,T)] = L[C_0(X,T)] + L[-1]L[(C_0)_T - (1-AT)(C_0)_{XX} + (1-AT)(C_0)_X]. \tag{4.6}$$

Using equation (4.5),

$$L[C_1(X,T)] = L[1-MX] + L[-1]L[(1-MX)_T - (1-AT)(1-MX)_{XX} + (1-AT)(1-MX)_X]. \tag{4.7}$$

Applying the inverse Laplace transform to equation (4.7), obtained result is

$$C_1(X,T) = 1 + M\left(T - \frac{AT^2}{2} - X\right). \tag{4.8}$$

Applying the boundary condition (equation (2.13)) to equation (4.8), the value of parameter A is given by

$$A = \frac{2\alpha}{T} \quad \textit{where} \quad \alpha = 1 - \frac{B}{M}. \tag{4.9}$$

Equation (4.8) can be written as

$$C_1(X,T) = 1 + M\left[(1-\alpha)T - X\right]. \tag{4.10}$$

Using Mathematica, next two iterations are given by,

$$C_2(X,T) = 1 + M\left[(1-2\alpha)T - X\right], \tag{4.11}$$

$$C_3(X,T) = 1 + M\left[(1-2\alpha)T - X\right]. \tag{4.12}$$

The iteration $C_2(X,T)$ and $C_3(X,T)$ are coincide and also reaming. The analytic solution of equation (2.9) is given as

$$c(x,t) = 1 + t\left(2b - \frac{dm}{k}\right) - mx. \tag{4.13}$$

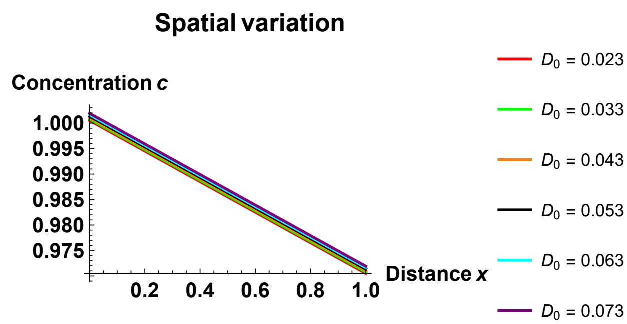

FIGURE 2. Spatial variation of concentration (c) with dispersion coefficient (D_0).

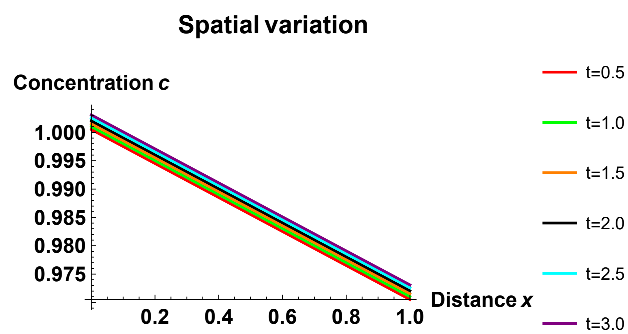

FIGURE 3. Spatial variation of concentration (c) with time (t).

5. Result and Discussion

The concentration profile of contaminate transport equation (2.9) together with equation (4.13) for linearly increasing concentration at a source point is graphically present in Figures 2 and 3. The contaminant concentration is found for six different values of dispersion coefficient D_0 $(km^2/year)$ (i.e. $D_0 = 0.022, 0.033, 0.043, 0.053, 0.063, 0.073$). The flow velocity is assumed as $u_0 = 0.03$ $(km/year)$ and the initial concentration as $c_0 = 1$. Initially, the concentration is decreasing with a constant parameter $m = 0.03$ (km^{-1}). The linearly increasing rate of the concentration at a source point is taken as $b = 0.0010$ $(year^{-1})$, $k = 0.7$ and $l = 1$.

As shown in Figure 2 the contaminant concentration is found in a finite domain $x = 0$ to $x = 1.0$ (km) at the fixed time $t = 0.5$ $(year)$ for six different values of dispersion coefficient. The concentration is decreasing with the space variable for all six dispersion values. Further, it is also clear from the Figure 2 that the concentration is found to increase with an increase in the dispersion. Figure 3 shows the concentration profile for six values of time (t) (0.5, 1.0, 1.5, 2.0, 2.5, 3.0) for fixed $D_0 = 0.023$. The concentration decreases with the space variable for all six values of time (t). Out of the six values of time for which the plots have been given, the highest concentration is obtained at $t = 3.0$, whereas the lowest concentration is obtained at $t = 0.5$. Thus, the concentration is increasing with time in the depicted boundary of space.

Figure 4 shows the variation in the concentration (c) with the time $t = 0$ to 1.0 $(year)$. All the parameters in the calculation are taken equally as in the spatial variation. The contaminant concentration (c) is derived with fixed $x = 0.5$ (km). In order to depict the effect of dispersion on concentration variation, the plots for the concentration (c) vs. time (t) have been given for the same six dispersion (D_0) as in the case of spatial variation of concentration. As in the natural conditions, presently the concentration is also obtained linearly increases with time. Moreover,

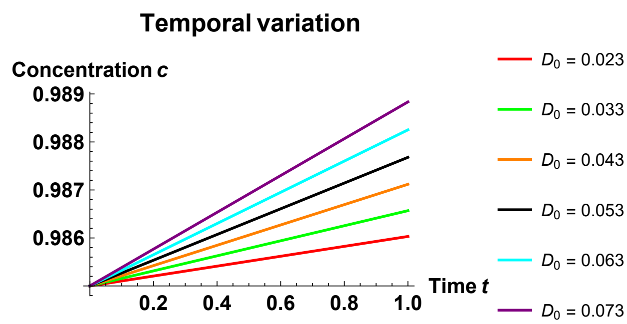

FIGURE 4. Temporal variation of concentration (c) with dispersion coefficient (D_0).

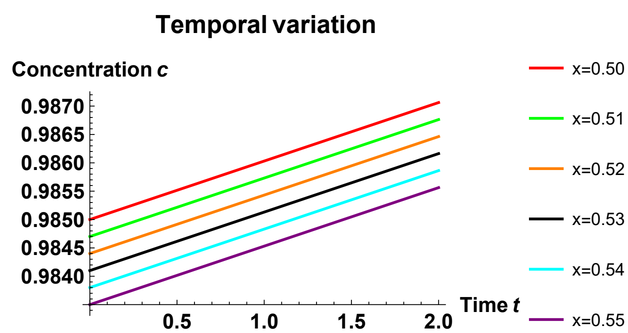

FIGURE 5. Temporal variation of concentration (c) with space variable (x).

concentration is found to increase with dispersion.

Figure 5 shows the temporal variation of concentration with time for six different values of space variable (x) (0.50, 0.51, 0.52, 0.53, 0.54, 0.55) with fixed $D_0 = 0.023$. The concentration (c) is found increasing with time (t). Moreover, the highest concentration (c) is obtained at ($x = 0.50$) and lowest at ($x = 0.55$). Comparing all lines of the plots for different x's, it is clear that lower the x, higher the concentration (c). In order to show the combined effect of space (x) and time (t) on the concentration, 3D plot is provided in Figure 6. Initially ($t = 0$) at source point ($x = 0$), the concentration of the contaminant is $c_0 = 1$. As it can be seen from the concentration profile of contaminant concentration given in Figure 6, the blue colour represents a lower concentration value, whereas the red colour represents a higher concentration. Thus, at a given time (t), c decreases with x. Using the 3D plot, it is clearly observed that this holds true for all values of t from $0 < t < 1$. Further, Figure 6 also shows that at any point at a distance $0 < x < 1$ from a source point, the contaminant concentration (c) increases as the time laps.

6. CONCLUSION

A mathematical model of one-dimensional contaminant transport through a finite homogeneous porous medium has been presented in this research. The said model is proposed for the situation where the dispersion is linearly proportional to flow velocity and decreases with time. Initially, a linearly decreasing concentration with space is assumed. Further, the increase in the concentration of the containment is taken increasing with the time at a source point. Application of the LVIM method for solving the containment transport in the presently depicted situation has been given in the present work. The solution of the equation has been provided using LVIM without any transformation and without converting it into an ordinary differential equation. The concentration variation with the space and time at different dispersions have been presented through the manuscript. The behavior of the contaminate concentration in

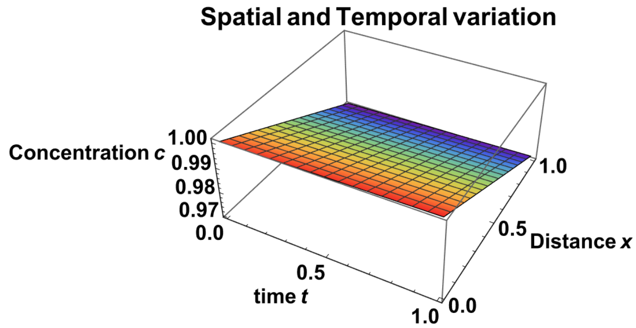

FIGURE 6. Temporal variation of concentration (c) with space variable (x).

obtained solution gives the idea for the prediction of dispersed pollutants in groundwater under certain conditions. The present study opens the scope for future research on the contaminant transport study in various realistic conditions that includes space and time dependent dispersion in two and three-dimensional medium. The study will also serve as a platform for the researchers working in the theoretical and experimental study of pollutant transportation with two and three directional flows.

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