NUMERICAL SIMULATIONS TO A ONE-DIMENSIONAL GROUNDWATER POLLUTION MESUREMENT MODEL THROUGH HETEROGENEOUS SOIL

WASU TIMPITAK

A THESIS SUBMITTED IN PARTIAL FULFILLMENT OF THE REQUIREMENT FOR THE DEGREE OF MASTER IN SCIENCE (APPLIED MATHEMATICS)

DEPARTMENT OF MATHEMATICS FACULTY OF SCIENCE

KING MONGKUTS INSTITUTE OF TECHNOLOGY LADKRABANG

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Thesis Title	Numerical Simulations to a One-dimensional Groundwater Pollution Mesurement Model Through Heterogeneous Soil
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Abstract

The problem of toxic contaminants in groundwater with groundwater pollution measurement model. A advection-diffusion equation is used to describe the concerned model. The theoretical solution of the advection-diffusion equation is limited only in ideal topography. Applications of numerical solutions are influenced in several initial and boundary conditions when dealing with complex geometries. In this research, numerical simulations for one-dimensional groundwater pollution measurement around landfills model through heterogeneous soil are focused. The forward time center space and Saulyev finite difference techniques are used to approximate the solutions. The accuracy of proposed techniques are to examine by comparing the approximated solutions with the analytical solution. The purposed technique gives good agreement approximated solution.

Keywords : groundwater pollution, advection-diffusion, landfills, saulyev finite difference method, heterogeneous soil.

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Wasu Timpitak

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Chapter 1

Introduction

1.1 Research Motivation

Groundwater is important to people. The rural population is used groundwater for consumption, agriculture and industrial processes. Groundwater is an important reserve water source to support expansion the population and source of recharge for lakes, rivers, and wetlands. In industrial processes, groundwater is an important component due to it is used as a raw material for production. Groundwater is found in the cracks and spaces in soil, community have to pump up it for use. It is important that groundwater is not contaminated. The quality of groundwater depend on depth and geological soil condition, it is vulnerable to contamination from a range of activities of industrial and agricultural plants. In Thailand, groundwater source are divided into two types groundwater basin and groundwater in rock source area. The groundwater basin originate from sediment deposits in the Chao Phraya River Basin, It consists of a layer of gravel sand and clay. The groundwater in rock source area are located in north and eastern of the Chao Phraya River Basin, It consists of volcanic rocks, sandstone, limestone and shale. The main groundwater source are the Chao Phraya basin, Lower Upper Chao Phraya Basin and Chiang Mai-Lamphun Basin etc. Drilling groundwater wells in Singburi as show in Fig 1.1-1.2. At Prachuap Khiri Khan has drilling groundwater wells in Kuiburi District, to solve the water shortage problem of wild animal, tourist and park staff at Kuiburi national park as show in Fig 1.3.

The groundwater pollution is almost the biggest problem in the world. Groundwater is susceptible to pollutants and contaminant occurs from industrial factory, agriculture and manufacture products. Groundwater not safe enough for use, When the contaminant flows down the soil. If people drinking groundwater contaminated, they may get directly affected to health. Ratchaburi villagers are affected by contaminants in groundwater sources from waste disposal plants as show in Fig 1.4. Potential sources of groundwater contamination such as storage tanks, septic systems, uncontrolled hazardous waste, landfills, chemicals, Road Salts and atmospheric contaminants. This research focuses on the problem of groundwater contamination caused by landfills where people take the garbage. Contaminants from the landfill can flow into the groundwater due to there is no layer to prevent contaminants or it is cracked in soil. In Fig.1.5 as show landfills, people live near this landfills are most affected by groundwater pollution sources.

Figure 1.1: Groundwater wells in Singburi to solve drought problems [15]

Figure 1.2: Excavation of groundwater in Sing Buri [15]

Figure 1.3: Groundwater wells in Kuiburi to solve the water shortage problem [16]

Figure 1.4: The affected of contaminants in groundwater sources [17]

Figure 1.5: Landfills [18]

The effect of contaminated groundwater consumption is life threatening. If receiving a lot of toxic substances, it is cause diseases. Blue baby syndrome is a disease caused by baby who receive groundwater contaminated with nitrates. Nitrate interrupts the oxygen pathway into the body, this causes made the skin take on a blue color as show in Fig 1.6. Quality of groundwater is important for consumption then it must pass the groundwater standard as show in table 1.1.

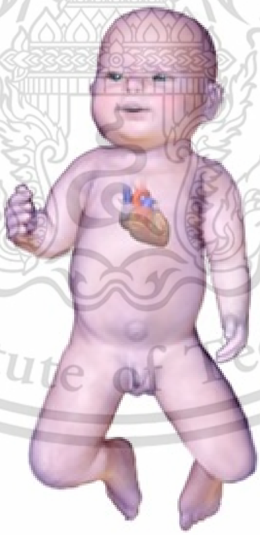


Figure 1.6: Blue baby syndrome [19]

Table 1.1: Groundwater standard for consumption

attribute	index of water quality	Unit	standard score	
			Appropriate criteria	Max grace criteria
physical	Colour	Platinum-cobalt	5	15
	Turbidity	Turbidity unit	5	20
	pH	-	7.0-8.5	6.5-9.2
Chemical	steel(Fe)	mg/l	No more than 0.5	1.0
	manganese(Fe)	mg/l	No more than 0.3	0.5
	copper(cu)	mg/l	No more than 1.0	1.5
	zinc(Zn)	mg/l	No more than 5.0	15.0
	Sulfate(SO_4)	mg/l	No more than 200	250
	Chloride(Cl)	mg/l	No more than 250	600
	Fluoride(F)	mg/l	No more than 0.7	1.0
	Nitrate(SO_3)	mg/l	No more than 45	45
	Total Hardness as $CaCO_3$	mg/l	No more than 300	500
	Non carbonate hardness as $CaCO_3$	mg/l	No more than 200	250
	Total dissIved solids	mg/l	No more than 600	1200
Toxic substance	Arsenic(As)	mg/l	none	0.05
	Cyanide(Cn)	mg/l	none	0.1
	Lead(Pb)	mg/l	none	0.05
	Mercury(Hg)	mg/l	none	0.001
	Cadmium(Cd)	mg/l	none	0.01
	Selenium(Se)	mg/l	none	0.01
Bacteria	Standard plate count	Colony per cc	No more than 500	-
	Most Probable Number (MPN)	M.P.N per cc	Less than 2.2	-
	E.coli	-	none	-

Contaminant flow down from landfills to groundwater and it spread to the surround area. Advection and diffusion of contaminants in groundwater makes the surrounding area to be affected. We don't know the exact time of contaminants measurement in groundwater, because contaminants have a very slow flow velocity. If there have community near landfills then contaminants measurement in groundwater is difficult. Mathematical model is used measurement contaminants in groundwater from landfills to community.

Figure 1.7: Diffusion phenomenon in water [20]

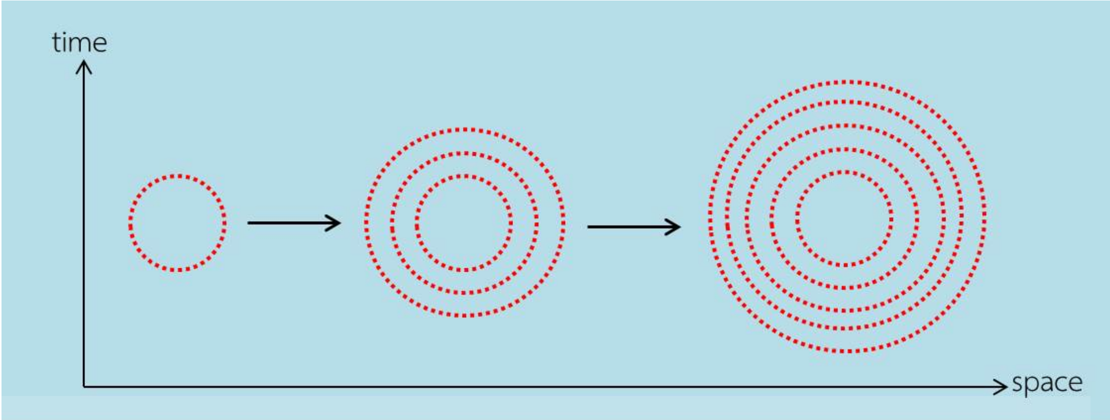


Figure 1.8: Advection-Diffusion phenomenon in water

1.2 Literature review

There are several use of the advection-diffusion equation (ADE), including heat transfer, sediment transport and water pollutant concentration measurement. [1] introduced a explicit and implicit forms of differential quadrature method for approximating ADE with constant coefficient. The developed scheme was based on a mathematical combine both Siemieniuch and Gradwell approximation for time and Dehghan's approximation for spatial variable. In [2], they have solved ADE with an explicit approach of finite difference method (EFDM) and variable coefficients in semi-infinite domain. This equation can analyze three dispersion problems:

(i) Solute dispersion along poised flow through inhomogeneous medium.

(ii) Temporarily dependent solute dispersion along uniform flow through homogeneous medium.

(iii) Solute dispersion along temporarily dependent not poised flow through inhomogeneous medium.

In [3], they have solved the one-dimensional (1D) ADE with variable coefficients in semi- infinite media by using EFDM for two dispersion problems:

(i) Temporarily dependent dispersion in uniform flow.

(ii) Spatially dependent dispersion in non-uniform flow, uniform pulse-type input condition and initial solute concentration, that decreasing function of distance were considered.

In [4], the EFDM to obtain the dispersion through a heterogeneous horizontal semi-infinite medium. The heterogeneous nature of the medium was discoursed by a position dependency linear nonhomogeneous expression for velocity with not poised exponential variation with time. Velocity and dispersion was zero at the origin. In [5], an analytical solution to one-dimensions ADE with several point sources through arbitrary time-dependent discharging rate is proposed. They reported that the results had indicated, the proposed analytical solution could offer an accurate estimation of the contemplation. The limitations of the proposed solution were valid only for the constant-parameters condition, and was not computational performance for problems involving a high temporal or a high spatial resolution.

The inhomogeneity of the medium causes variation in the flow velocity, [2, 6]. In [7], studied on the variation of the increasing nature. In this research, we will propose an explicit finite difference technique for an advection-diffusion equation with variable coefficient in a semi-infinite domain. Due to the low advection groundwater flow, the contaminated groundwater flow measurement need very long term transition time. The effective time of prediction will be larger than a year. The simulation of contaminated groundwater level in faraway point need to be introduced.

In this research, the transient contaminated groundwater dispersion measurement around landfills model will be introduced. The inhomogeneous soil by the bottom topography will be also concerned in the proposed model. The finite difference technique that is used to obtain the approximated solutions are purposed. The accuracy of the purposed numerical methods are tested by comparison them with an analytical solution in an ideal case.

1.3 Objectives of the study

1) To propose mathematical model of problem of toxic contaminants in groundwater measurement.
2) To define initial condition and boundary condition consistent with realistic simulations of toxic contaminants in groundwater.
3) To define functions of contaminated groundwater dispersion coefficient and functions of contaminated groundwater flow velocity through considered heterogeneous soil.
4) To propose numerical method to obtain the approximated groundwater pollutant concentration in long term of time.
5) To propose realistic numerical simulation.

1.4 Scopes of the study

1) To study the one-dimension advection-diffusion equation (ADE)
2) To long term simulation of toxic contaminants in groundwater.
3) To study problem of toxic contaminants in groundwater through heterogeneous soil.
4) To approximate solution of toxic contaminants in groundwater.

1.5 Methodology

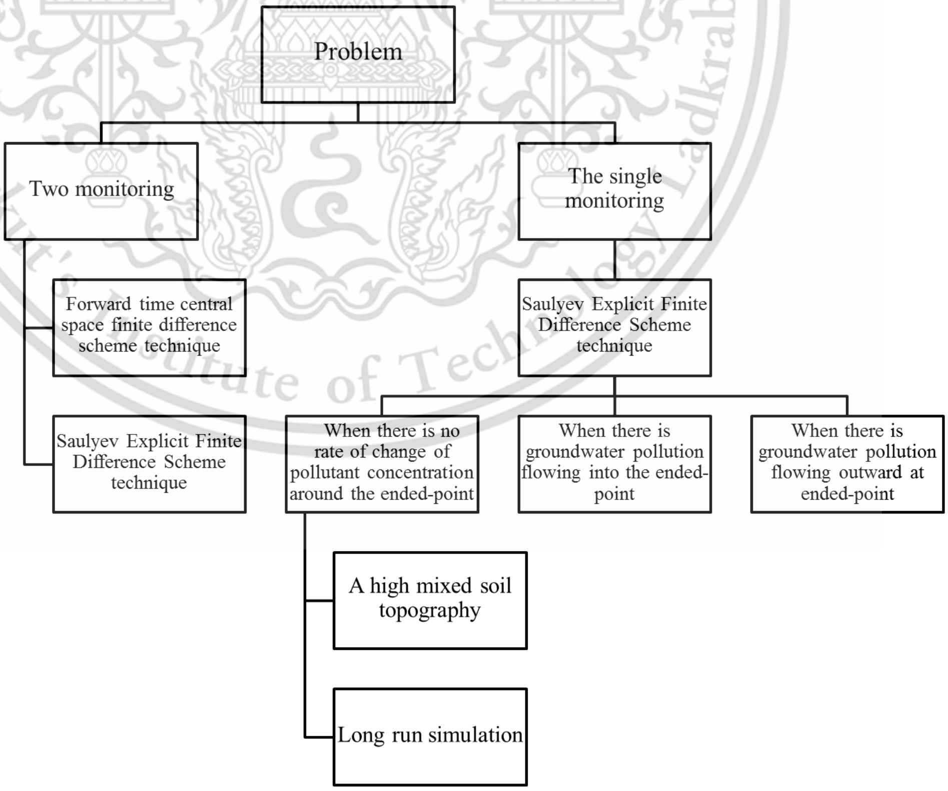
1) Study mathematical model of problem of toxic contaminants in groundwater.
2) Define initial condition and boundary condition consistent with problem of toxic contaminants in groundwater.
3) Define functions of contaminated groundwater dispersion coefficient and functions of contaminated groundwater flow velocity through considered heterogeneous soil.
4) Using numerical methods to simulate the groundwater quality measurement.

1.6 Benefits of the study

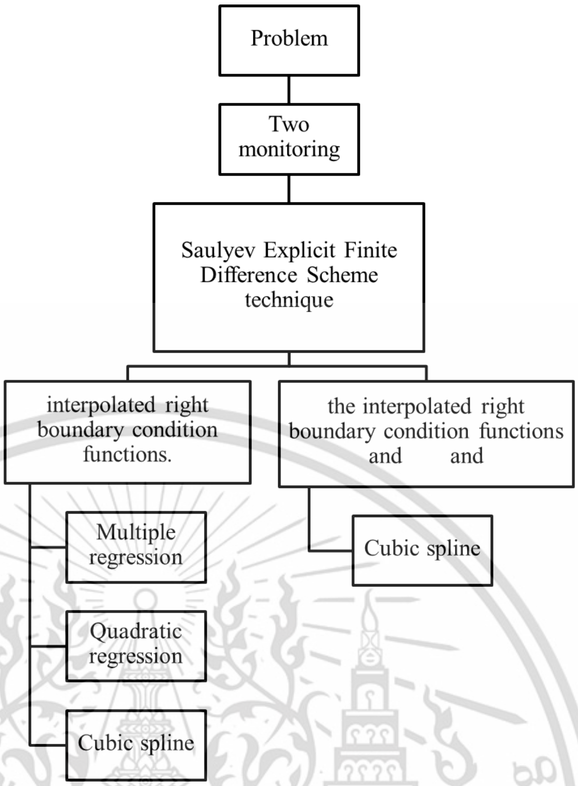
1) We can measure groundwater pollution in long run.
2) We can forecast groundwater quality and other effects in the future.
3) We can forecast some affect of a landfill to surrounding community.

1.7 Plan of the thesis

1.7.1 first part



1.7.2 Second part



Chapter 2

Governing Equation

Groundwater pollutant contaminant can predict by the groundwater pollution measurement model. Groundwater pollution problem as show in Fig 2.1, contaminant flow from landfills to groundwater and it disperse to the community area. In this research, predict pollutant contaminant in groundwater from landfill to community through heterogeneous soil. The soil is divided into 3 types such as clay, sandy soil, combination of clay. Heterogeneous soil is mixed soil, it causes the diffusion coefficient and flow velocity field are unequal in each area as show in Fig 2.2.

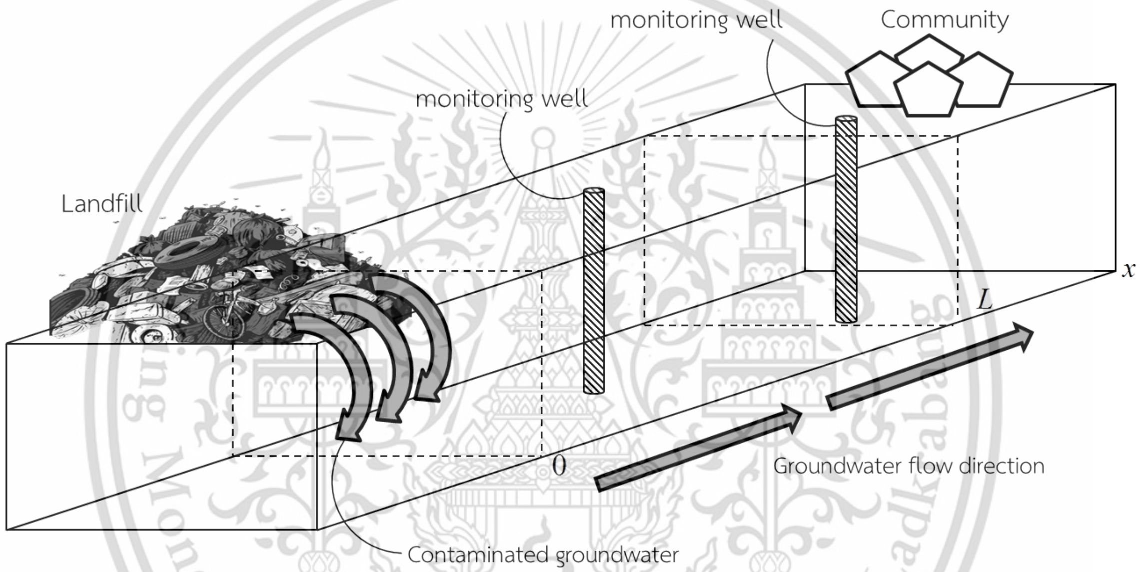


Figure 2.1: Groundwater pollution problem

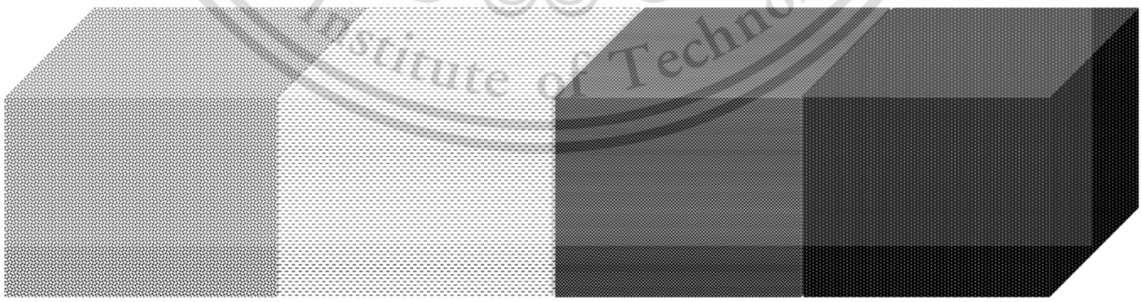


Figure 2.2: Heterogeneous soil

2.1 Contaminated groundwater dispersion along unsteady flow through general soil

The one-dimension advection-diffusion equation (ADE) is expressed as follows [6],

$$\frac{\partial C(x,t)}{\partial t} = \frac{\partial}{\partial x}\left(D(x,t)\frac{\partial C(x,t)}{\partial x}\right) - \frac{\partial u(x,t)\,C(x,t)}{\partial x}, \tag{2.1}$$

for all $(x,t) \in \Omega$ such that $\Omega = [0,L] \times [0,T]$, where are $C(x,t)$ the dispersing solute concentration, the longitudinal axis, and time, respectively.

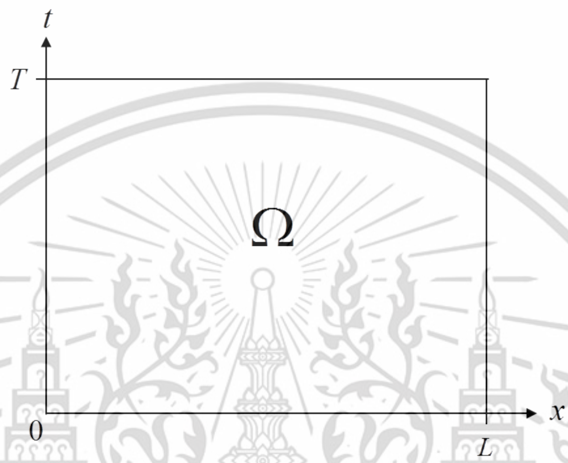


Figure 2.3: Domain diagram

2.2 Contaminated groundwater dispersion along unsteady flow through inhomogeneous soil

If the considered area has inhomogeneous soil properties, the diffusion term and the advective term can be assumed by [1],

$$D = D_0 f_1(x,t), \tag{2.2}$$

$$u = u_0 f_2(x,t), \tag{2.3}$$

where D_0 and u_0 are given the diffusion contaminated groundwater pollutant coefficient constant and the advective contaminated groundwater pollutant coefficient constant, and $f_1(x,t)$, $f_2(x,t)$ are given fuctions which are represent the diffusive term and the advective term due to the inhomogeneous soil. the Eq.(2.1) becomes [1],

$$\frac{\partial C(x,t)}{\partial t} = D_0\frac{\partial}{\partial x}\left(f_1(x,t)\frac{\partial C(x,t)}{\partial x}\right) - \frac{u_0 \partial f_2(x,t)\,C(x,t)}{\partial x}, \tag{2.4}$$

for all $(x,t) \in [0,L]\times[0,T]$, where D_0 and u_0 are constant values whose dimensions depend upon the expressions $f_1(x,t)$ and $f_2(x,t)$ and $f_1(x,t)$ and $f_2(x,t)$ are given functions. The analytical solutions of ADE for the previously mentioned two hydrodynamic dispersion problems were introduced by [6].

2.3 The initial and boundary conditions

The initial condition is defined by an interpolation function of measured raw data. The boundary conditions can be classified into two cases.

2.3.1 Potential contaminated groundwater

An initially solute free condition is assumed for both of the problems in the semi-infinite domain. Meanwhile, a uniform distribution of nodes is applied at the origin of the domain. The initial condition, is assumed by

$$C(x,0) = f(x)\,, \tag{2.5}$$

for all $x \in [0, L]$, where $f(x)$ is an initially pollutant concentration function.

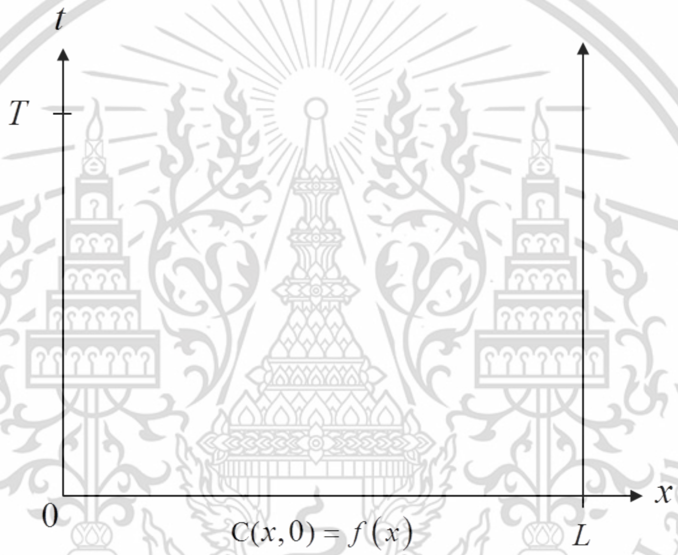


Figure 2.4: The initial condition

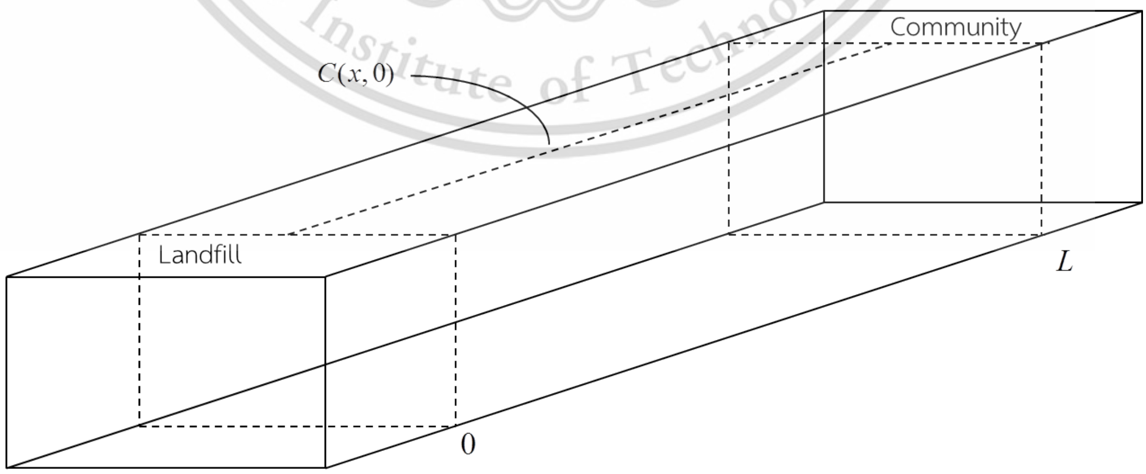


Figure 2.5: The initial condition in groundwater pollution problem

2.3.2 Contaminated groundwater at two monitoring points

The boundary conditions, are also assumed by

$$C(0,t) = g_1(t), \quad (2.6)$$

$$C(L,t) = g_2(t), \quad (2.7)$$

for all $t \in [0,T]$, where $g_1(t)$ and $g_2(t)$ boundary sources of pollutant concentration on the starting point and the end point of the radius of considered area, respectively.

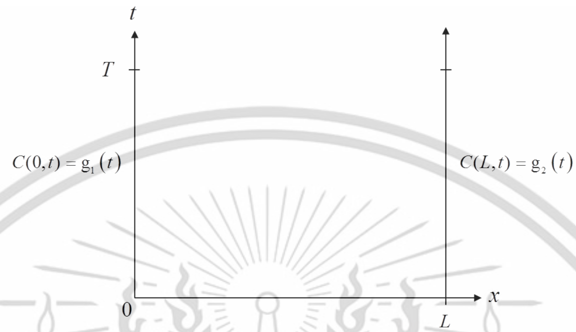


Figure 2.6: The boundary conditions of two monitoring points

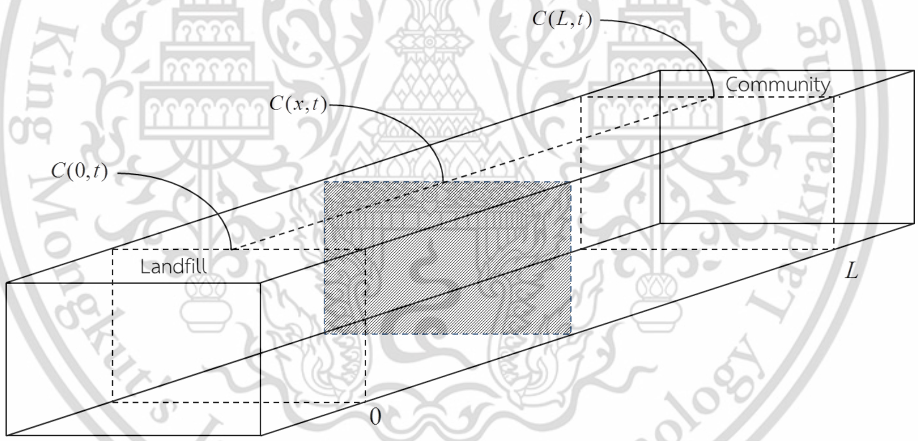


Figure 2.7: The boundary conditions of two monitoring points in groundwater pollution problem

2.3.3 Contaminated groundwater at the single static monitoring point

The left boundary condition is assumed by the interpolation function of measured raw data at the considered landfill. The right boundary condition is assumed by the averaged rate of change of pollutant concentration around the right ended point. The boundary conditions, are also assumed by

$$C(0,t) = g_1(t), \quad (2.8)$$

$$\frac{\partial C(L,t)}{\partial x} = \kappa, \quad (2.9)$$

for all $t \in [0, T]$, where $g_1(t)$ and κ boundary sources of pollutant concentration on the starting point and the rate of change of pollutant concentration with respect to distance around the ended point on the considered area, respectively.

$\kappa = 0$ (there is no rate of change of pollutant concentration around the ended-point)

$\kappa > 0$ (the increasing rate of change of pollutant concentration around the ended-point)

$\kappa < 0$ (the reducing rate of change of pollutant concentration around the ended-point)

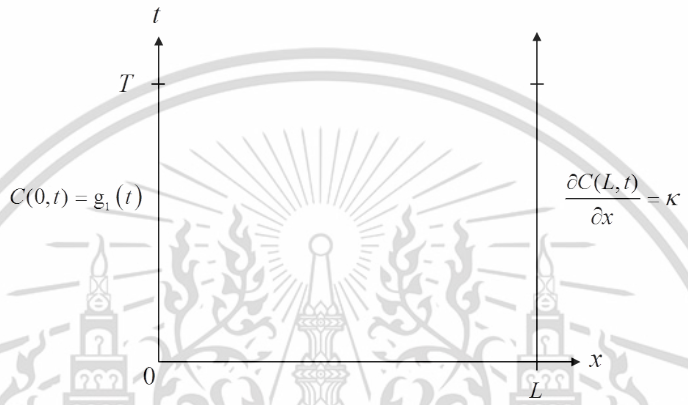


Figure 2.8: The boundary conditions of the single monitoring point

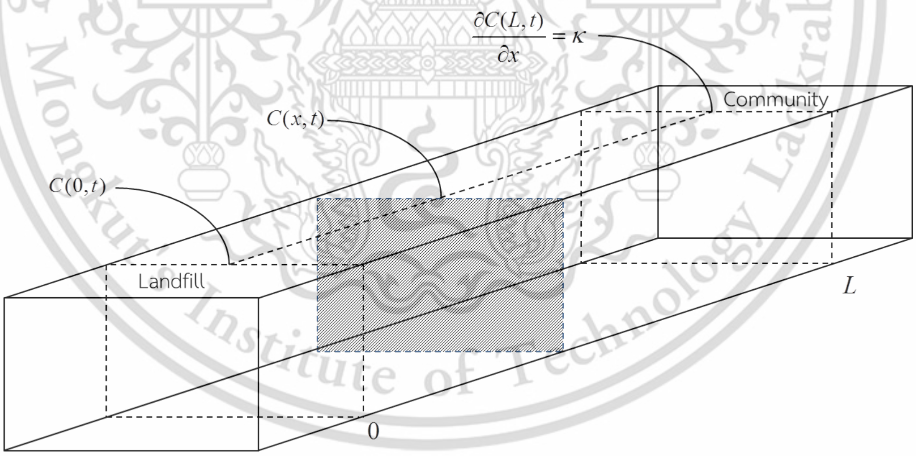


Figure 2.9: The boundary conditions of the single monitoring point in groundwater pollution problem

Chapter 3

Numerical Techniques

We now discretize the domain by dividing the interval $[0, L]$ into M subintervals such that $M\Delta x = L$ and the time interval $[0, T]$ 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 $i = 1, 2, 3, \ldots, M$ and $t_n = n\Delta t$ for all $n = 1, 2, 3, \ldots, N$ in which M and N are positive integers as show in Fig 3.1. 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 $0 \le n \le N$.

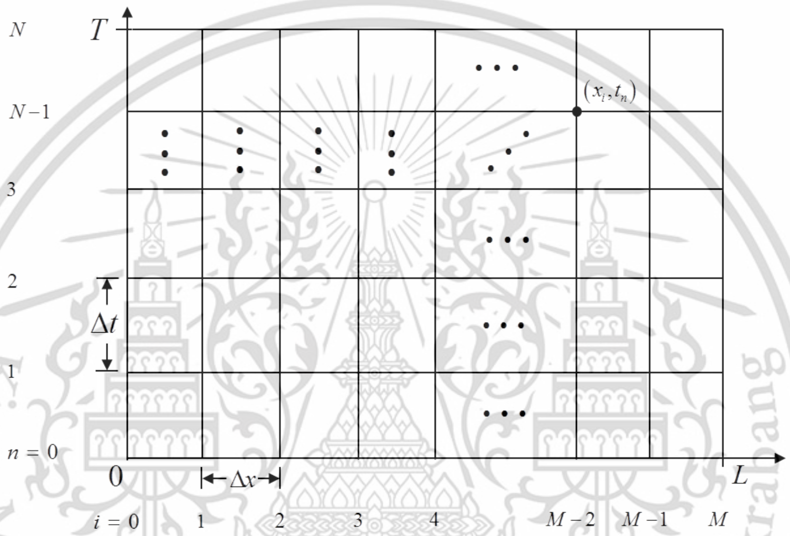


Figure 3.1: Grid spacing

3.1 Forward time central space finite difference scheme

Taking the forward time central space technique into Eq.(2.4), it can be obtained the following discretization:

$$C(x_i, t_n) \cong C_i^n, \tag{3.1}$$

$$\left.\frac{\partial C}{\partial t}\right|_{(x_i, t_n)} \cong \frac{C_i^{n+1} - C_i^n}{\Delta t}, \tag{3.2}$$

$$\left.\frac{\partial C}{\partial x}\right|_{(x_i, t_n)} \cong \frac{C_{i+1}^n - C_{i-1}^n}{2\Delta x}, \tag{3.3}$$

$$\left.\frac{\partial^2 C}{\partial x^2}\right|_{(x_i, t_n)} \cong \frac{C_{i+1}^n + C_{i-1}^n - 2C_i^n}{(\Delta x)^2}, \tag{3.4}$$

$$f_1(x_i, t_n) = {f_1}_i^n, \tag{3.5}$$

$$f_2(x_i, t_n) = {f_2}_i^n. \tag{3.6}$$

Substituting Eqs.(3.1)-(3.6) into Eq.(2.4), we get the finite difference equation,

$$\frac{C_i^{n+1}-C_i^n}{\Delta t} = \left(D_0 \cdot \left.\frac{\partial f_1}{\partial x}\right|_{(x_i,t_n)} - u_0 f_{2_i}^n\right)\left(\frac{C_{i+1}^n - C_{i-1}^n}{2\Delta x}\right) - u_0 \cdot \left.\frac{\partial f_2}{\partial x}\right|_{(x_i,t_n)} C_i^n$$

$$+D_0 f_{1_i}^n \left(\frac{C_{i-1}^n - 2C_i^n + C_{i+1}^n}{(\Delta x)^2}\right), \tag{3.7}$$

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

$$C_i^{n+1} = \left[\lambda_i^n - \frac{1}{2}\gamma_i^n + \frac{1}{2}\beta_i^n\right] C_{i-1}^n + \left[1 - \Delta t\alpha_i^n - 2\lambda_i^n\right] C_i^n + \left[\lambda_i^n + \frac{1}{2}\gamma_i^n - \frac{1}{2}\beta_i^n\right] C_{i+1}^n, \tag{3.8}$$

where

$$\lambda_i^n = \frac{\Delta t\, D_0 f_{1_i}^n}{(\Delta x)^2}, \tag{3.9}$$

$$\beta_i^n = \frac{\Delta t\, u_0 f_{2_i}^n}{\Delta x}, \tag{3.10}$$

$$\gamma_i^n = \frac{\Delta t\, D_0}{\Delta x} \left.\frac{\partial f_1}{\partial x}\right|_{(x_i,t_n)}, \tag{3.11}$$

$$\alpha_i^n = u_0 \cdot \left.\frac{\partial f_2}{\partial x}\right|_{(x_i,t_n)}, \tag{3.12}$$

the explicit finite difference Eq.(3.8) can be written in a compact form as,

$$V_i^n = \lambda_i^n - \frac{1}{2}\gamma_i^n + \frac{1}{2}\beta_i^n, \tag{3.13}$$

$$G_i^n = 1 - \Delta t\alpha_i^n - 2\lambda_i^n, \tag{3.14}$$

$$P_i^n = \lambda_i^n + \frac{1}{2}\gamma_i^n - \frac{1}{2}\beta_i^n. \tag{3.15}$$

Then

$$C_i^{n+1} = V_i^n C_{i-1}^n + G_i^n C_i^n + P_i^n C_{i+1}^n. \tag{3.16}$$

The Stencil diagram of the finite difference equation Eq.3.16 is shown in Fig.3.2. According to the right boundary condition Eq.(2.9), if $i = M$, substituting the approximate unknown value of the right boundary [9], we can let

$$C_{M+1}^n = 2\kappa\Delta x + C_{M-1}^n \tag{3.17}$$

and by rearranging, we obtain

$$C_M^{n+1} = (V_M^n + P_M^n)\, C_{M-1}^n + G_M^n C_M^n + 2\Delta x \cdot \kappa P_M^n. \tag{3.18}$$

The forward time central space scheme is conditionally stable subject to constraints in Eq.(3.8). The stability requirements for the scheme are [9, 10]

$$\lambda_i^n = \frac{\Delta t\, D_0 f_1(x_i, t_n)}{(\Delta x)^2} < \frac{1}{2},$$

$$\beta_i^n,\ \gamma_i^n,\ \alpha_i^n < 1,$$

where λ_i^n is the diffusion number (dimensionless) and β_i^n is the advection number (dimensionless). It can be obtained that the strictly stability requirements are the main disadvantage of this scheme.

The finite difference formula Eq.(3.16) has been derived in [11] that the truncation error for this method is $O\left\{(\Delta x)^2, \Delta t\right\}$

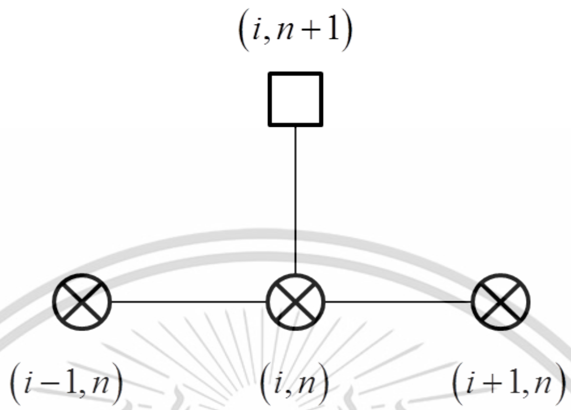


Figure 3.2: Stencil diagram of forward time central space finite difference scheme

3.2 Saulyev Explicit Finite Difference Scheme

The Saulyev scheme is unconditionally stable [12]. It is clear that the nonstrictly stability requirement of Saulyev scheme is the main of advantage and economical to use. Taking Saulyev technique [12] into Eq.(2.4), it can be obtained the following discretization:

$$C\left(x_i, t_n\right) \cong C_i^n, \tag{3.19}$$

$$\left.\frac{\partial C}{\partial t}\right|_{(x_i,t_n)} \cong \frac{C_i^{n+1} - C_i^n}{\Delta t}, \tag{3.20}$$

$$\left.\frac{\partial C}{\partial x}\right|_{(x_i,t_n)} \cong \frac{C_{i+1}^n - C_{i-1}^{n+1}}{2\Delta x}, \tag{3.21}$$

$$\left.\frac{\partial^2 C}{\partial x^2}\right|_{(x_i,t_n)} \cong \frac{C_{i+1}^n - C_i^n - C_i^{n+1} + C_{i-1}^{n+1}}{\left(\Delta x\right)^2}, \tag{3.22}$$

$$f_1\left(x_i, t_n\right) = f_{1\,i}^{\,n}, \tag{3.23}$$

$$f_2\left(x_i, t_n\right) = f_{2\,i}^{\,n}. \tag{3.24}$$

Substituting Eqs.(3.19)-(3.24) into Eq.(2.4), we get the finite difference equation,

$$\frac{C_i^{n+1} - C_i^n}{\Delta t} = \left(D_0 \cdot \left.\frac{\partial f_1}{\partial x}\right|_{(x_i,t_n)} - u_0 f_{2\,i}^{\,n}\right)\left(\frac{C_{i+1}^n - C_{i-1}^{n+1}}{2\Delta x}\right) - u_0 \cdot \left.\frac{\partial f_2}{\partial x}\right|_{(x_i,t_n)} C_i^n$$
$$+ D_0 f_{1\,i}^{\,n}\left(\frac{C_{i+1}^n - C_i^n - C_i^{n+1} + C_{i-1}^{n+1}}{\left(\Delta x\right)^2}\right), \tag{3.25}$$

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

$$C_i^{n+1} = \frac{1}{1+\lambda_i^n}\left[\left(\lambda_i^n - \frac{1}{2}\gamma_i^n + \frac{1}{2}\beta_i^n\right)C_{i-1}^{n+1} + \left(1 - \Delta t\alpha_i^n - \lambda_i^n\right)C_i^n\right.$$
$$\left.+\left(\lambda_i^n + \frac{1}{2}\gamma_i^n - \frac{1}{2}\beta_i^n\right)C_{i+1}^n\right], \tag{3.26}$$

where

$$\lambda_i^n = \frac{\Delta t\, D_0 f_{1\,i}^{\,n}}{\left(\Delta x\right)^2}, \tag{3.27}$$

$$\beta_i^n = \frac{\Delta t\, u_0 f_{2\,i}^{\,n}}{\Delta x}, \tag{3.28}$$

$$\gamma_i^n = \frac{\Delta t\, D_0}{\Delta x}\left.\frac{\partial f_1}{\partial x}\right|_{(x_i,t_n)}, \tag{3.29}$$

$$\alpha_i^n = u_0 \cdot \left.\frac{\partial f_2}{\partial x}\right|_{(x_i,t_n)}, \tag{3.30}$$

the explicit finite difference Eq.(3.26) can be written in a compact form as,

$$A_i^n = \frac{1}{1+\lambda_i^n}, \tag{3.31}$$

$$B_i^n = \lambda_i^n - \frac{1}{2}\gamma_i^n + \frac{1}{2}\beta_i^n, \tag{3.32}$$

$$Q_i^n = 1 - \Delta t \alpha_i^n - 2\lambda_i^n, \tag{3.33}$$

$$Z_i^n = \lambda_i^n + \frac{1}{2}\gamma_i^n - \frac{1}{2}\beta_i^n. \tag{3.34}$$

Then

$$C_i^{n+1} = A_i^n \left(B_i^n C_{i-1}^{n+1} + Q_i^n C_i^n + Z_i^n C_{i+1}^n \right). \tag{3.35}$$

The Stencil diagram of the finite difference equation Eq.(3.35) is shown in Fig.3.3. According to the right boundary condition Eq.(2.9), if $i = M$, substituting the approximate unknown value of the right boundary [9], we can let

$$C_{M+1}^n = 2\kappa\Delta x + C_{M-1}^n \tag{3.36}$$

and by rearranging, we obtain

$$C_M^{n+1} = A_M^n \left(B_M^n C_{M-1}^{n+1} + Q_M^n C_M^n + Z_M^n C_{M-1}^n + 2\Delta x \cdot \kappa Z_M^n \right). \tag{3.37}$$

Using Taylor series expansions on the approximation, [13] has shown that the truncation error is $O\left\{(\Delta x)^2 + (\Delta t)^2 + (\Delta t/\Delta x)^2\right\}$ or $O\left\{2, 2, (1/1)^2\right\}$.

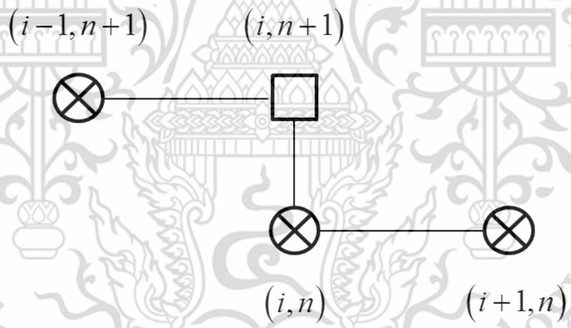


Figure 3.3: Stencil diagram of saulyev explicit finite difference scheme

3.3 Quadratic regression

Due to the soil physics affect diffusion (D) and advection (u), it can be represented by given functions. In this research, the least-squares regression is used to represent their diffusion term and advection term. First the quadratic regression is introduced as follows.

The lest-squares procedure can be readily extended to fit the data to a higher-order polynomial. Suppose that we fit a second-order polynomial or quadratic:

$$y = a_0 + a_1 x + a_2 x^2 + e. \tag{3.38}$$

For this case the sum of the squares of the residuals is

$$S_r = \sum_{i=1}^{n} \left(y_i - a_0 - a_1 x_i - a_2 {x_i}^2 \right)^2. \tag{3.39}$$

Following the procedure of the previous section, we take the derivative of Eq.(3.39) with respect to each of the unknown coefficients of the polynomial, as in

$$\frac{\partial S_r}{\partial a_0} = -2\sum \left(y_i - a_0 - a_1 x_i - a_2 {x_i}^2\right)^2, \tag{3.40}$$

$$\frac{\partial S_r}{\partial a_1} = -2\sum x_i \left(y_i - a_0 - a_1 x_i - a_2 {x_i}^2\right)^2, \tag{3.41}$$

$$\frac{\partial S_r}{\partial a_2} = -2\sum x_i^2 \left(y_i - a_0 - a_1 x_i - a_2 {x_i}^2\right)^2. \tag{3.42}$$

These equations can be set equal to zero and rearranged to develop the following set of normal equations:

$$(n)\, a_0 + \left(\sum x_i\right) a_1 + \left(\sum x_i^2\right) a_2 = \sum y_i \tag{3.43}$$

$$\left(\sum x_i\right) a_0 + \left(\sum x_i^2\right) a_1 + \left(\sum x_i^3\right) a_2 = \sum x_i y_i\,, \tag{3.44}$$

$$\left(\sum x_i^2\right) a_0 + \left(\sum x_i^3\right) a_1 + \left(\sum x_i^4\right) a_2 = \sum x_i^2 y_i\,, \tag{3.45}$$

where all $i = 1$ summation are from through n. Note that the above three equations are linear and have three unknowns: a_0 , a_1 and a_2. The coefficients of the unknowns can be calculated directly from the observed data.

3.4 Multiple linear regression

A useful extension of linear regression is the case where y is a linear function of two or more independent variables. y might be a linear function of x_1 and x_2 as in

$$y = a_0 + a_1 x_1 + a_2 {x_2}^2 + e. \tag{3.46}$$

Such an equation is particularly useful when fitting experimental data where the variable being studied is often a function of two other variables. For this two-dimensional case, the regression "line" becomes a "plane".

As with the previous cases, the "best" values of the coefficients are determined by setting up the sum of the squares of the residuals

$$S_r = \sum_{i=1}^{n} \left(y_i - a_0 - a_1 x_{1i} - a_2 {x_{2i}}^2\right)^2, \tag{3.47}$$

and differentiating with respect to each of the unknown coefficient,

$$\frac{\partial S_r}{\partial a_0} = -2\sum \left(y_i - a_0 - a_1 x_{1i} - a_2 {x_{2i}}^2\right)^2, \tag{3.48}$$

$$\frac{\partial S_r}{\partial a_1} = -2\sum x_{1i} \left(y_i - a_0 - a_1 x_{1i} - a_2 {x_{2i}}^2\right)^2, \tag{3.49}$$

$$\frac{\partial S_r}{\partial a_2} = -2\sum x_{2i}^2 \left(y_i - a_0 - a_1 x_{1i} - a_2 {x_{2i}}^2\right)^2. \tag{3.50}$$

The coefficients yielding the minimum sum of the squares of the residuals are obtained by setting the partial derivatives equal to zero ad expressing the result in matrix form as

$$\begin{bmatrix} n & \sum x_{1i} & \sum x_{2i} \\ \sum x_{1i} & \sum x_{1i}^2 & \sum x_{1i}x_{2i} \\ \sum x_{2i} & \sum x_{1i}x_{2i} & \sum x_{2i}^2 \end{bmatrix} \begin{Bmatrix} a_0 \\ a_1 \\ a_2 \end{Bmatrix} = \begin{Bmatrix} \sum y_i \\ \sum x_{1i}y_i \\ \sum x_{2i}y_i \end{Bmatrix}$$

3.5 Cubic splines

The most common piecewise-polynomial approximation uses cubic polynomials between each successive pair of nodes and is called cubic spine interpolation. A general cubic polynomial involves four constants, so there is sufficient flexibility in the cubic spline procedure to ensure that the interpolant is not only continuously differentiable on the interval, but also has a continuous second derivative. The construction of the cubic spline does not, however, assume that the derivatives of the interpolant agree with those of the function it is approximating, even at the nodes as show in Fig.3.4.

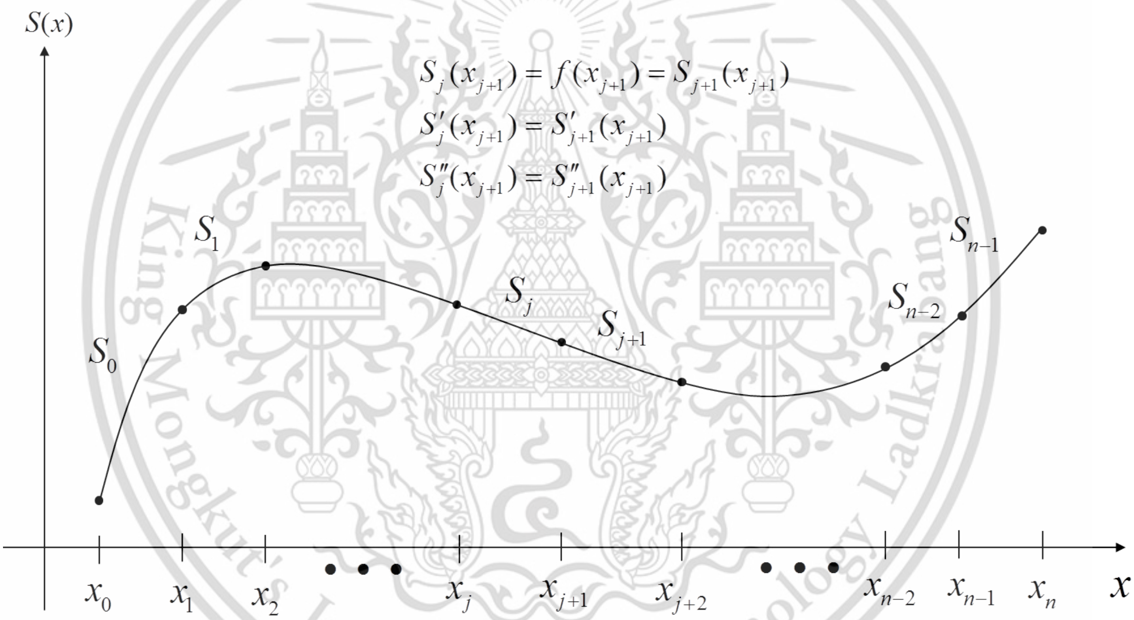


Figure 3.4: Cubic spline interpolant

Definition 3.1. Given a function f defined on $[a,b]$ and a set of nodes $a = x_0 < x_1 < \cdots < x_n = b$, a cubic spine interpolant S for f is a function that satisfies the following conditions:

(a) $S(x)$ is a cubic polynomial, denoted $S_j(x)$, on the subinterval $[x_j, x_{j+1}]$ for each $j = 0, 1, \ldots, n-1$.

(b) $S_j(x_j) = f(x_j)$ and $S_j(x_{j+1}) = f(x_{j+1})$ for each $j = 0, 1, \ldots, n-1$.

(c) $S_{j+1}(x_{j+1}) = S_j(x_{j+1})$ for each $j = 0, 1, \ldots, n-2$. (Implied by (b).)

(d) $S'_{j+1}(x_{j+1}) = S'_j(x_{j+1})$ for each $j = 0, 1, \ldots, n-2$.

(e) $S''_{j+1}(x_{j+1}) = S''_j(x_{j+1})$ for each $j = 0, 1, \ldots, n-2$.

(f) One of the following sets of boundary conditions is satisfied:

(i) $S''(x_0) = S''(x_n) = 0$ (natural (or free) boundary).

(ii) $S'(x_0) = f'(x_0)$ and $S'(x_n) = f'(x_n)$ (clamped boundary.)

Although cubic splines are defined with other boundary conditions, the conditions given if (f) are sufficient for our purposes. When the free boundary conditions occur, the spine is called a natural spline, and its graph approximates the shape that a long flexible rod would assume if forced to go through the data points $\{(x_0, f(x_0)), (x_1, f(x_1)), \ldots, (x_n, f(x_n))\}$.

In general, clamped boundary conditions lead to more accurate approximations because they include more information about the function. However, for this type of boundary condition to hold, it is necessary to have either the values of the derivative at the endpoints or an accurate approximation to those values.

3.5.1 Construction of a Cubic Spline

As the preceding example demonstrates, a spline defined on an interval that is divided into n subintervals will require determining $4n$ constants. To construct the cubic spline interpolant for a given function f, the conditions in the definition are applied to the cubic polynomials

$$S_j(x) = a_j + b_j(x - x_j) + c_j(x - x_j)^2 + d_j(x - x_j)^3, \tag{3.51}$$

for each $j = 0, 1, \ldots, n-1$. Since $S_j(x_j) = a_j = f(x_j)$, condition (c) can be applied to obtain,

$$a_{j+1} = S_{j+1}(x_{j+1}) = a_j + b_j(x_{j+1} - x_j) + c_j(x_{j+1} - x_j)^2 + d_j(x_{j+1} - x_j), \tag{3.52}$$

for $j = 0, 1, \ldots, n-2$.

Thus terms $x_{j+1} - x_j$ are used repeatedly in this development, so it is convenient to introduce the simpler notation

$$h_j = x_{j+1} + x_j$$

for each $j = 0, 1, \ldots, n-1$. If we also define $a_n = f(x_n)$, then the equation

$$a_{j+1} = a_j + b_j h_j + c_j h_j^2 + d_j h_j^3 \tag{3.53}$$

holds for each $j = 0, 1, \ldots, n-1$. In a similar manner, define $b_n = S'(x_n)$ and observe that

$$S_j'(x) = b_j + 2c_j(x - x_j) + 3d_j(x - x_j)^2.$$

Implines $S_j'(x) = b_j$, for each $j = 0, 1, \ldots, n-1$. Applying condition (d) gives

$$b_{j+1} = b_j + 2c_j h_j + 3d_j h_j^2, \tag{3.54}$$

for each $j = 0, 1, \ldots, n-1$. Another relationship between the coefficients of S_j is obtained by defining $c_n = S''(x_n)/2$ and applying condition Then,for each $j = 0, 1, \ldots, n-1$,

$$c_{j+1} = c_j + 3d_j h_j. \tag{3.55}$$

Solving for d_j in Eq.eqCubicC and substituting this value into Eqs.eqCubicA and eqCubicB gives, for each $j = 0, 1, \ldots, n-1$, the new equations

$$a_{j+1} = a_j + b_j h_j + \frac{{h_j}^2}{3}\left(2c_j + c_{j+1}\right), \tag{3.56}$$

and

$$b_{j+1} = b_j + h_j\left(c_j + c_{j+1}\right). \tag{3.57}$$

The final relationship involving the coefficients is obtained by solving the appropriate equation in the form of equation eqCubicAjplus1, first for b_j,

$$b_{j+1} = \frac{1}{h_j}\left(a_{j+1} - a_j\right) - \frac{h_j}{3}\left(2c_j + c_{j+1}\right). \tag{3.58}$$

and then, with a reduction of the index, for b_{j-1}. This gives

$$b_{j-1} = \frac{1}{h_{j-1}}\left(a_j - a_{j-1}\right) - \frac{h_{j-1}}{3}\left(2c_{j-1} + c_j\right).$$

Substituting these values into the equation derived from Eq.eqCubicBjplus1, with the index reduced by one, gives the linear system of equations,

$$h_{j-1}c_{j-1} + 2\left(h_{j-1} + h_j\right)c_j + h_j c_{j+1} = \frac{3}{h_j}\left(a_{j+1} - a_j\right) - \frac{3}{h_{j-1}}\left(a_j - a_{j-1}\right), \tag{3.59}$$

for each $j = 0, 1, \ldots, n-1$. This system involves only the $\{c_j\}_{j=0}^{n}$ as unknowns. The values of $\{h_j\}_{j=0}^{n-1}$ and $\{a_j\}_{j=0}^{n}$ are given, respectively, by the spacing of the nodes $\{x_j\}_{j=0}^{n}$ and the values of f at the nodes. So once the values of $\{c_j\}_{j=0}^{n}$ are determined, it is a simple matter to find the reminder of the constant $\{b_j\}_{j=0}^{n-1}$ from Eq.eqCubicBjplus11 and $\{d_j\}_{j=0}^{n-1}$ from Eq.eqCubicCplus1, Then we can construct the cubic polynomials $\{S_j(x)\}_{j=0}^{n-1}$

Theorem 3.1. If f is defined at $a = x_0 < x_1 < \cdots < x_n = b$, then f has a unique natural soline interpolant S on the nodes $x_0, x_1, \ldots, x_n$; that is, a spline interpolant that satisfies the natural boundary conditions $S''(a) = 0$ and $S''(b) = 0$.

Example 1 : At the beginning of Chapter 3 we gave some Taylor polynomials to approximate the exponential $f(x) = e^x$. Use the data points $(0,1), (1,e), (2,e^2)$, and $(3,e^3)$ to form a natural spline $S(x)$ that approximates $f(x) = e^x$. We have $n = 3, h_0 = h_1 = h_2 = 1, a_0 = 1, a_1 = e, a_2 = e^2$, and $a_3 = e^3$. So the matrix A and the vectors v and given in Theorem 3.1 have the forms

$A = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 1 & 4 & 1 & 0 \\ 0 & 1 & 4 & 1 \\ 0 & 0 & 0 & 1 \end{bmatrix}, v = \begin{bmatrix} 0 \\ 3\left(e^2 - 2e + 1\right) \\ 3\left(e^3 - 2e^2 + e\right) \\ 0 \end{bmatrix}$, and $x_c = \begin{bmatrix} c_0 \\ c_1 \\ c_2 \\ c_3 \end{bmatrix}$. The vector-matrix equation $Ax_c = v$ is equivalent to the system of equations

$$\begin{aligned} c_0 &= 0 \\ c_0 + 4c_1 + c_2 &= 3\left(e^2 - 2e + 1\right), \\ c_1 + 4c_2 + c_3 &= 3\left(e^3 - 2e^2 + e\right), \\ c_0 &= 0 \end{aligned}$$

This system has the solution $c_0 = c_3 = 0$, and to 5 decimal places,
$c_1 = \frac{1}{5}\left(-e^3 + 6e^2 - 9e + 4\right) \approx 0.75685$, and $c_2 = \frac{1}{5}\left(4e^3 - 9e^2 + 6e - 1\right) \approx 5.83007$.
Solving for the remaining constants gives

$$\begin{aligned}
b_0 &= \frac{1}{h_0}\left(a_1 - a_0\right) - \frac{h_0}{3}\left(c_1 + 2c_0\right) \\
&= (e-1) - \frac{1}{15}\left(-e^3 + 6e^2 - 9e + 4\right) \approx 1.46600, \\
b_1 &= \frac{1}{h_1}\left(a_2 - a_1\right) - \frac{h_1}{3}\left(c_2 + 2c_1\right) \\
&= \left(e^2 - e\right) - \frac{1}{15}\left(2e^3 + 3e^2 - 12e + 7\right) \approx 2.22285, \\
b_2 &= \frac{1}{h_2}\left(a_3 - a_2\right) - \frac{h_2}{3}\left(c_3 + 2c_2\right) \\
&= \left(e^3 - e^2\right) - \frac{1}{15}\left(8e^3 - 18e^2 + 12e - 2\right) \approx 8.80977, \\
d_0 &= \frac{1}{3h_0}\left(c_1 - c_0\right) = \frac{1}{15}\left(-e^3 + 6e^2 - 9e + 4\right) \approx 0.25228, \\
d_1 &= \frac{1}{3h_1}\left(c_2 - c_1\right) = \frac{1}{15}\left(e^3 - 3e^2 + 3e - 1\right) \approx 1.69107, \\
d_2 &= \frac{1}{3h_2}\left(c_3 - c_2\right) = \frac{1}{15}\left(-4e^3 + 9e^2 - 6e + 1\right) \approx -1.94336.
\end{aligned}$$

The natural cubic spine is described piecewise by

$$S\left(x\right) = \begin{cases} 1 + 1.46600x + 0.25228x^3, & for\, x \in [0,1] \\ 2.71828 + 2.22285\left(x-1\right) + 0.75685(x-1)^2 + 1.69107(x-1)^3, & for\, x \in [1,2] \\ 7.38906 + 8.80977\left(x-2\right) + 5.83007(x-2)^2 - 1.94336(x-2)^3, & for\, x \in [2,3] \end{cases}$$

The spline and its agreement with $f\left(x\right) = e^x$

Chapter 4

Numerical experiments and results

4.1 The accuracy of the proposed numerical technique

The variation in velocity is assumed as small order to insure that it can satisfy the essential conditions for velocity parameter in the ADE. Additionally, as the second assumption, dispersion parameter is considered proportional to the square of the velocity [9]. Thus, for Eq.(2.4), the expressions of $f_1(x,t)$ and $f_2(x,t)$ are assumed by [6]:

$$f_1(x,t) = (1+ax)^2, \tag{4.1}$$

$$f_2(x,t) = 1+ax, \tag{4.2}$$

where a is a parameter that accounts for the inhomogeneity of the domain with dimension $(length)^{-1}$ In [6] , they have introduced an analytical solution that satisfies the specific $f_1(x,t)$ and $f_2(x,t)$ as in Eq.(4.1) and Eq.(4.2) ,

$$C = \frac{c_0}{2}\left[(1+ax)^{-1}\textit{\textbf{erfc}}\left(\frac{\ln(1+ax)}{2a\sqrt{D_0T}} - \beta\sqrt{t}\right) + (1+ax)^{\delta}\textit{\textbf{erfc}}\left(\frac{\ln(1+ax)}{2a\sqrt{D_0T}} + \beta\sqrt{t}\right)\right], \tag{4.3}$$

where

$$\omega_0 = (au_0 - a^2D_0) \tag{4.4}$$

$$\delta = \frac{u_0}{aD_0}, \tag{4.5}$$

$$\beta = \sqrt{\frac{\omega_0^2}{4a^2D_0} + au_0} = \frac{u_0 + aD_0}{2\sqrt{D_0}}. \tag{4.6}$$

4.2 Simulation 1: Two monitoring contaminated groundwater points; forward time central space finite difference scheme technique for an ideal contaminated groundwater dispersion measurement.

Assuming that the chemical dispersion through inhomogeneous soil the diffusion coefficient and flow velocity field are averaged to be $D_0 = 0.71$ (km²/year) and $u_0 = 0.6$ (km/year), respectively. The parameter that accounts for the inhomogeneity of the soil is assumed by $a = 1.0$ (km^{-1}) and $f_1(x,t) = (1+x)^2$ and $f_2(x,t) = 1+x$. The boundary conditions and the initial condition are assumed by Eq.(4.3). By employing the propose finite difference technique Eq.(3.16), we get the chemical concentration in Tables 4.1-4.3 when time increment (Δt) are varied and $\lambda = \Delta t \big/ (\Delta x)^2$ is divided by a half. The surface of approximated solutions is illustrated in Fig 4.1.

Table 4.1: The approximated chemical concentration in a heterogeneous soil ($\Delta x = 0.05\ (km)$, $\Delta t = 0.000125\,(year)$, $\lambda = 0.2$), where $\lambda = \Delta t/\Delta x^2$.

t/x	0.1	0.2	0.3	0.4	0.5	0.6	0.7	0.8	0.9	1.0
0.2	0.83862	0.70228	0.58759	0.49144	0.41106	0.34398	0.28806	0.24146	0.20263	0.17027
0.5	0.88114	0.78073	0.69509	0.62143	0.55765	0.50210	0.45347	0.41069	0.37291	0.33942
0.7	0.89079	0.79881	0.72039	0.65285	0.59416	0.54281	0.49757	0.45749	0.42181	0.38990

Table 4.2: The approximated chemical concentration in a heterogeneous soil ($\Delta x = 0.05\ (km)$, $\Delta t = 0.000125\,(year)$, $\lambda = 0.1$), where $\lambda = \Delta t/\Delta x^2$.

t/x	0.1	0.2	0.3	0.4	0.5	0.6	0.7	0.8	0.9	1.0
0.2	0.83856	0.70217	0.58745	0.49130	0.41092	0.34386	0.28796	0.24139	0.20260	0.17027
0.5	0.88113	0.78073	0.69508	0.62142	0.55764	0.50209	0.45346	0.41068	0.37291	0.33942
0.7	0.89079	0.79881	0.72039	0.65284	0.59416	0.54280	0.49756	0.45749	0.42181	0.38990

Table 4.3: The approximated chemical concentration in a heterogeneous soil ($\Delta x = 0.05\ (km)$, $\Delta t = 0.000125\,(year)$, $\lambda = 0.05$), where $\lambda = \Delta t/\Delta x^2$.

t/x	0.1	0.2	0.3	0.4	0.5	0.6	0.7	0.8	0.9	1.0
0.2	0.83853	0.70212	0.58738	0.49122	0.41085	0.34380	0.28791	0.24136	0.20258	0.17027
0.5	0.88113	0.78072	0.69507	0.62141	0.55763	0.50209	0.45345	0.41068	0.37291	0.33942
0.7	0.89079	0.79881	0.72038	0.65284	0.59416	0.54280	0.49756	0.45749	0.42181	0.38990

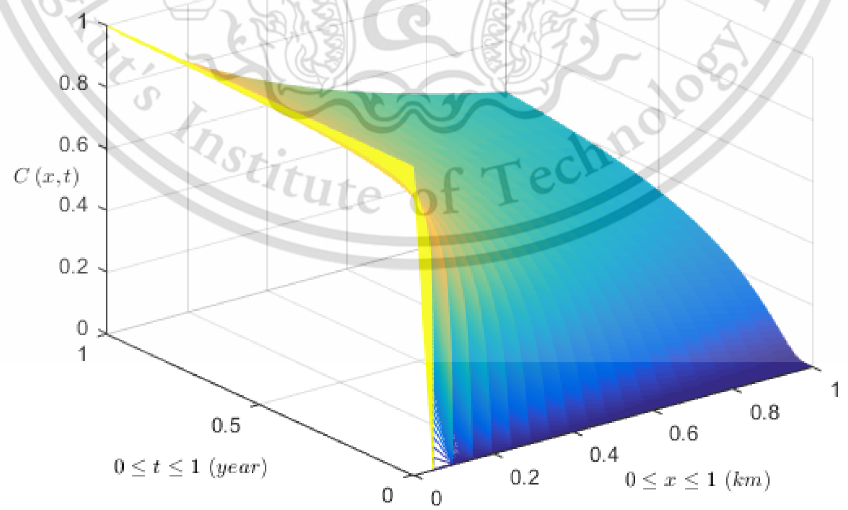


Figure 4.1: The surface plot of computed chemical concentrations $\tilde{C}\,(x,t)$ for all $(x,t) \in [0,1]\times[0,1]$.

4.3 Simulation 2: Two monitoring contaminated groundwater points; Saulyev Explicit Finite Difference Scheme technique for an ideal contaminated groundwater dispersion measurement.

Assuming that the chemical dispersion through inhomogeneous soil the diffusion coefficient and flow velocity field are averaged to be $D_0 = 0.71$ (km²/year) and $u_0 = 0.6$ (km/year), respectively. The parameter that accounts for the inhomogeneity of the soil is assumed by $a = 1.0$ (km^{-1}) and $f_1(x,t) = (1+x)^2$ and $f_2(x,t) = 1 + x$. The boundary conditions and the initial condition are assumed by Eq.(4.3). By employing the propose finite difference technique Eq.(3.35), we get the chemical concentration in Tables 4.4-4.6 when time increment (Δt) are varied and $\lambda = \Delta t \big/ (\Delta x)^2$ is divided by a half. The surface of approximated solutions is illustrated in Fig 4.2.

Table 4.4: The approximated chemical concentration in a heterogeneous soil ($\Delta x = 0.05\ (km)$, $\Delta t = 0.000125\,(year)$, $\lambda = 0.2$), where $\lambda = \Delta t/\Delta x^2$.

t/x	0.1	0.2	0.3	0.4	0.5	0.6	0.7	0.8	0.9	1.0
0.2	0.83801	0.70138	0.58663	0.49057	0.41034	0.34344	0.28769	0.24124	0.20253	0.17027
0.5	0.88084	0.78024	0.69449	0.62080	0.55704	0.50156	0.45303	0.41038	0.37275	0.33942
0.7	0.89063	0.79854	0.72006	0.65249	0.59382	0.54250	0.49732	0.45731	0.42172	0.38990

Table 4.5: The approximated chemical concentration in a heterogeneous soil ($\Delta x = 0.05\ (km)$, $\Delta t = 0.000125\,(year)$, $\lambda = 0.1$), where $\lambda = \Delta t/\Delta x^2$.

t/x	0.1	0.2	0.3	0.4	0.5	0.6	0.7	0.8	0.9	1.0
0.2	0.83825	0.70172	0.58697	0.49086	0.41056	0.34359	0.28777	0.24128	0.20255	0.17027
0.5	0.88098	0.78048	0.69478	0.62110	0.55734	0.50182	0.45324	0.41053	0.37283	0.33942
0.7	0.89071	0.79868	0.72022	0.65266	0.59399	0.54265	0.49744	0.45740	0.42176	0.38990

Table 4.6: The approximated chemical concentration in a heterogeneous soil ($\Delta x = 0.05\ (km)$, $\Delta t = 0.000125\,(year)$, $\lambda = 0.05$), where $\lambda = \Delta t/\Delta x^2$.

t/x	0.1	0.2	0.3	0.4	0.5	0.6	0.7	0.8	0.9	1.0
0.2	0.83837	0.70189	0.58714	0.49100	0.41067	0.34366	0.28782	0.24130	0.20256	0.17027
0.5	0.88106	0.78060	0.69492	0.62125	0.55748	0.50195	0.45334	0.41060	0.37287	0.33942
0.7	0.89075	0.79874	0.72030	0.65275	0.59407	0.54272	0.49750	0.45744	0.42179	0.38990

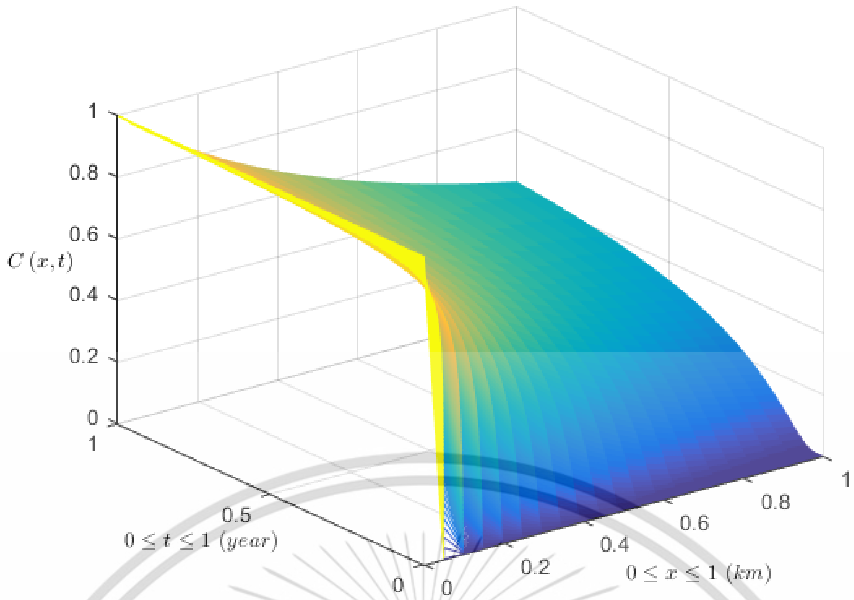


Figure 4.2: The surface plot of computed chemical concentrations $\tilde{C}(x,t)$ for all $(x,t) \in [0,1]\times[0,1]$.

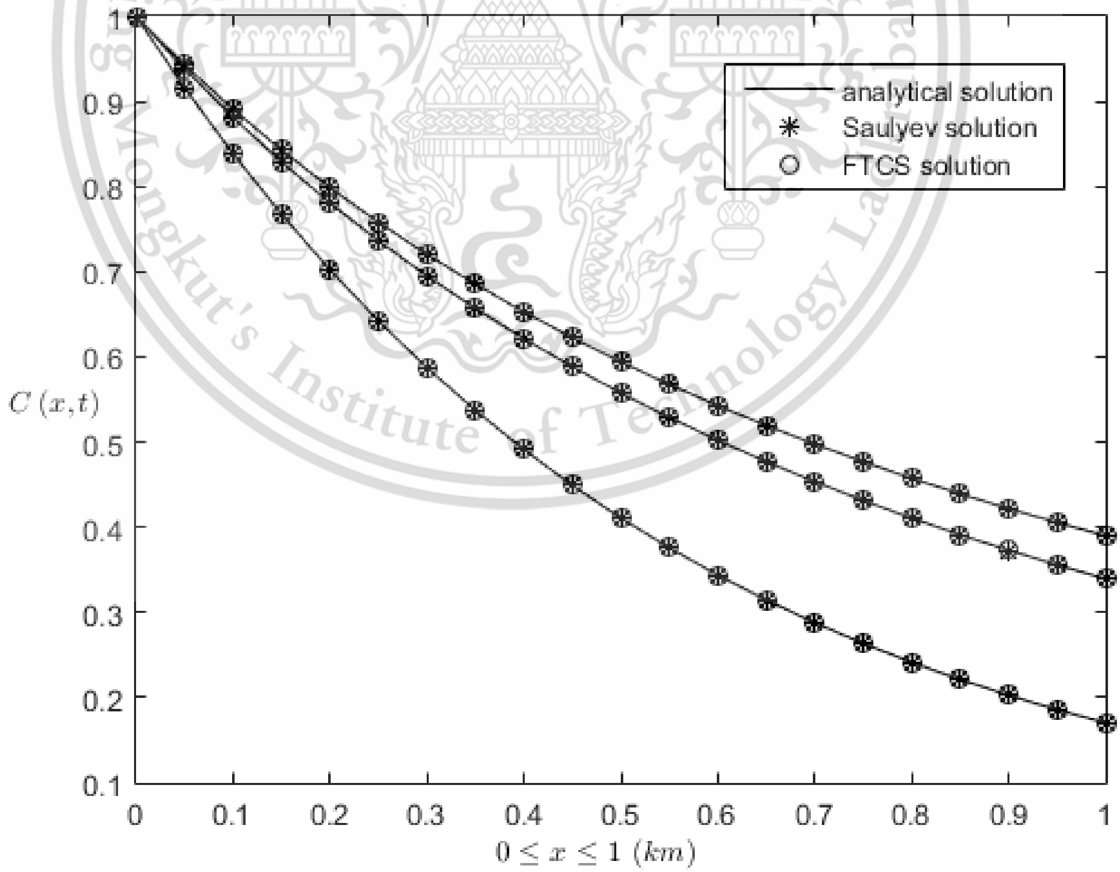


Figure 4.3: The comparison of FTCS scheme and the Saulyev scheme and the analytical solution when $t = 0.2$, 0.5 and 0.7

Table 4.7: The comparison the root mean square error of FTCS solutions and Saulyev solutions

λ	Δx	Δt	$FTCS\ RSME_{\text{max}}$	$Saulyev\ RSME_{\text{max}}$
0.025	0.050	6.2500×10^{-5}	1.2361×10^{-2}	1.5604×10^{-2}
	0.025	1.5625×10^{-5}	8.5507×10^{-3}	1.0739×10^{-2}
0.050	0.050	1.2500×10^{-4}	8.9331×10^{-3}	1.5631×10^{-2}
	0.025	3.1250×10^{-5}	6.2175×10^{-3}	1.0755×10^{-2}
0.100	0.050	2.5000×10^{-4}	2.5368×10^{-3}	1.5170×10^{-2}
	0.025	6.2500×10^{-5}	1.9303×10^{-3}	1.0466×10^{-2}
0.200	0.050	5.0000×10^{-4}	1.5331×10^{-2}	1.5476×10^{-2}
	0.025	1.2500×10^{-4}	1.0200×10^{-2}	1.0649×10^{-2}
0.400	0.050	1.0000×10^{-3}	Unstable	1.4332×10^{-2}
	0.025	2.5000×10^{-4}	Unstable	9.4084×10^{-3}
0.800	0.050	2.0000×10^{-3}	Unstable	2.4844×10^{-2}
	0.025	5.0000×10^{-4}	Unstable	1.5746×10^{-2}

Table 4.8: The maximum error of approximated pollutant concentration at $x = 0.25, 0.50, 0.75$ for all $t \in [0, 1]$

Δx	Δt	Maximum error		
		$x = 0.25$	$x = 0.50$	$x = 0.75$
0.1	6.2500×10^{-5}	4.7209×10^{-3}	2.5689×10^{-3}	1.4949×10^{-3}
0.050	3.1250×10^{-5}	2.9954×10^{-3}	1.4627×10^{-3}	8.2912×10^{-4}
0.025	1.5625×10^{-5}	2.1662×10^{-3}	9.1606×10^{-4}	4.9769×10^{-4}

4.4 Simulation 3: The single monitoring contaminated groundwater when there is no rate of change of pollutant concentration around the ended-point; Saulyev Explicit Finite Difference Scheme technique for an ideal contaminated groundwater dispersion measurement.

Assuming that the chemical dispersion through inhomogeneous soil the diffusion coefficient and flow velocity field are averaged to be $D_0 = 0.71$ (km²/year) and $u_0 = 0.6$ (km/year), respectively. The parameter that accounts for the inhomogeneity of the soil is assumed by $a = 1.0$ (km^{-1}) and $f_1(x,t) = (1+x)^2$ and $f_2(x,t) = 1 + x$. The boundary conditions and the initial condition are assumed $C(0,t) = 1,\ \frac{\partial C}{\partial x}(1,t) = 0$, for all $t \in [0,1]$ and $C(x,0) = 0$, for all $x \in [0,1]$, respectively. By employing the propose finite difference technique Eq.(3.35) and Eq.(3.37), we get the chemical concentration in Tables 4.9. The surface of approximated solutions is illustrated in Fig 4.4.

Table 4.9: The approximated chemical concentration in a heterogeneous soil ($\Delta x = 0.05\ (km)$, $\Delta t = 0.000125\,(year)$, $\lambda = 0.05$), where $\lambda = \Delta t/\Delta x^2$.

t/x	0.1	0.2	0.3	0.4	0.5	0.6	0.7	0.8	0.9	1.0
0.2	0.84921	0.72410	0.62234	0.54142	0.47886	0.43232	0.39967	0.37899	0.36860	0.36700
0.5	0.92416	0.86342	0.81526	0.77767	0.74899	0.72786	0.71313	0.70384	0.69918	0.69846
0.7	0.94083	0.89443	0.85824	0.83034	0.80926	0.79384	0.78314	0.77642	0.77305	0.77254

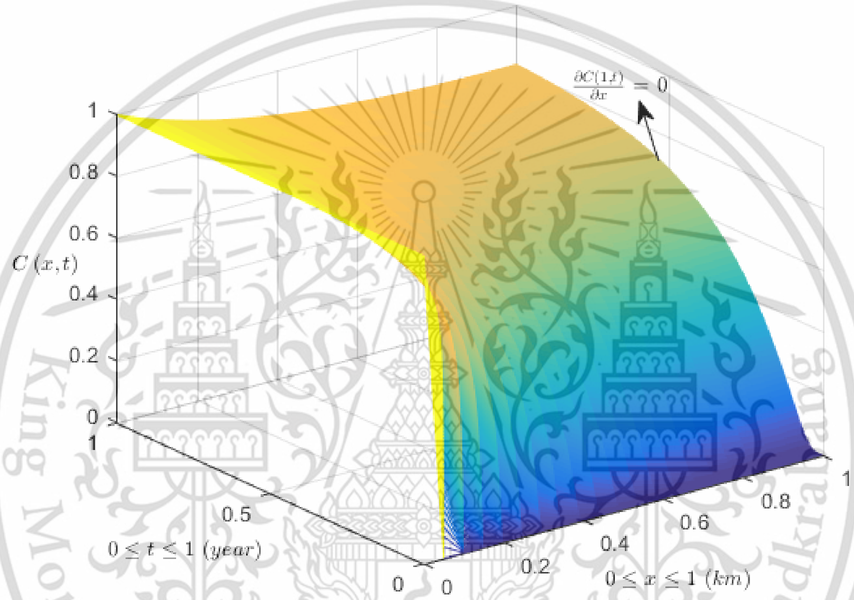


Figure 4.4: The surface plot of computed chemical concentrations $\tilde{C}\,(x,t)$ for all $(x,t) \in [0,1]\times[0,1]$.

4.5 Simulation 4: The single monitoring contaminated groundwater point when there is groundwater pollution flowing into the ended-point; Saulyev Explicit Finite Difference Scheme technique for an ideal contaminated groundwater dispersion measurement.

Assuming that the chemical dispersion through inhomogeneous soil the diffusion coefficient and flow velocity field are averaged to be $D_0 = 0.71$ (km^2/year) and $u_0 = 0.6$ (km/year), respectively. The parameter that accounts for the inhomogeneity of the soil is assumed by $a = 1.0$ (km^{-1}) and $f_1\,(x,t) = (1+x)^2$ and $f_2\,(x,t) = 1+x$. The boundary conditions and the initial condition are assumed $C(0,t) = 1$, $\frac{\partial C}{\partial x}(1,t) = 0.015$, for all $t \in [0,1]$ and $C(x,0) = 0$, for all $x \in [0,1]$, respectively. By employing the propose finite difference technique Eq.(3.35) and Eq.(3.37), we get the chemical concentration in Tables 4.10. The surface of approximated solutions is illustrated in Fig 4.5.

Table 4.10: The approximated chemical concentration in a heterogeneous soil ($\Delta x = 0.05\ (km)$, $\Delta t = 0.000125\,(year)$, $\lambda = 0.05$), where $\lambda = \Delta t / \Delta x^2$.

t/x	0.1	0.2	0.3	0.4	0.5	0.6	0.7	0.8	0.9	1.0
0.2	0.84922	0.72413	0.62238	0.54148	0.47894	0.43242	0.39978	0.37913	0.36875	0.36717
0.5	0.92419	0.86347	0.81534	0.77777	0.74912	0.72801	0.71330	0.70403	0.69939	0.69869
0.7	0.94087	0.89449	0.85832	0.83045	0.80940	0.79400	0.78332	0.77662	0.77328	0.77278

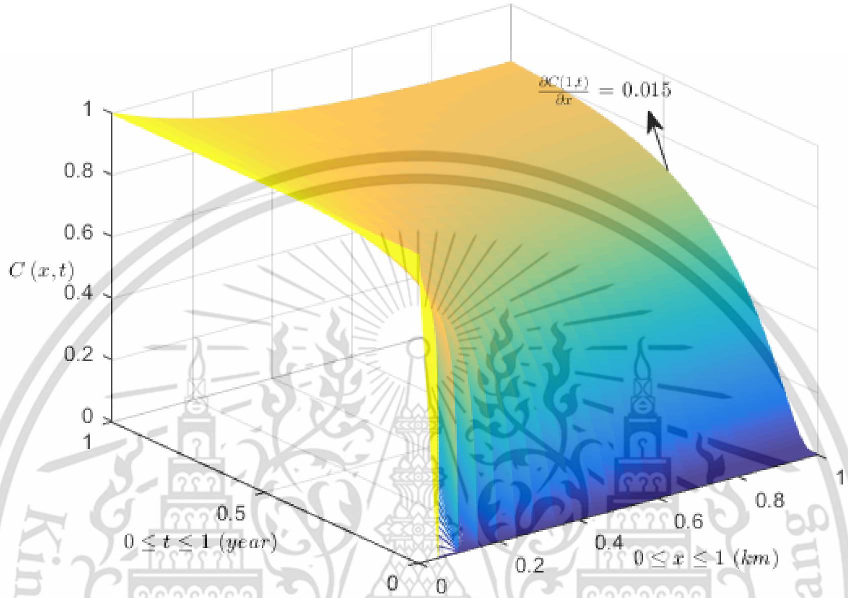


Figure 4.5: The surface plot of computed chemical concentrations $\tilde{C}(x,t)$ for all $(x,t) \in [0,1]\times[0,1]$.

4.6 Simulation 5: The single monitoring contaminated groundwater point when there is groundwater pollution flowing outward at ended-point; Saulyev Explicit Finite Difference Scheme technique for an ideal contaminated groundwater dispersion measurement.

Assuming that the chemical dispersion through inhomogeneous soil the diffusion coefficient and flow velocity field are averaged to be $D_0 = 0.71$ (km^2/year) and $u_0 = 0.6$ (km/year), respectively. The parameter that accounts for the inhomogeneity of the soil is assumed by $a = 1.0$ (km^{-1}) and $f_1(x,t) = (1+x)^2$ and $f_2(x,t) = 1 + x$. The boundary conditions and the initial condition are assumed $C(0,t) = 1$, $\frac{\partial C}{\partial x}(1,t) = -0.015$, for all $t \in [0,1]$ and $C(x,0) = 0$, for all $x \in [0,1]$, respectively. By employing the propose finite difference technique Eq.(3.35) and Eq.(3.37), we get the chemical concentration in Tables 4.11. The surface of approximated solutions is illustrated in Fig 4.6.

Table 4.11: The approximated chemical concentration in a heterogeneous soil ($\Delta x = 0.05\ (km)$, $\Delta t = 0.000125\,(year)$, $\lambda = 0.05$), where $\lambda = \Delta t/\Delta x^2$.

t/x	0.1	0.2	0.3	0.4	0.5	0.6	0.7	0.8	0.9	1.0
0.2	0.84919	0.72407	0.62229	0.54136	0.47878	0.43223	0.39956	0.37886	0.36845	0.36683
0.5	0.92413	0.86336	0.81518	0.77757	0.74886	0.72771	0.71296	0.70365	0.69897	0.69823
0.7	0.94080	0.89437	0.85815	0.83023	0.80912	0.79368	0.78296	0.77621	0.77283	0.77229

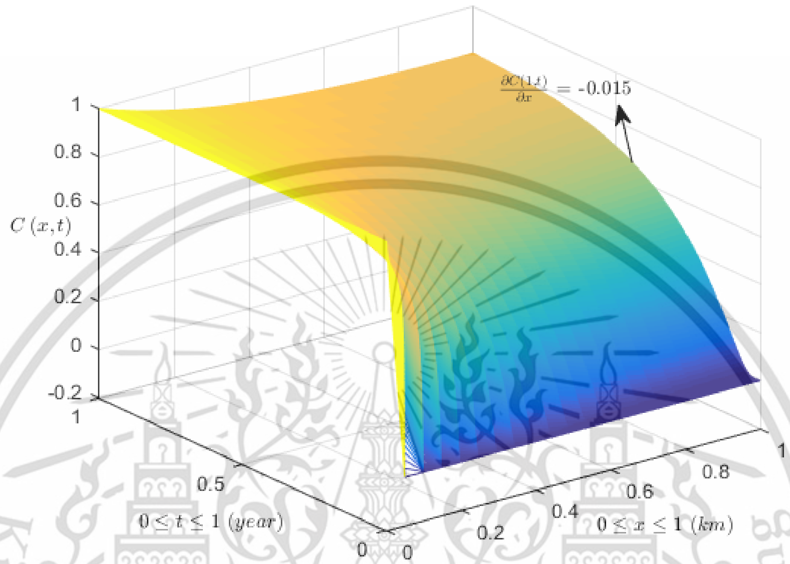


Figure 4.6: The surface plot of computed chemical concentrations $\tilde{C}\,(x,t)$ for all $(x,t) \in [0,1]\times[0,1]$.

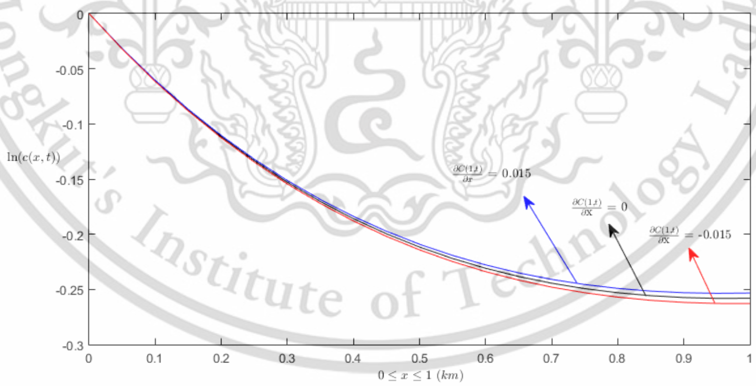


Figure 4.7: The comparison of FTCS solutions of solution 2 , solution 3 and solution 4 when $t = 0.7$

4.7 Simulation 6: The single monitoring contaminated groundwater point when there is no rate of change of pollutant concentration around the ended-point in a high mixed soil topography; Saulyev Explicit Finite Difference Scheme technique for an ideal contaminated groundwater dispersion measurement.

Assuming that the chemical dispersion through high mixed inhomogeneous soil $f_1(x,t) = \sin(x)(1+x)^2$, and $f_2(x,t) = \sin(x)(1+x)$. The diffusion coefficient and flow velocity field are averaged to be $D_0 = 0.71$ (km^2/year) and $u_0 = 0.6$ (km/year), respectively. The parameter that accounts for the inhomogeneity of the soil is assumed by $a = 1.0$ (km^{-1}). The boundary conditions and the initial condition are assumed $C(0,t) = 1$, $\frac{\partial C}{\partial x}(1,t) = 0$, for all $t \in [0,1]$, and $C(x,0) = 0$, for all $x \in [0,1]$, respectively. By employing the propose finite difference technique Eq.(3.35) and Eq.(3.37), we get the chemical concentration in Tables 4.12. The surface of approximated solutions is illustrated in Fig 4.8.

Table 4.12: The approximated chemical concentration in a heterogeneous soil ($\Delta x = 0.05\ (km)$, $\Delta t = 0.000125\ (year)$, $\lambda = 0.05$), where $\lambda = \Delta t/\Delta x^2$.

t/x	0.1	0.2	0.3	0.4	0.5	0.6	0.7	0.8	0.9	1.0
0.2	0.13435	0.03968	0.01457	0.00609	0.0028	0.00139	0.00075	0.00044	0.00031	0.00027
0.5	0.23427	0.11088	0.06247	0.03896	0.026294	0.01909	0.01493	0.01261	0.01147	0.01115
0.7	0.26724	0.14103	0.08805	0.06073	0.04527	0.03614	0.03072	0.02763	0.02610	0.02566

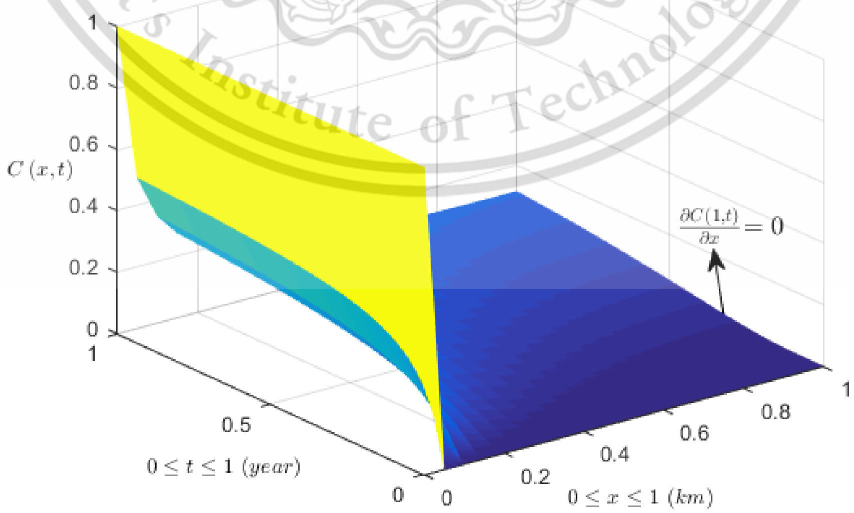


Figure 4.8: The surface plot of computed chemical concentrations $\tilde{C}(x,t)$ for all $(x,t) \in [0,1]\times[0,1]$.

4.8 Simulation 7: The single monitoring contaminated groundwater point when there is no rate of change of pollutant concentration around the ended-point; Saulyev Explicit Finite Difference Scheme technique for an ideal contaminated groundwater dispersion measurement with long run simulation.

Assuming that the chemical dispersion through inhomogeneous soil the diffusion coefficient and flow velocity field are averaged to be $D_0 = 0.71$ (km²/year) and $u_0 = 0.6$ (km/year), respectively. The parameter that accounts for the inhomogeneity of the soil is assumed by $a = 1.0$ (km^{-1}) and $f_1(x,t) = (1+x)^2$, and $f_2(x,t) = (1+x)$. The boundary conditions and the initial condition are assumed $C(0,t) = 1$, $\frac{\partial C}{\partial x}(3,t) = 0$, for all $t \in [0, 16.67]$, and $C(x,0) = 0$, for all $x \in [0,3]$, respectively. By employing the propose finite difference technique Eq.(3.35) and Eq.(3.37), we get the chemical concentration in Tables 4.13. The surface of approximated solutions is illustrated in Fig 4.9.

Table 4.13: The approximated chemical concentration in a heterogeneous soil ($\Delta x = 0.05\ (km)$, $\Delta t = 0.000125\,(year)$, $\lambda = 0.05$), where $\lambda = \Delta t/\Delta x^2$.

t/x	0.1	0.2	0.3	0.4	0.5	0.6	0.7	0.8	0.9	1.0
0.2	0.76944	0.62509	0.52613	0.45404	0.39931	0.35679	0.32373	0.29912	0.28337	0.27849
0.5	0.76952	0.62536	0.52672	0.45508	0.40091	0.35900	0.3266	0.30250	0.28713	0.28238
0.7	0.76952	0.62536	0.52673	0.45508	0.40091	0.35900	0.32657	0.30250	0.28714	0.28238

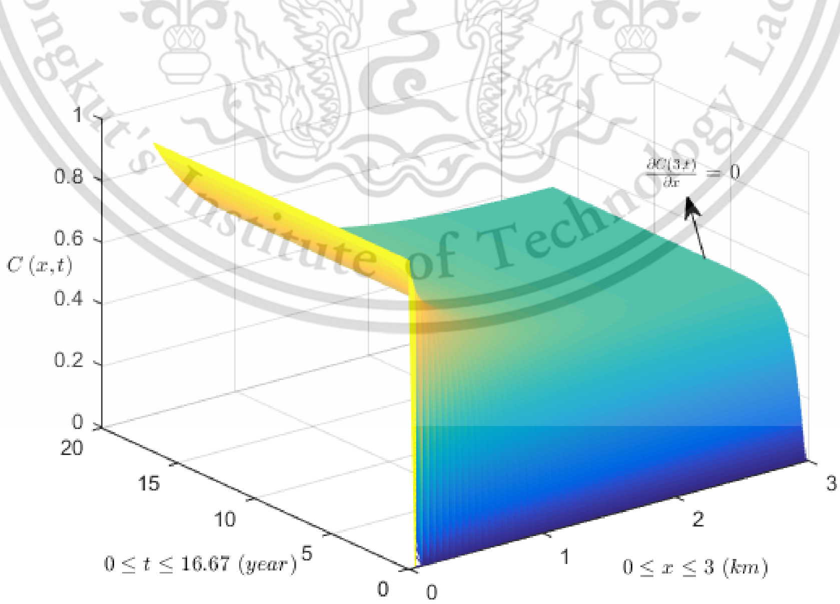


Figure 4.9: The surface plot of computed chemical concentrations $\tilde{C}(x,t)$ for all $(x,t) \in [0,3] \times [0, 16.67]$.

4.9 Simulation 8: Two monitoring contaminated groundwater points; Saulyev Explicit Finite Difference Scheme technique for an ideal contaminated groundwater dispersion measurement with the interpolated right boundary condition functions.

Assuming that the chemical dispersion through inhomogeneous soil the diffusion coefficient and flow velocity field are averaged to be $D_0 = 0.71$ (km²/year) and $u_0 = 0.6$ (km/year), respectively. The parameter that accounts for the inhomogeneity of the soil is assumed by $a = 1.0$ (km^{-1}) and $f_1(x,t) = (1+x)^2$ and $f_2(x,t) = 1+x$. The left boundary condition and the initial condition are assumed by Eq.(4.3) and The right boundary condition is interpolated functions. By employing the propose finite difference technique Eq.(3.35), prediction of a field data at the boundary can be obtained by using an multiple regression, the quadratic regression and the cubic splines interpolated right boundary condition Eqs.(3.38),(3.46) and (3.51). The interpolation is used to interpolate the right boundary condition,

$$C(1,t) = \tilde{g}_2(t) \tag{4.7}$$

at $t \in [0,1]$, where $\tilde{g}_2(t)$ is interpolated function.

We get the chemical concentration in Tables.4.14-4.16. The maximum root mean square error of approximated pollutant concentration with the interpolated right boundary condition functions is shown in Table.4.17 and the root mean square error of interpolated right boundary condition functions is shown in Table.4.18. The maximum error of interpolated right boundary condition functions is shown in Table.4.19. The surface plot of computed chemical concentration in a heterogeneous soil with the multiple regression, the quadratic regression and the the cubic splines interpolated as show in Figs.4.10-4.12 respectively. The comparison of the multiple regression, the quadratic regression and the the cubic splines interpolated right boundary condition functions and the analytical solution as show in Figs.4.13-4.16 respectively.

Table 4.14: The approximated chemical concentration in a heterogeneous soil with the multiple regression interpolated right boundary condition functions. ($\Delta x = 0.05\ (km)$, $\Delta t = 0.000125\,(year)$, $\lambda = 0.05$), where $\lambda = \Delta t/\Delta x^2$.

t/x	0.1	0.2	0.3	0.4	0.5	0.6	0.7	0.8	0.9	1.0
0.2	0.84462	0.71317	0.60200	0.50785	0.42779	0.35932	0.30029	0.24890	0.20370	0.16350
0.5	0.87462	0.76826	0.67707	0.59819	0.52949	0.46933	0.41639	0.36967	0.32831	0.29165
0.7	0.88627	0.79045	0.70891	0.63899	0.57868	0.52642	0.48101	0.44148	0.40705	0.37708

Table 4.15: The approximated chemical concentration in a heterogeneous soil with the quadratic regression interpolated right boundary condition functions. ($\Delta x = 0.05\ (km)$, $\Delta t = 0.000125\ (year)$, $\lambda = 0.05$), where $\lambda = \Delta t/\Delta x^2$.

t/x	0.1	0.2	0.3	0.4	0.5	0.6	0.7	0.8	0.9	1.0
0.2	0.83950	0.70383	0.58945	0.49316	0.41212	0.34380	0.28606	0.23708	0.19535	0.15963
0.5	0.87988	0.77848	0.69212	0.61806	0.55420	0.49888	0.45079	0.40887	0.37225	0.34019
0.7	0.89179	0.80082	0.72346	0.65707	0.59964	0.54961	0.50575	0.46709	0.43284	0.40233

Table 4.16: The approximated chemical concentration in a heterogeneous soil with the cubic splines interpolated right boundary condition functions. ($\Delta x = 0.05\ (km)$, $\Delta t = 0.000125\ (year)$, $\lambda = 0.05$)

t/x	0.1	0.2	0.3	0.4	0.5	0.6	0.7	0.8	0.9	1.0
0.2	0.83837	0.70189	0.58714	0.49100	0.41067	0.34366	0.28782	0.24130	0.20256	0.17027
0.5	0.88106	0.78060	0.69492	0.62125	0.55748	0.50195	0.45334	0.41060	0.37287	0.33942
0.7	0.89075	0.79874	0.7203	0.65275	0.59407	0.54272	0.49750	0.45744	0.42179	0.38990

Table 4.17: The maximum root mean square error of approximated pollutant concentration with the interpolated right boundary condition functions to the analytical solution (Eq.4.3) for all $t \in [0, 1]$.

Δx	Δt	$RMSE_{max}(C)$		
		multiple regression	quadratic regression	cubic splines
0.050	5.00×10^{-4}	4.6636×10^{-2}	1.5553×10^{-2}	1.5476×10^{-2}
0.050	2.50×10^{-4}	4.5052×10^{-2}	1.5246×10^{-2}	1.5170×10^{-2}
0.050	1.25×10^{-4}	1.5681×10^{-2}	1.5681×10^{-2}	1.5631×10^{-2}

Table 4.18: The root mean square error of interpolated right boundary condition functions to the analytical solution (Eq.4.3). $RMSE(T_{g_2}) = \sqrt{\frac{\sum_{n=0}^{T}(\tilde{g}_2(t_n)-g_2(t_n))}{N}}$ for all $t \in [0, 1]$

Δx	Δt	$RMSE(T_{g_2})$		
		multiple regression	quadratic regression	cubic splines
0.050	5.00×10^{-4}	4.4944×10^{-2}	1.1555×10^{-2}	2.1187×10^{-10}
0.050	2.50×10^{-4}	4.4934×10^{-2}	1.1552×10^{-2}	3.6933×10^{-11}
0.050	1.25×10^{-4}	4.4929×10^{-2}	1.1550×10^{-2}	6.5177×10^{-12}

Table 4.19: The maximum error of interpolated right boundary condition functions to the analytical solution (Eq.4.3). $E(T_{g_2}) = max\,|\tilde{g}_2(t) - g_2(t)|$ for all $t \in [0, 1]$.

Δx	Δt	$E(T_{g_2})$		
		multiple regression	quadratic regression	cubic splines
0.050	5.00×10^{-4}	9.1775×10^{-2}	2.3918×10^{-2}	8.9845×10^{-9}
0.050	2.50×10^{-4}	9.1796×10^{-2}	2.3952×10^{-2}	2.2461×10^{-9}
0.050	1.25×10^{-4}	9.1806×10^{-2}	2.3969×10^{-2}	5.6153×10^{-10}

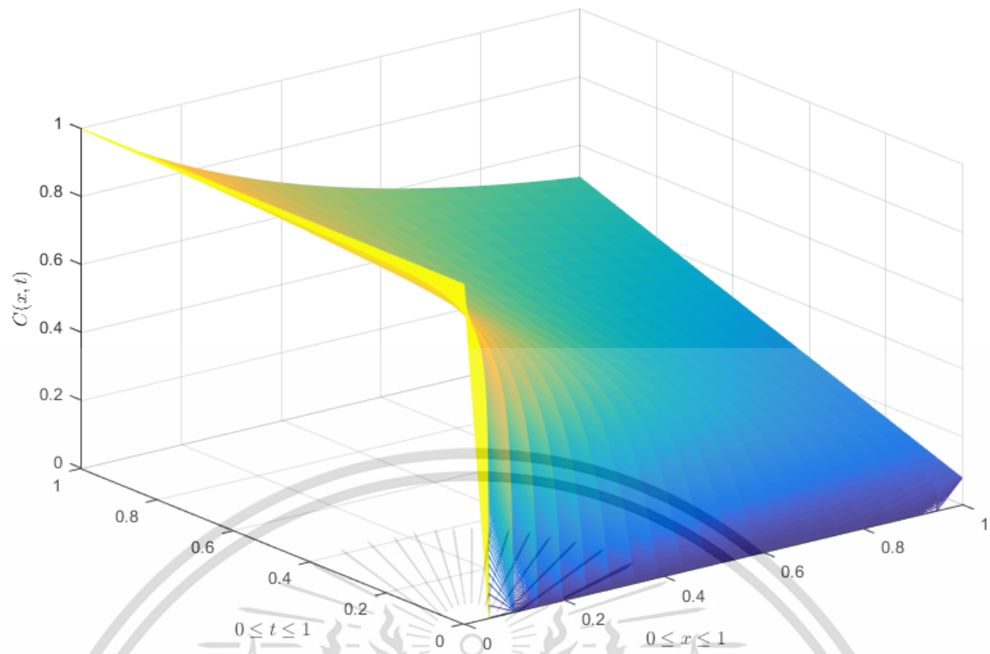


Figure 4.10: The surface plot of computed chemical concentration $\tilde{C}(x,t)$ for all $(x,t) \in [0,1] \times [0,1]$, in a heterogeneous soil with the multiple regression interpolated right boundary condition functions.

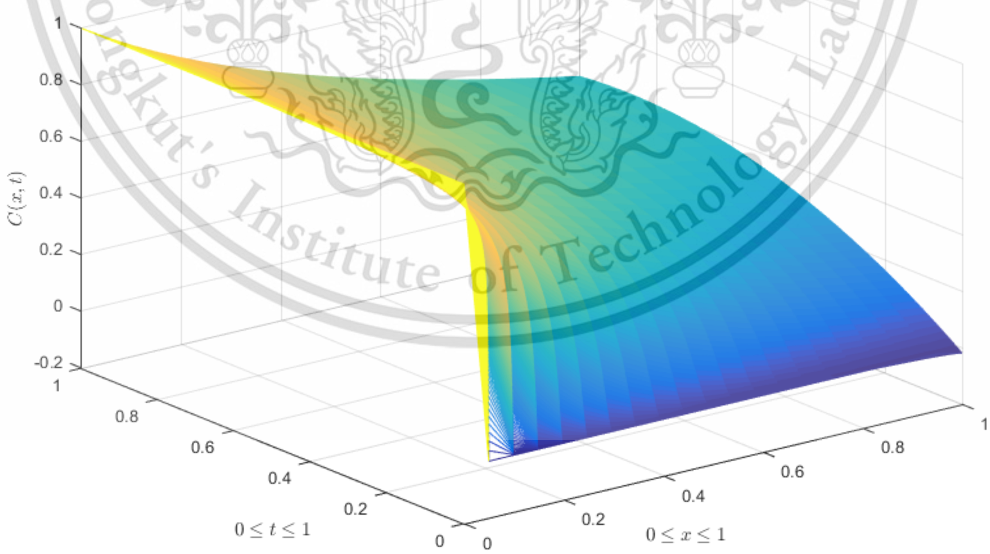


Figure 4.11: The surface plot of computed chemical concentration $\tilde{C}(x,t)$ for all $(x,t) \in [0,1] \times [0,1]$, in a heterogeneous soil with the quadratic regression interpolated right boundary condition functions.

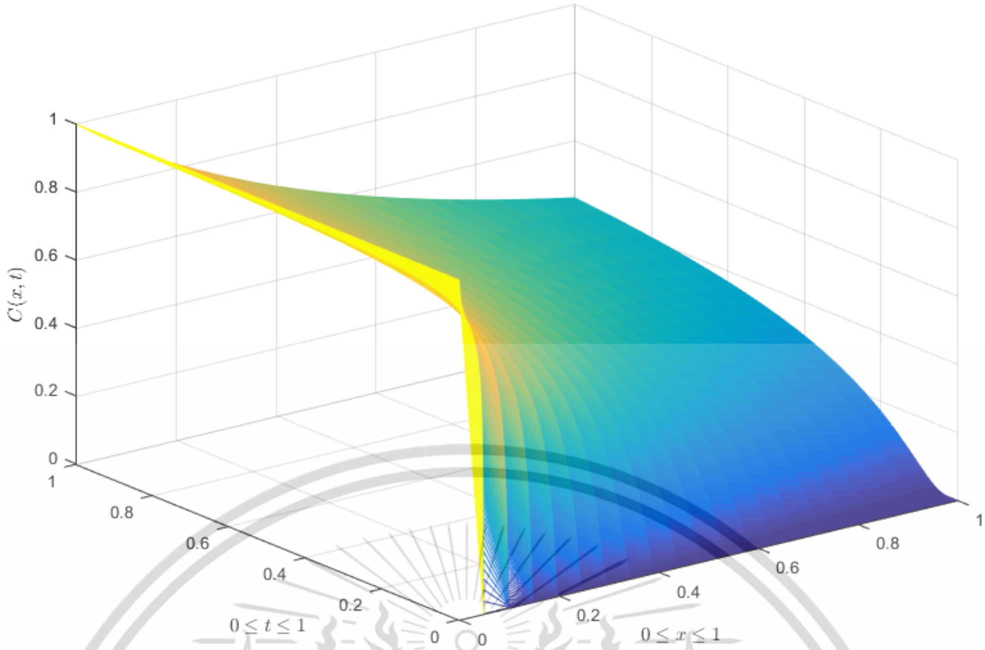


Figure 4.12: The surface plot of computed chemical concentration $\tilde{C}(x,t)$ for all $(x,t) \in [0,1] \times [0,1]$, in a heterogeneous soil with the cubic splines interpolated right boundary condition functions.

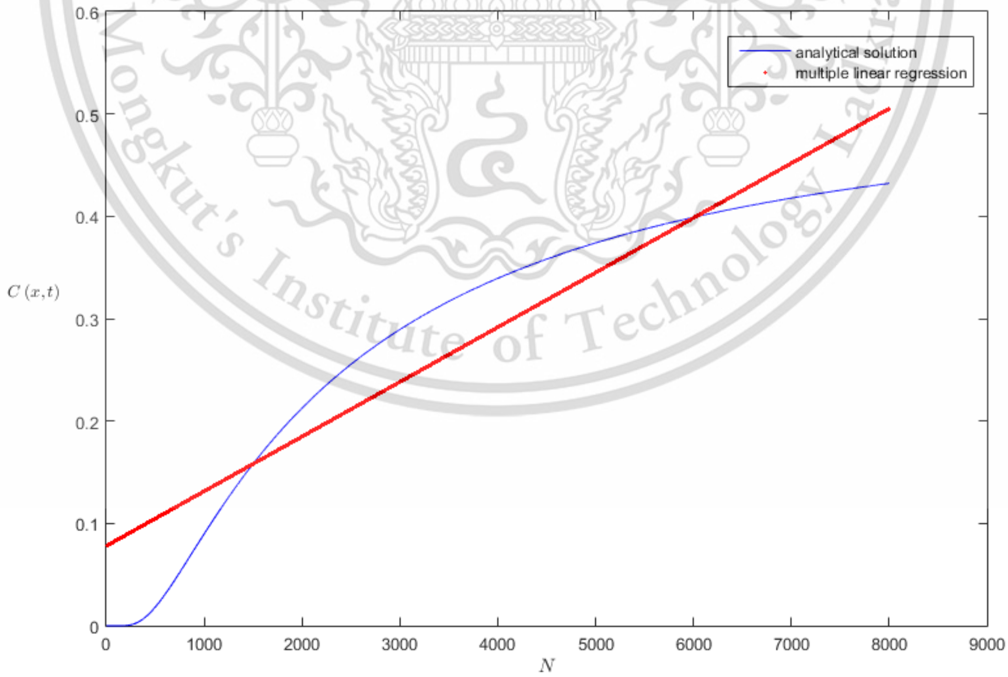


Figure 4.13: The comparison of the multiple regression interpolated right boundary condition functions and the analytical solution for all $0 \leq t \leq 1$

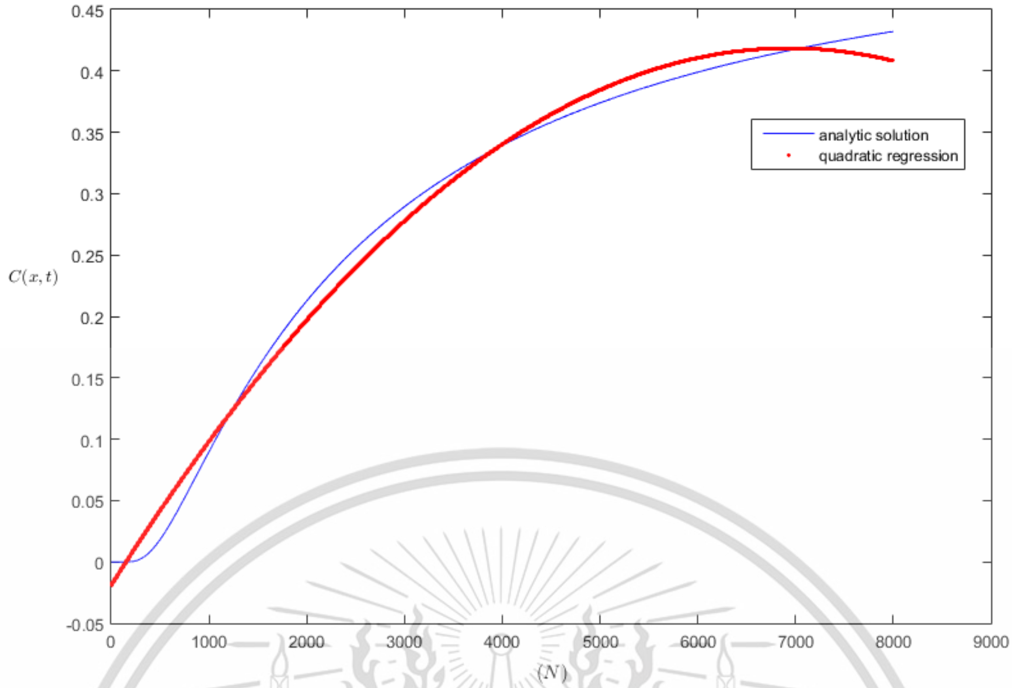


Figure 4.14: The comparison of the quadratic regression interpolated right boundary condition functions and the analytical solution for all $0 \le t \le 1$

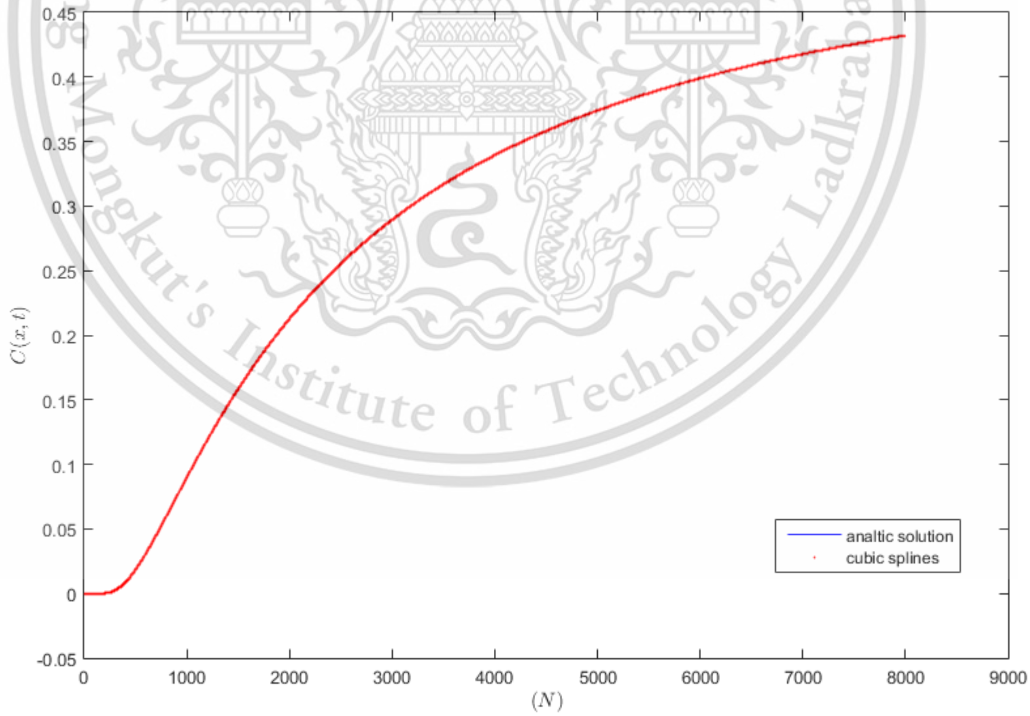


Figure 4.15: The comparison of the cubic splines interpolated right boundary condition functions and the analytical solution for all $0 \le t \le 1$

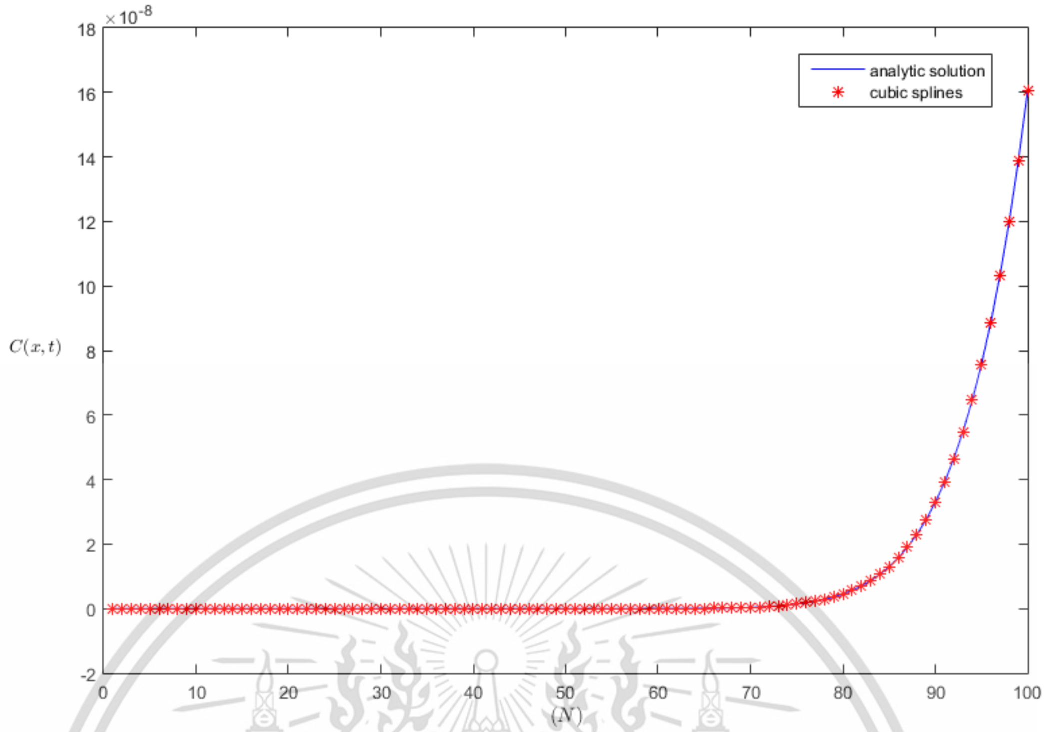


Figure 4.16: The comparison of the cubic splines interpolated right boundary condition functions and the analytical solution for all $0 \leq t \leq 0.0124$

4.10 Simulation 9: Two monitoring contaminated groundwater points; Saulyev Explicit Finite Difference Scheme technique for an ideal contaminated groundwater dispersion measurement with the interpolated right boundary condition functions and the diffusive term $(f_1(x,t))$ and the advective term $(f_2(x,t))$.

Assuming that the chemical dispersion through inhomogeneous soil the diffusion coefficient and flow velocity field are averaged to be $D_0 = 0.71$ (km²/year) and $u_0 = 0.6$ (km/year), respectively. The parameter that accounts for the inhomogeneity of the soil is assumed by $a = 1.0$ (km^{-1}) The left boundary condition and the initial condition are assumed by Eq.(4.3) and The right boundary condition and the diffusive term and the advective term are interpolated functions. By employing the propose finite difference technique Eq.(3.35), prediction of a field data at the boundary can be obtained by using the cubic splines Eq.(3.51). The interpolation is used to interpolate the right boundary condition and the diffusive term and the advective term,

$$C(1,t) = \tilde{g}_2(t), \tag{4.8}$$

$$f_1(x,t) = \tilde{f}_1(x,t), \tag{4.9}$$

$$f_2(x,t) = \tilde{f}_2(x,t). \tag{4.10}$$

at $x \in [0,1]$, and $t \in [0,1]$, where $\tilde{g}_2\,(t)$, $\tilde{f}_1\,(x,t)$ and $\tilde{f}_2\,(x,t)$ are interpolated function.

We get the chemical concentration with the cubic splines interpolated in Table.4.20. The maximum root mean square error of approximated pollutant concentration with the interpolated right boundary condition functions is shown in Table.4.22 and the root mean square error of interpolated right boundary condition functions and the diffusive term and the advective term is shown in Table.4.21. The surface plot of computed chemical concentration in a heterogeneous soil with the cubic splines interpolated as show in Fig.4.17. The comparison of the cubic splines interpolated the diffusion term and the advective term and the analytical solution as shown in Figs.4.18-4.19.

Table 4.20: The approximated chemical concentration in a heterogeneous soil with the cubic splines interpolated right boundary condition functions and the diffusion term and the advective term ($\Delta x = 0.05\ (km)$, $\Delta t = 0.000125\,(year)$, $\lambda = 0.05$), where $\lambda = \Delta t/\Delta x^2$.

t/x	0.1	0.2	0.3	0.4	0.5	0.6	0.7	0.8	0.9	1.0
0.2	0.91406	0.76630	0.64107	0.53615	0.44836	0.37511	0.31405	0.26320	0.22087	0.18570
0.5	0.93667	0.82816	0.73549	0.65624	0.58783	0.52845	0.47660	0.43112	0.39105	0.35570
0.7	0.94177	0.84229	0.75746	0.68486	0.62204	0.56728	0.51919	0.47672	0.43901	0.40546

Table 4.21: The root mean square error of interpolated right boundary condition functions and the diffusive term and the advective term to the analytical solution (Eq.4.3). $RMSE(T_{g_2}) = \sqrt{\frac{\sum_{n=0}^{N}(\tilde{g}_2(t_n)-g_2(t_n))}{N}}$ for all $t \in [0,1]$, $RMSE(T_{f_1}) = \sqrt{\frac{\sum_{i=0}^{M}\left(\tilde{f}_1(x_i,t_n)-f_1(x_i,t_n)\right)}{M}}$ and $RMSE(T_{f_2}) = \sqrt{\frac{\sum_{i=0}^{M}\left(\tilde{f}_2(x_i,t_n)-f_2(x_i,t_n)\right)}{M}}$ for all $x \in [0,1]$

Δx	Δt	$RMSE(T_{f_1})$	$RMSE(T_{f_2})$	$RMSE(T_{g_2})$
0.050	5.00×10^{-4}	6.8959×10^{-6}	1.5956×10^{-10}	2.1187×10^{-10}
0.050	2.50×10^{-4}	4.8741×10^{-6}	8.5384×10^{-17}	3.6933×10^{-11}
0.050	1.25×10^{-4}	3.4458×10^{-6}	1.3951×10^{-18}	6.5177×10^{-12}

Table 4.22: The maximum root mean square error of approximated pollutant concentration with the interpolated right boundary condition functions and the diffusive term and the advective term and τ is the maximum RMSE time.

Δx	Δt	$RMSE_{max}(C)$	τ
0.050	5.00×10^{-4}	3.3723×10^{-4}	5.0000×10^{-4}
0.050	2.50×10^{-4}	2.3366×10^{-4}	5.0000×10^{-4}
0.050	1.25×10^{-4}	1.7135×10^{-4}	3.7500×10^{-4}

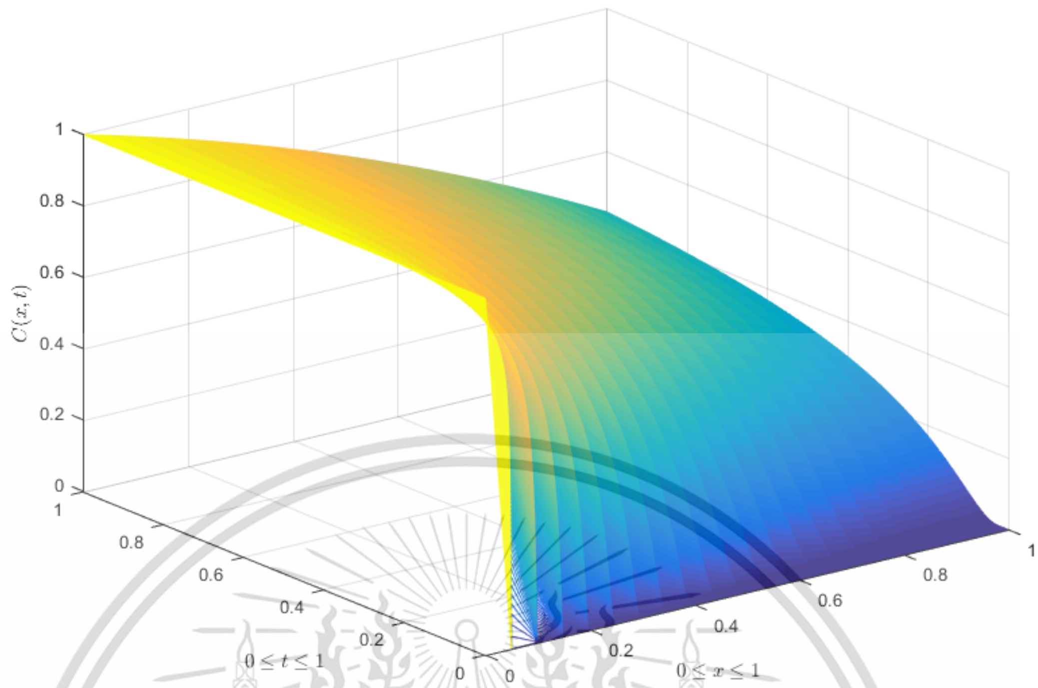


Figure 4.17: The surface plot of computed chemical concentration in a heterogeneous soil with the cubic splines interpolated right boundary condition functions and the diffusion term and the advective term. $\tilde{C}(x,t)$ for all $(x,t) \in [0,1] \times [0,1]$.

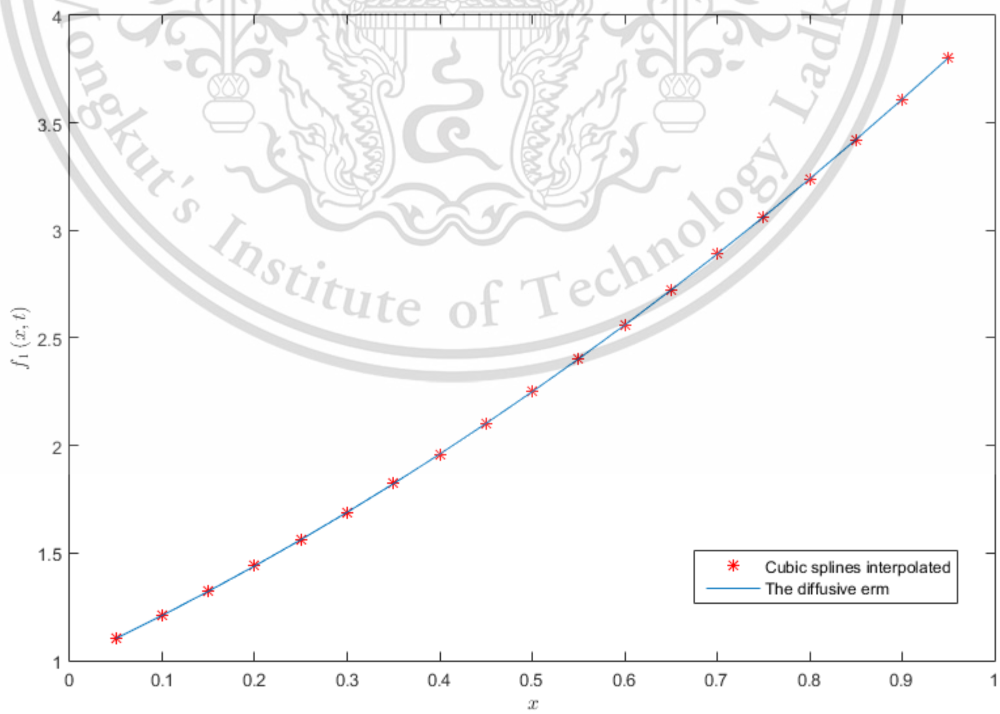


Figure 4.18: The comparison of the cubic splines interpolated the diffusion term and the analytical solution for all $0 \le x \le 1$

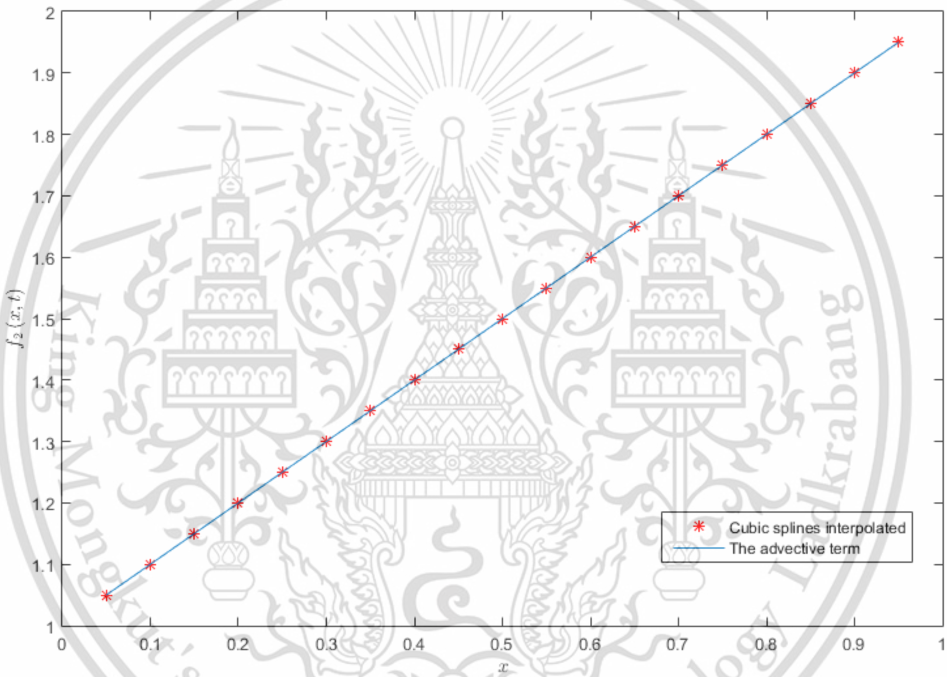


Figure 4.19: The comparison of the cubic splines interpolated the advective term and the analytical solution for all $0 \leq x \leq 1$

Chapter 5

Conclusion and Discussion

5.1 Discussion

In simulation 1, the approximated FTCS solutions are good agreement when is divided b a half in 3 cases as show in Tables 4.1-4.1. In simulation 2, if the Saulyev method is employ to approximate the groundwater pollutant concentration, it turn out that the solutions are closed to the FTCS solutions as show in Tables 4.4-4.6. The comparison of both approximation techniques are illustrated in Fig 4.3. Both method give accurately approximated groundwater pollutant concentration but the FTCS gives unstable solutions when greater than 0.4 as show in Table 4.7. Although, The proposed Saulyev method still gives accurately groundwater pollutant concentration that is free from illustrated grid spacing.

In simulations 3-5, the problems of the single monitoring contaminated groundwater point when there is no rate of change, there is positive rate of change and there is negative rate of change of pollutant concentration a the ended point are simulated as show in Tables 4.9-4.11 and Fig 4.4-4.6 we can see that the groundwater pollutant concentration in simulation 4 is higher than simulation 3 and 5, respectively as show Fig 4.7.

In simulation 6, the realistic heterogeneous soil function are experimented such as f_1 and f_2, we can get the approximated groundwater pollutant concentration by using the proposed Saulyev method as show in Table 4.12 and Fig 4.8.

In simulation 7, the long-term situation is experimented. The considered domain is large as the realistic area, 3 km. The simulation time is long as prediction requirement, 16.67 year.

In simulations 8, The approximated chemical concentration in a heterogeneous soil with the multiple regression, quadratic regression and cubic splines interpolated right boundary condition function are simulated as show in Tables 4.14-4.16. The cubic splines interpolated right boundary condition function give accurately approximated groundwater pollutant concentration than the multiple regression and quadratic regression, respectively as show Tables 4.17-4.19 and Fig 4.13-4.16.

In the last simulations, The approximated chemical concentration in a heterogeneous soil with the cubic splines interpolated right boundary condition functions and the diffusion term and the advective term is simulated as show in Table 4.20. The cubic splines interpolated right boundary condition function give accurately approximated groundwater pollutant concentration as show Tables 4.21-**??** and Fig 4.18-4.19.

5.2 Conclusion

The numerical simulations to a one-dimensional groundwater pollution measurement model through heterogeneous soil are simulated. The numerical solutions for approximating the chemical concentration in heterogeneous medium are proposed. The forward time center space method and Saulyev finite difference technique are used to approximate the solution of the several simulations. The multiple regression, quadratic regression and cubic spline are used to represent the diffusion term, the advective term and the right boundary condition for filed data. The proposed finite difference technique gives good agreement approximated solutions under different conditions. We can see that the computed solutions are applicable to the real-world problems.

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Appendix

Appendix A

Numerical Simulations for a One-dimensional Dispersion Measurement Model Through Heterogeneous Medium

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Abstract

There are many natural phenomenas concern with the mass transport model. The advection-diffusion equation is used to describe the concerned model. The theoretical solution of the advection-diffusion equation is limited only in ideal geometries. Applications of numerical solutions are influenced in several initial and boundary conditions when dealing with complex geometries. In this research, an explicit finite difference technique for an advection-diffusion equation with variable coefficients in a semi-infinite domain is proposed. The accuracy of the proposed technique is to examine by comparing the approximated solutions with the analytical solution. The technique gives good agreement approximated solution.

Keywords: advection, diffusion, semi-infinite domain, finite difference method, variable coefficient.

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1. Introduction

There are several use of the advection-diffusion equation (ADE), including heat transfer, sediment transport and water pollutant concentration measurement. [1] introduced a numerical technique for approximating ADE with constant coefficient. The developed scheme was based on a mathematical combine both Siemieniuch and Gradwell approximation for time and Dehghan's approximation for spatial variable. In [2], they have solved ADE with an explicit approach of finite difference method (EFDM) and variable coefficients in semi-infinite domain. This equation can analyze three dispersion problems: (i) solute dispersion along poised flow through inhomogeneous medium, (ii) temporarily dependent solute dispersion along uniform flow through homogeneous medium, and (iii) solute dispersion along temporarily dependent not poised flow through inhomogeneous medium. In [3], they have solved the one-dimensional (1D) ADE with variable coefficients in semi- infinite media by using EFDM for two dispersion problems: (i) temporarily dependent dispersion in uniform flow and (ii) spatially dependent dispersion in non-uniform flow, uniform pulse-type input condition and initial solute concentration, that decreasing function of distance were considered. In [4], the EFDM to obtain the dispersion through a heterogeneous horizontal semi-infinite medium. The heterogeneous nature of the medium was discoursed by a position dependency linear nonhomogeneous expression for velocity with not poised exponential variation with time. Velocity and dispersion was zero at the origin. In [5], an analytical solution to one-dimensions ADE with several point sources through arbitrary time-dependent discharging rate is proposed. They reported that the results had indicated, the proposed analytical solution could offer an accurate estimation of the contemplation. The limitations of the proposed solution were valid only for the constant-parameters condition, and was not computational performance for problems involving a high temporal or a high spatial resolution.

The inhomogeneity of the medium causes variation in the flow velocity, [2,6]. In [7], studied on the variation of the increasing nature. In this research, we will propose an explicit finite difference technique for an advection-diffusion equation with variable coefficient in a semi-infinite domain.

2 Governing equation

2.1 Solute dispersion along steady flow through inhomogeneous domain

The one-dimension advection-diffusion equation (ADE) is expressed as follows [6]

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

for all $(x,t)\in\Omega$ such that $\Omega=[0,L]\times[0,T]$, where are $c(x,t)$ the dispersing solute concentration, the longitudinal axis, and time, respectively. If the values of D and u assumed as constants, then these values are named dispersion coefficient and uniform velocity of the flow field, respectively. In this study preferred to use Eq. (1) as follows:

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

for all $(x,t) \in [0,L] \times [0,T]$, where D_0 and u_0 are constant values whose dimensions depend upon the expressions $f_1(x,t)$ and $f_2(x,t)$, and $f_1(x,t)$ and $f_2(x,t)$ are given function. The analytical solutions of ADE for the previously mentioned two hydrodynamic dispersion problems were introduced by [6].

2.2 The initial and boundary conditions

An initially solute free condition is assumed for both of the problems in the semi-infinite domain. Meanwhile, a uniform distribution of nodes is applied at the origin of the domain. The initial condition, is assumed by

$$c(x,0) = f(x), \text{ for all } x \in [0,L], \tag{3}$$

and the boundary conditions, are also assumed by

$$c(0,t) = g_1(t), \text{ for all } t \in [0,T], \tag{4}$$

$$c(L,t) = g_2(t), \text{ for all } t \in [0,T], \tag{5}$$

where $f(x)$ is an initially pollutant concentration function, $g_1(t)$ and $g_2(t)$ boundary sources of pollutant concentration on the left and the right end of the consider domain, respectively.

3 Numerical technique

We now discretize the domain by dividing the interval $[0,L]$ into M subintervals such that $M\Delta x = L$ and the time interval $[0,T]$ 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 $i = 1,2,3,\ldots,M$ and $t_n = n\Delta t$ for all $n = 1,2,3,\ldots,N$ 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)

3.1 Forward Time Central Space Finite Difference Scheme

$$C(x_i,t_n) \cong C_i^n, \tag{6}$$

$$\left.\frac{\partial C}{\partial t}\right|_{(x_i,t_n)} \cong \frac{C_i^{n+1} - C_i^n}{\Delta t}, \tag{7}$$

$$\left.\frac{\partial C}{\partial t}\right|_{(x_i,t_n)} \cong \frac{C_{i+1}^n - C_{i-1}^n}{2\Delta x}, \tag{8}$$

$$\left.\frac{\partial^2 C}{\partial x^2}\right|_{(x_i,t_n)} \cong \frac{C_{i+1}^n + C_{i-1}^n - 2C_i^n}{\Delta x^2}, \tag{9}$$

$$f_1(x_i,t_n) = f_{1_i}^n, \tag{10}$$

$$f_2(x_i,t_n) = f_{2_i}^n. \tag{11}$$

Substituting Eqs. (6)-(11) into Eq. (2), we get the finite difference equation,

$$\frac{C_i^{n+1} - C_i^n}{\Delta t} = \left(D_0 \cdot \left.\frac{\partial f_1}{\partial x}\right|_{(x_i,t_n)} - u_0 f_2(x_i,t_n) \right)\left(\frac{C_{i+1}^n - C_{i-1}^n}{2\Delta x} \right)$$

$$- u_0 \cdot \left.\frac{\partial f_2}{\partial x}\right|_{(x_i,t_n)} C_i^n + D_0 f_1(x_i,t_n)\left(\frac{C_{i-1}^n - 2C_i^n + C_{i+1}^n}{\Delta x^2} \right), \tag{12}$$

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

$$C_i^{n+1} = \left[\lambda_i^n - \frac{1}{2}\gamma_i^n + \frac{1}{2}\beta_i^n \right] C_{i-1}^n + \left[1 - \Delta t \alpha_i^n - 2\lambda_i^n \right] C_i^n$$

$$+ \left[\lambda_i^n + \frac{1}{2}\gamma_i^n - \frac{1}{2}\beta_i^n \right] C_{i+1}^n, \tag{13}$$

where $\lambda_i^n = \frac{\Delta t\, D_0 f_1(x_i,t_n)}{(\Delta x)^2}$, $\beta_i^n = \frac{\Delta t\, u_0 f_2(x_i,t_n)}{\Delta x}$, $\gamma_i^n = \frac{\Delta t\, D_0}{\Delta x} \left.\frac{\partial f_1}{\partial x}\right|_{(x_i,t_n)}$, and $\alpha_i^n = u_0 \cdot \left.\frac{\partial f_2}{\partial x}\right|_{(x_i,t_n)}$, the explicit finite difference Eq. (13) can be written in a compact form as,

$$V_i^n = \lambda_i^n - \frac{1}{2}\gamma_i^n + \frac{1}{2}\beta_i^n, \tag{14}$$

$$G_i^n = 1 - \Delta t \alpha_i^n - 2\lambda_i^n, \tag{15}$$

$$P_i^n = \lambda_i^n + \frac{1}{2}\gamma_i^n - \frac{1}{2}\beta_i^n. \tag{16}$$

Then

$$C_i^{n+1} = V_i^n C_{i-1}^n + G_i^n C_i^n + P_i^n C_{i+1}^n. \tag{17}$$

The forward time central space scheme is conditionally stable subject to constraints in (13).

The stability requirements for the scheme are [9,10]

$$\lambda_i^n = \frac{\Delta t\, D_0 f_1(x_i,t_n)}{(\Delta x)^2} < \frac{1}{2},$$

$$\beta_i^n, \gamma_i^n, \alpha_i^n < 1,$$

where λ_i^n is the diffusion number (dimensionless) and β_i^n is the advection number (dimensionless). It can be obtained that the strictly stability requirements are the main disadvantage of this scheme.

The finite difference formula (17) has been derived in [11] that the truncation error for this method is $O\{(\Delta x)^2, \Delta t\}$.

4 The accuracy of the proposed numerical technique

The variation in velocity is assumed as small order to insure that it can satisfy the essential conditions for velocity parameter in the ADE. Additionally, as the second assumption, dispersion parameter is considered proportional to the square of the velocity [8]. Thus, for Eq. (2), the expressions of $f_1(x,t)$ and $f_2(x,t)$ are assumed by [6]:

$$f_1(x,t) = (1 + ax)^2, \tag{18}$$

$$f_2(x,t) = 1 + ax, \tag{19}$$

where a is a parameter that accounts for the inhomogeneity of the domain with dimension (length)$^{-1}$. In [6], they have introduced an analytical solution that satisfies the specific $f_1(x,t)$ and $f_2(x,t)$ as in Eq. (18) and Eq. (19),

$$C = \frac{c_0}{2}\left[(1+ax)^{-1} erfc\left(\frac{\ln(1+ax)}{2a\sqrt{D_0 T}} - \beta\sqrt{t}\right) + (1+ax)^{\delta} erfc\left(\frac{\ln(1+ax)}{2a\sqrt{D_0 T}} + \beta\sqrt{t}\right)\right], \quad (20)$$

Where

$$\omega_0 = \left(au_0 - a^2 D_0\right),\ \beta = \sqrt{\frac{\omega_0^2}{4a^2 D_0} + au_0} = \frac{u_0 + aD_0}{2\sqrt{D_0}}$$

and $\delta = \frac{u_0}{aD_0}$.

5 Numerical experiments and results

Assuming that the chemical dispersion through inhomogeneous soil the diffusion coefficient and flow velocity field are averaged to be $D_0 = 0.71$ (km^2/year) and $u_0 = 0.6$ (km/year), respectively. The parameter that accounts for the inhomogeneity of the soil is assumed by $a = 1.0$ (km^{-1}). The boundary conditions and the initial condition are assumed by Eq. (20). By employing the propose finite difference technique Eq. (17), we get the chemical concentration in Tables 1-3 when time increment (Δt) are varied and λ is divided by a half. The comparison of computed results, when the proposed numerical technique and the theoretical solution Eq. (11) are used, is shown in Fig1. The maximum error when λ is divided by a half is shown in Table 4. We can see that the maximum error of the approximation is decreased when λ is also reduced. The surface of approximated solutions is illustrated in Fig 2.

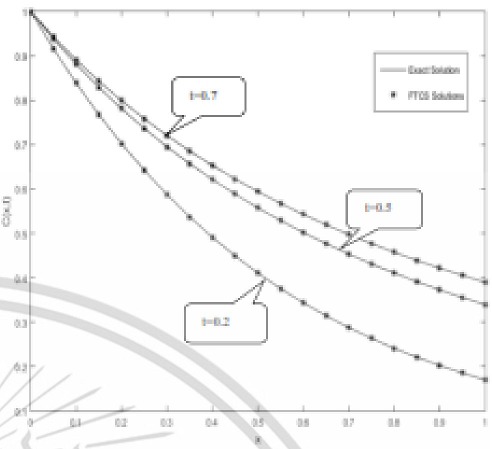

Figure 1: The caparison of FTCS solutions and the analytical solution when $t = 0.2, 0.5$ and 0.7

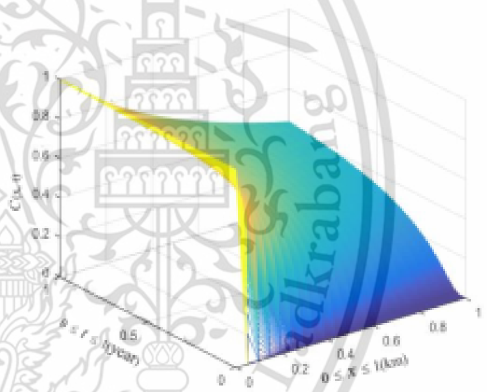

Figure 2: The surface plot of computed chemical concentrations $C(x,t)$ for all $(x,t) \in [0,1]\times[0,1]$.

Table 1: The approximated chemical concentration in a heterogeneous medium ($\Delta x = 0.05$ (km), $\Delta t = 0.0005$ (year), $\lambda = 0.2$)

t\x	0	0.1	0.2	0.3	0.4	0.5	0.6	0.7	0.8	0.9	1
0.2	1	0.83862	0.70228	0.58759	0.49144	0.41106	0.34398	0.28806	0.24146	0.20263	0.17027
0.5	1	0.88114	0.78073	0.69509	0.62143	0.55765	0.50210	0.45347	0.41069	0.37291	0.33942
0.7	1	0.89079	0.79881	0.72039	0.65285	0.59416	0.54281	0.49757	0.45749	0.42181	0.38990

Table 2: The approximated chemical concentration in a heterogeneous medium ($\Delta x = 0.05$ (km), $\Delta t = 0.00025$(year), $\lambda = 0.1$)

t\x	0	0.1	0.2	0.3	0.4	0.5	0.6	0.7	0.8	0.9	1
0.2	1	0.83856	0.70217	0.58745	0.49130	0.41092	0.34386	0.28796	0.24139	0.20260	0.17027
0.5	1	0.88113	0.78073	0.69508	0.62142	0.55764	0.50209	0.45346	0.41068	0.37291	0.33942
0.7	1	0.89079	0.79881	0.72039	0.65284	0.59416	0.54280	0.49756	0.45749	0.42181	0.38990

Table 3: The approximated chemical concentration in a heterogeneous medium
($\Delta x = 0.05$ (km), $\Delta t = 0.000125$ (year), $\lambda = 0.05$)

t/x	0	0.1	0.2	0.3	0.4	0.5	0.6	0.7	0.8	0.9	1
0.2	1	0.83853	0.70212	0.58738	0.49122	0.41085	0.34380	0.28791	0.24136	0.20258	0.17027
0.5	1	0.88113	0.78072	0.69507	0.62141	0.55763	0.50209	0.45345	0.41068	0.37291	0.33942
0.7	1	0.89079	0.79881	0.72038	0.65284	0.59416	0.54280	0.49756	0.45749	0.42181	0.38990

Table 4 : The maximum error of the computed solutions with the analytical solution at $T = 0.7$, where $E_T = \left\{ e_i \middle| e_i = \left| C_i^n - \tilde{C}_i^n \right|, \right.$ for all $i = 1, 2, 3, \ldots, M-1$ and $n = N \}$.

λ	Δx	Δt	Max $E_{0.7}$
0.20	0.05	0.000500	5.0513×10^{-5}
0.10	0.05	0.000250	4.6388×10^{-5}
0.05	0.05	0.000125	4.4323×10^{-5}

6 Conclusion

The one-dimensional dispersion measurement model through heterogeneous medium is simulated. The numerical solutions for approximating the chemical concentration in heterogeneous medium is proposed. The proposed finite difference technique gives good agreement approximated solutions. We can see that the computed solutions are applicable to the real-world problems.

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