A Numerical Groundwater Quality Assessment Model Using the Cubic Spline Method

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Abstract— **Human activities on the surface, including municipal garbage disposal, pesticide usage, and fertilizer use, can contaminate groundwater. Long-term groundwater quality investigations near landfill sites necessitate the use of mathematical models. Research on the environmental impacts of projects, including landfills, depends on the long-term expansion of groundwater quality. Analyzing the quality of groundwater employed an advection-diffusion equation (ADE) in one dimension to describe the quantity of pollution in the groundwater. In this research, numerical simulations for a one-dimensional mathematical model for a long-term contaminated groundwater pollution measurement around landfills are proposed. The finite difference and the natural cubic spline techniques are approximated by the model solution. In a given scenario, the approximate solutions are compared with the exact solutions. The proposed finite difference analysis provides close-to-exact and properly accurate solutions. Numerous varieties of soil physics can be used for the suggested numerical simulation. The simulations can be used to assess the quality of groundwater that becomes contaminated in the future. It is demonstrated that the cubic spline method yields acceptable approximations. It is an alternate finite difference technique.**

Index Terms—**groundwater pollution, contamination, advection-diffusion equation, finite difference method, natural cubic spline method**

I. INTRODUCTION

Pollutants are released into the ground and into aquifers, which are natural underground water reserves, causing groundwater contamination. When contaminants that are discharged enter groundwater, they contaminate it. Groundwater pollution is an issue that has numerous causes, including trash dumping, municipal solid waste, hazardous materials from industry and landfills, etc. There are several mathematical models used to save the environment for humans, such as [1-5]. In [6], we analyze nitrogen pollutant models from the advection-dispersion-reaction equation to estimate pollutant concentrations in terms of total nitrogen, organic nitrogen, ammonia, nitrite, and nitrate concentrations. In [7], a mathematical simulation of water quality over a long period of flooding is performed using a couple of different models: the one-dimensional shallow water equations that provide the water's elevation and velocity, and the one-dimensional advection-dispersion equation that provides the water's pollutant concentrations after the sandbag dike has been destroyed. [8] The purpose of this research was to develop a numerical model of the one-dimensional advection-diffusion equation for estimating salinity levels in the Lower Chao Phraya River, Thailand.

Recent research involves mathematical models for groundwater-quality assessment. The mathematical model [9-11] is used to simulate the salinity in the groundwater with varied flow velocities. The mathematical simulation of groundwater management in drought areas is used to optimize the management of the water injection stations to achieve minimum cost [12]. The transient two-dimensional groundwater flow model and the transient two-dimensional advection diffusion equation use the explicit method, which was described in [13]. In [14], they have presented a measured nitrogen dispersion on total nitrogen transformation effects models. The mathematical models [15] presented the effects of landfill construction on groundwater quality in rural areas. In [16], they explain the one-dimensional groundwater pollution measurement around landfills through heterogeneous soil. In [17], they have used mathematical models to explain the groundwater contamination with chloride and its substances. Two-level explicit methods and the Lax-Wendroff method [18] are used to approximate groundwater quality assessment. In [19], they proposed the effects of pumping water to adjacent settlements on groundwater flow and the quality of the water. In this case, long-term groundwater quality investigations near waste sites necessitate the use of mathematical models. Reports on the environmental effects of projects, including landfills, are based on the growth of long-term groundwater quality. Analyzing the quality of groundwater employed an advection-diffusion equation (ADE) in one dimension to describe the quantity of pollution in the groundwater. The groundwater pollutant concentration is expressed using the one-dimensional advection-diffusion equation (ADE).

In this research, we studied the groundwater dispersion flow through an inhomogeneous soil model. The finite difference method, which is the natural cubic spline, is used to obtain the approximated solutions. The accuracy of the intended numerical methods is tested by an analytical solution.

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II. GOVERNING EQUATION

A. The inhomogeneous soil model allows groundwater contamination dispersion flow to occur

A partial differential equation of one-dimensional advection-diffusion governs a groundwater efficiency model as [20];

$$\frac{\partial C(x,t)}{\partial t}=\frac{\partial}{\partial x}\left(D(x,t)\frac{\partial C(x,t)}{\partial x}-u(x,t)C(x,t)\right), \quad (1)$$

for all $(x,t)\in[0,L]\times[0,T]$, where $C(x,t)$ is the dispersing concentration of groundwater pollutant at position x along the longitudinal direction at time t, D is the pollutant method' s dispersion coefficient, u is a uniform flow velocity, L is the distance in the examined region measured from the origin of the pollution to the endpoint, and T is the rate of change simulation time. The in homogeneity of the soil causes variation in the groundwater flow velocity. Kumar et al. [20] proposed a variation of increasing nature. They also believed that functions were given to the dispersion parameter and the velocity parameter $f_1(x,t)$ and $f_2(x,t)$. It is possible to rewrite Eq. (1) as [21];

$$\frac{\partial C(x,t)}{\partial t}=\frac{\partial}{\partial x}\left(D_0 f_1(x,t)\frac{\partial C(x,t)}{\partial x}-u_0 f_2(x,t)C(x,t)\right), \quad (2)$$

Eq. (2) can be written in the following form;

$$\frac{\partial C(x,t)}{\partial t}=\frac{\partial}{\partial x}\left(D_0\frac{\partial f_1(x,t)}{\partial x}-u_0 f_2(x,t)C(x,t)\right)$$
$$+D_0 f_1(x,t)\frac{\partial^2 C(x,t)}{\partial x^2}-u_0\frac{\partial f_2(x,t)}{\partial x}C(x,t). \quad (3)$$

In the equation above, D_0 and u_0 are constants, the dimensions of which depend on the expression $f_1(x,t)$ and $f_2(x,t)$. The inhomogeneity of the soil allows the rate of flow to differ. A difference in the growing dispersion of groundwater contaminants in heterogeneous soil has been considered by Kumar et al. [21]. The dispersion parameter is often believed to be proportional to the velocity square. Consequently, Eq. (2) is becoming;

$$f_1(x,t)=(1+ax)^2, \text{ and } f_2(x,t)=1+ax, \quad (4)$$

the parameter a with the $(length)^{-1}$ dimension accounts for the inhomogeneity of the soil, Eq. (3) is becoming;

$$\frac{\partial C(x,t)}{\partial t}=\left[(1+ax)(2aD_0-u_0)\right]\frac{\partial C(x,t)}{\partial x}$$
$$+D_0(1+ax)^2\frac{\partial^2 C(x,t)}{\partial x^2}-u_0aC(x,t), \quad (5)$$

$$\frac{\partial C(x,t)}{\partial t}=g(x)\frac{\partial C(x,t)}{\partial x}+h(x)\frac{\partial^2 C(x,t)}{\partial x^2}-KC(x,t). \quad (6)$$

where

$$g(x)=(1+ax)(2aD_0-u_0), \quad (7)$$

$$h(x)=D_0(1+ax)^2, \quad (8)$$

$$K=au_0, \quad (9)$$

$$-\beta=g(x), \quad (10)$$

$$\alpha=h(x). \quad (11)$$

B. Initial and boundary conditions

The initial condition described by the soil's groundwater-contaminated free state of concentration is as follows:

$$C(x,0)=r(x),\ 0\le x\le L,\ t=0. \quad (12)$$

where $r(x)$ is a given initially measured groundwater pollutant function. The average chance rate of groundwater pollutant concentration surrounding them, which is described by the following boundary conditions, determines the concentration gradient at the end point; at the origin, groundwater pollutant concentration is introduced due to a continuous input;

$$C(0,t)=C_0,\ t>0, \quad (13)$$

$$\frac{\partial C(x,t)}{\partial x}=C_s,\ x=L,\ t\ge 0. \quad (14)$$

where C_0 is a given average groundwater pollutant concentration at the considered landfill, and C_s is the rate of change of the pollutant concentration in the area around the far field monitoring station.

III. NUMERICAL TECHNIQUES

The domain is now discretized by dividing the interval $[0,L]$ into M subintervals such that $M\Delta x=L$ and the time interval $[0,L]$ into N subintervals such that $N\Delta t=T$. The grid points (x_i,t_n) are defined by $x_i=i\Delta x$ for all $i=0,1,2,...,M$ and $t_n=n\Delta t$ for all $n=0,1,2,...,N$ in which M and N are positive integers. We can then approximate $C(x_i,t_n)$ by C_i^n, value of the difference approximation of $C(x,t)$ at point $x=i\Delta x$ and $t=n\Delta t$, where $0\le i\le M$ and $0\le n\le N$. We will employ the forward time central space finite difference scheme (FTCS) into Eq. (2).

A. Forward Time Central Space Finite Difference Scheme

$$C(x_i,t_n)\cong C_i^n, \quad (15)$$

$$\left.\frac{\partial C}{\partial t}\right|_{(x_i,t_n)}\cong\frac{C_i^{n+1}-C_i^n}{\Delta t}, \quad (16)$$

$$\left.\frac{\partial C}{\partial x}\right|_{(x_i,t_n)}\cong\frac{C_{i+1}^n-C_{i-1}^n}{2\Delta x}, \quad (17)$$

$$\left.\frac{\partial^2 C}{\partial x^2}\right|_{(x_i,t_n)}\cong\frac{C_{i+1}^n-C_{i-1}^n-2C_i^n}{(\Delta x)^2}, \quad (18)$$

Substituting Eqs. (15)-(18) into Eq. (6), we get the finite difference equation,

$$\frac{C_i^{n+1}-C_i^n}{\Delta t}=g(x)\frac{C_{i+1}^n-C_{i-1}^n}{2\Delta x}+h(x)\frac{C_{i+1}^n-2C_i^n+C_{i-1}^n}{(\Delta x)^2}-KC_i^n, \tag{19}$$

for all $i=1,2,3,...,M$ and $n=0,1,2,...,N-1$ Then the explicit finite difference equation becomes

$$C_i^{n+1}=\frac{\Delta t}{2\Delta x}g(x)\left(C_{i+1}^n-C_{i-1}^n\right)+\frac{\Delta t}{(\Delta x)^2}h(x)\left(C_{i+1}^n-2C_i^n+C_{i-1}^n\right)-\Delta tKC_i^n+C_i^n, \tag{20}$$

$$C_i^{n+1}=pg(x)C_{i+1}^n-pg(x)C_{i-1}^n+qh(x)C_{i+1}^n-2qh(x)C_i^n+qh(x)C_{i-1}^n-\Delta tKC_i^n+C_i^n, \tag{21}$$

Thus

$$C_i^{n+1}=\left(qh(x)-pg(x)\right)C_{i-1}^n+\left(1-2qh(x)-\Delta tK\right)C_i^n+\left(qh(x)+pg(x)\right)C_{i+1}^n, \tag{22}$$

where

$$p=\frac{\Delta t}{2\Delta x}, \tag{23}$$

$$q=\frac{\Delta t}{(\Delta x)^2}, \tag{24}$$

The initial condition Eq. (12) for Eq. (19) can be expressed in the finite difference form as;

$$C_i^0=r(x)=r(i\Delta x)=r_i,\ \ x\geq 0,\ \ t=0. \tag{25}$$

In the finite difference form, Boundary Condition Eq. (13) can be written as;

$$C_0^n=C_0. \tag{26}$$

If we utilize the forward space method in Eq. (14) to the right boundary condition, we have;

$$C_N^n=C_{N-1}^n+\Delta xC_s. \tag{27}$$

The finite difference formula Eq. (22) has been derived in [22] that the truncation error for this method is $O\left\{(\Delta x)^2,\Delta t\right\}$

B. The Natural Cubic Spline Method

The definition of the natural cubic spline for this study includes:

(i) The interpolating spline regions are cubic polynomial functions on each sub-interval $\left[x_j,x_{j+1}\right],\ j=1,2,...,N,$ and all of them match the function values at the grid-points;

(ii) The first and second derivatives of the cubic spline regions are continuous at the inner points; and

(iii) The second derivatives of the cubic spline regions are equal to zero at the first and last grid points.

In employing the cubic spline approach, the approximate solution of the governing problem satisfies:

$$\frac{\partial C(x,t)}{\partial t}=g(x)P_j^n+h(x)Q_j^n-KC(x,t), \tag{28}$$

$$\frac{C_j^{n+1}-C_j^n}{\Delta t}=g(x)P_j^n+h(x)Q_j^n-KC_j^n, \tag{29}$$

for $j=1,2,...,N+1;\ n=0,1,2,...$ where P_j^n is the first derivative and Q_j^n the second derivative of the cubic spline function at the point x_j at time $n\Delta t$. Eq. (29) can be written in the explicit form:

$$C_j^{n+1}=\Delta t\cdot g(x)P_j^n+\Delta t\cdot h(x)Q_j^n+\left(1-\Delta t\cdot K\right)C_j^n, \tag{30}$$

The values of the slopes P_j^n can be obtained by solving the following system of simultaneous equations (derived by manipulation of the equations which result from the continuity conditions for the spline segments; see [23] for details of algebraic working):

$$\begin{bmatrix} 2 & 1 & 0 & 0 & 0 & . & . & . & 0 & 0 & 0 \\ \alpha_2 & 2 & \mu_2 & 0 & 0 & . & . & . & 0 & 0 & 0 \\ 0 & \alpha_3 & 2 & \mu_3 & 0 & . & . & . & 0 & 0 & 0 \\ . & & & & & . & & & & & . \\ . & & & & & . & & & & & . \\ . & & & & & . & & & & & . \\ 0 & 0 & 0 & 0 & 0 & . & . & . & \alpha_{N-1} & 2 & \mu_{N-1} \\ 0 & 0 & 0 & 0 & 0 & . & . & . & 0 & 1 & 2 \end{bmatrix}\begin{bmatrix} P_1^n \\ P_2^n \\ P_3^n \\ . \\ . \\ . \\ P_N^n \\ P_{N+1}^n \end{bmatrix}=\begin{bmatrix} d_1^n \\ d_2^n \\ d_3^n \\ . \\ . \\ . \\ d_N^n \\ d_{N+1}^n \end{bmatrix}, \tag{31}$$

where

$$d_1^n=3\left(\frac{C_2^n-C_1^n}{x_2-x_1}\right)$$

$$d_i^n=3\frac{\mu_j}{h_{j+1}}\left(C_{j+1}^n-C_j^n\right)+3\frac{\alpha_j}{h_j}\left(C_j^n-C_{j-1}^n\right) \text{ for } j=2,3,...,N$$

$$d_{N+1}^n=3\left(\frac{C_{N+1}^n-C_N^n}{x_{N+1}-x_N}\right)$$

and where $\alpha_j=\frac{h_{j+1}}{\left(h_j+h_{j+1}\right)},\ \mu_j=1-\alpha_j=\frac{h_j}{\left(h_j+h_{j+1}\right)},$ $h_{j+1}=x_{j+1}-x_j$ and $h_j=x_j-x_{j-1}.$

The values of Q_j^n are the second derivatives of cubic spline at points x_j for $j=2,3,...,N,$ at time $n\Delta t.$ For the natural cubic spline it is assumed that $s_1''(x_1)=s_n''(x_{n+1})=0\ \left(i.e.\ Q_1^n=Q_{N+1}^n=0\right).$ Then we have:

$$Q_j^n=6\frac{C_{j+1}^n-C_j^n}{\left(x_{j+1}-x_j\right)^2}-4\frac{P_j^n}{x_{j+1}-x_j}-2\frac{P_{j+1}^n}{x_{j+1}-x_j} \tag{32}$$

for $j=2,3,...,N.$

In this research, the stability condition of the finite difference method is applied.

IV. Numerical Experiments

The measured concentration of groundwater pollutants C beneath a landfill and in the area around it. The studied area is 1.0 km long overall and aligned with the longitudinal distance. Leachate is a pollution source that is released underground from a landfill. The pollutant parameters at the considered landfill are $C_0\ kg/l,\ D_0=0.71\ km^{-2}/year,$ and $a=1\ km^{-1}.$ The numerical experiment divides time and space using $\Delta x=0.1\ km$ and $\Delta t=0.0001$ year, respectively. The concentration of groundwater is estimated using the finite difference method and the natural cubic spline method. We obtain an analytical solution of an ideal advection-diffusion equation, proposed in [29];

$$\tilde{C}(x,t)=\frac{C_0}{2}\left(\begin{array}{l}(1+ax)^{-1}\,erfc\left(\dfrac{\ln(1+ax)}{2a\sqrt{D_0 t}}-\beta_0\sqrt{t}\right)\\ +(1+ax)^{\delta}\,erfc\left(\dfrac{\ln(1+ax)}{2a\sqrt{D_0 t}}+\beta_0\sqrt{t}\right)\end{array}\right). \tag{33}$$

where

$$\omega_0=\left(au_0-a^2D_0\right), \tag{34}$$

$$\beta_0=\sqrt{\frac{\omega_0^2}{4a^2D_0}+au_0}=\frac{u_0+aD_0}{2\sqrt{D_0}}, \tag{35}$$

$$\delta=\frac{u_0}{aD_0}. \tag{36}$$

If we employ the finite difference method in Eqs. (19)–(22), we obtain the estimated groundwater pollution along the area under consideration for a period of one year, as shown in Table I and Figs. 1 and 2. If we use the Natural Cubic Spline method in Eqs. (28)–(32), Table II and Figs. 3 and 4 show the approximated groundwater pollutant concentration along the longitudinally considered area. The accuracy of the finite difference method and the natural cubic spline method are shown in Figs. 1 and 3. The accuracy of both approximations is tested by using the analytical solution and the absolute error, as shown in Tables III and IV and Fig. 5.

TABLE I
APPROXIMATE CONCENTRATION OF POLLUTANTS IN GROUNDWATER USING THE PARTIAL DIFFERENCE METHOD FOR A CONSIDERED AREA OF 0.1-1.0 YEARS

t \ x	0.0	0.1	0.2	0.3	0.4	0.5
0.1	1.0000	0.7862	0.6094	0.4675	0.3567	0.2723
0.3	1.0000	0.8799	0.7807	0.6997	0.6346	0.5834
0.5	1.0000	0.9181	0.8519	0.7987	0.7565	0.7236
0.7	1.0000	0.9358	0.8849	0.8446	0.8130	0.7886
1.0	1.0000	0.9463	0.9044	0.8717	0.8464	0.8270

t \ x	0.6	0.7	0.8	0.9	1.0
0.1	0.2097	0.1650	0.1349	0.1166	0.1083
0.3	0.5441	0.5152	0.4952	0.4828	0.4772
0.5	0.6986	0.6802	0.6675	0.6598	0.6562
0.7	0.7701	0.7567	0.7474	0.7418	0.7392
1.0	0.8125	0.8019	0.7947	0.7903	0.7882

As seen from Table I, the effect concentration of the pollutant at x = 0.5 and x = 1.0 is small. It can be seen in Fig. 1. that the numerical solution of the finite difference method indicates that the concentration of the pollutant increases while t increasing.

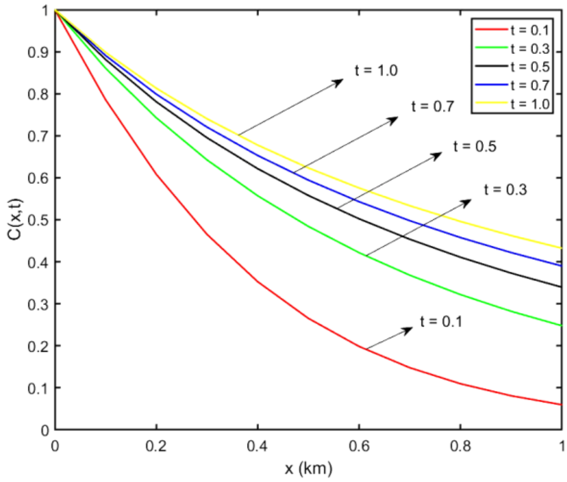

Fig 1. Groundwater contaminant at intervals of 0.1, 0.3, 0.5, 0.7 and 1.0 years using the finite difference method (FTCS).

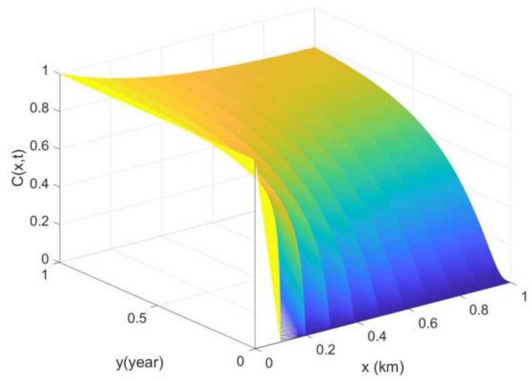

Fig 2. The surface plot of groundwater pollutant by using the finite difference method (FTCS).

TABLE II
APPROXIMATE CONCENTRATION OF POLLUTANTS IN GROUNDWATER USING THE NATURAL CUBIC SPLINE METHOD FOR A CONSIDERED AREA OF 0.1-1.0 YEARS

t \ x	0.0	0.1	0.2	0.3	0.4	0.5
0.1	1.0000	0.7936	0.6175	0.4762	0.3664	0.2841
0.3	1.0000	0.8930	0.8024	0.7297	0.6727	0.6293
0.5	1.0000	0.9310	0.8737	0.8287	0.7939	0.7678
0.7	1.0000	0.9463	0.9025	0.8686	0.8428	0.8236
1.0	1.0000	0.9540	0.9170	0.8887	0.8675	0.8518

t \ x	0.6	0.7	0.8	0.9	1.0
0.1	0.2252	0.1859	0.1629	0.1535	0.1532
0.3	0.5978	0.5765	0.5639	0.5587	0.5586
0.5	0.7489	0.7363	0.7288	0.7258	0.7257
0.7	0.8099	0.8007	0.7954	0.7932	0.7931
1.0	0.8406	0.8332	0.8289	0.8271	0.8271

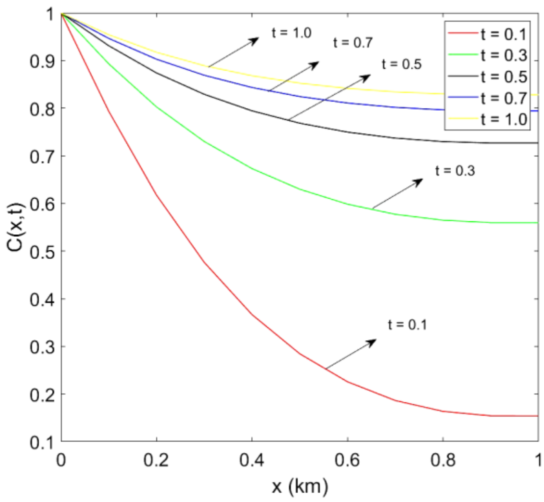

Fig 3. Groundwater contaminant at intervals of 0.1, 0.3, 0.5, 0.7 and 1.0 years using the natural cubic spline method.

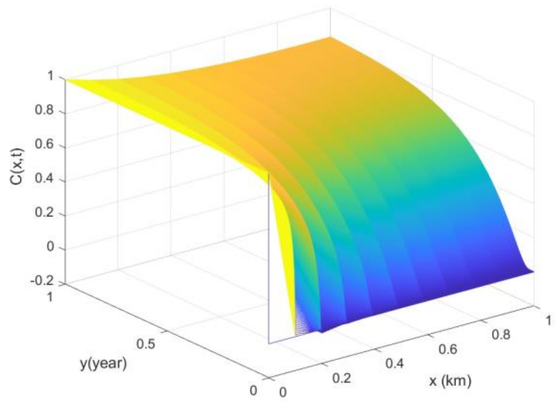

Fig 4. The surface plot of groundwater pollutant by using the natural cubic spline method.

TABLE III
THE ASOLUTE ERROR OF THE FINITE DIFFERENCE METHOD APPROXIMATION WHERE $e(x,t)=\left|C(x,t)-\tilde{C}(x,t)\right|$

t \ x	0.0	0.1	0.2	0.3	0.4	0.5
0.1	1.00000	0.00011	0.00009	0.00044	0.00077	0.00098
0.3	1.00000	0.00001	0.00002	0.00002	0.00002	0.00003
0.5	1.00000	0.00008	0.00012	0.00013	0.00013	0.00012
0.7	1.00000	0.00010	0.00015	0.00017	0.00017	0.00015
1.0	1.00000	0.00011	0.00017	0.00018	0.00018	0.00016
t \ x	**0.6**	**0.7**	**0.8**	**0.9**	**1.0**	
0.1	0.00102	0.00091	0.00067	0.00036	0.00000	
0.3	0.00003	0.00003	0.00002	0.00001	0.00000	
0.5	0.00010	0.00008	0.00006	0.00003	0.00000	
0.7	0.00013	0.00010	0.00007	0.00003	0.00000	
1.0	0.00014	0.00011	0.00007	0.00004	0.00000	

TABLE IV
THE ABSOLUTE ERROR OF THE NATURAL CUBIC SPLINE METHOD APPROXIMATION WHERE $e(x,t)=\left|C(x,t)-\tilde{C}(x,t)\right|$

t \ x	0.0	0.1	0.2	0.3	0.4	0.5
0.1	1.00000	0.00490	0.00245	0.00202	0.00880	0.01805
0.3	1.00000	0.00983	0.02282	0.03466	0.04550	0.05544
0.5	1.00000	0.00778	0.01834	0.02774	0.03615	0.04373
0.7	1.00000	0.00612	0.01500	0.02300	0.03018	0.03676
1.0	1.00000	0.00502	0.01278	0.01978	0.02617	0.03206
t \ x	**0.6**	**0.7**	**0.8**	**0.9**	**1.0**	
0.1	0.02987	0.04426	0.06111	0.04495	0.00000	
0.3	0.06454	0.07283	0.08035	0.05436	0.00000	
0.5	0.05058	0.05681	0.06249	0.04223	0.00000	
0.7	0.04281	0.04842	0.05364	0.03636	0.00000	
1.0	0.03754	0.04268	0.04753	0.03228	0.00000	

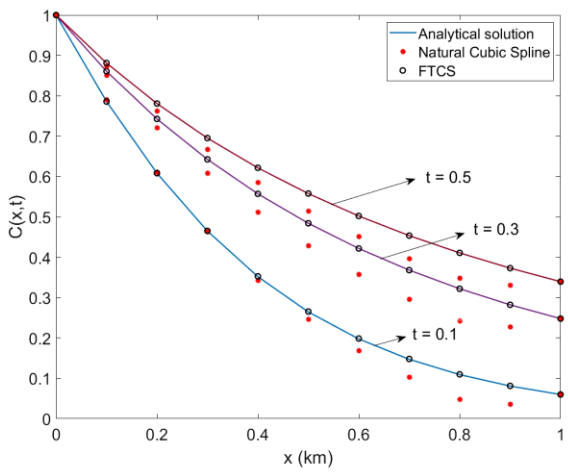

Fig 5. The comparison of finite difference method (FTCS) and the natural cubic spline method and analytical solution at 0.1, 0.3 and 0.5 years.

V. Discussion

In numerical experiment, the approximated groundwater pollutant concentration using the finite difference method and the natural cubic spline method are give good agreement in 5 cases as show in Table I-II and Fig.1 and Fig.3. The surface plot of groundwater pollutant by using the finite difference method and the natural cubic spline method as shown in Fig.2 and Fig.4. The absolute error of the approximation as shown in Table III-IV, the finite difference method gives better than the natural cubic spline method. The comparison of both approximation and analytic solution at 0.1, 0.3 and 0.5 years as shown in Fig.5.

VI. Conclusion

A one-dimensional groundwater pollutant concentration model was approximately simulated by the numerical model. Utilizing both the natural cubic spline approach and the finite difference method, the numerical solutions of contaminants in groundwater are approximated. An acceptable approximation was obtained by the alternative finite difference method, which uses a natural cubic spline technique. The quality of groundwater that has been contaminated for more than ten years can be assessed using the simulation that is being presented. The numerical methods that are suggested provide a good approximation. We can see that the cubic spline method gives acceptable approximate solutions. It is an alternative finite difference method.

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