

A proposed algorithm to solve a Finite Difference of Solute Transport Model in a Groundwater Flow

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Abstract

This research presents a theoretical study of solute transport in ground water flow. The molecular diffusion process is accompanied simultaneously with advection diffusion process which effect the solute transport process in ground water flow. Both diffusion processes can be described mathematically in terms of a partial differential equations models. This paper proposed an–algorithm that generates a numerical solution of a partial differential equations using MATLAB. Finite difference approximation is used to discretize the governed partial differential equations of dissolved salts transport in ground water flow at aquifer of the study area. The proposed algorithm showed an explicit finite difference to a discrete form of a partial differential equations.

Key Words: groundwater transport model, solute, differential equation , MATLAB

1- Introduction:

For several decades ago, the scientific community as well as nongovernmental organization have sought to raise an alarm concerning the unsustainable use of the planet's water available water resources. Rising world population and consumption inexorably increasing human demand for domestic, industrial, and agricultural water. Population and wealth along with other global stressors will have a direct and significant impact on the sustainability goals, technology selection, and governance strategies that are related to water quality and quantity [1].

Groundwater transport in porous media and solute diffusion has a large area of interest for hydrology and environment researchers. This movement is governed by established hydraulic principles. The flow through aquifers, most of which are natural porous media, can be expressed by what is known as Darcy's law, a French hydraulic engineer Henry Darcy [2]. Applications of Darcy's law through porous media to track the irregularities of flow behavior, also in the zone of aeration the presence of air adds complicated factor to the flow of water [3]. Natural geochemical weathering of substance soil has caused an unacceptable level of dissolved materials in groundwater in many regions of the world. Despite the quite high of rainfall in some geographical areas, the surface water is still not fit for drinking due to poor sanitation practices in that region with the potential for an

outbreak waterborne diseases [4]. Contamination of ground water by a pollutants has become an increasing concern in recent years. These pollutants enter the ground-water system by a wide variety of mechanisms, including accidental spills, land disposal of domestic and industrial waste, and application of agricultural fertilizers and pesticides [5]. Groundwater flow models are used as a tool for decision maker by evaluate impact assessment required for a water resource system. They may be also used to predict some future groundwater properties or behavior due to solute diffusion contamination [6]. The problem is most critical where the beneficial effects of water passing through fine grained rocks, such as basalt or limestone aquifers [7]. The modeling in these areas often leads to a partial differential equation (PDE), or transport equations, which parabolic in nature. Such equations may be linear, in which case analytic solutions are often achievable, but most of the transport equations are nonlinear and numerical solutions are used to solve and more understand the particular problem [8].

These equations can be applied to a particular groundwater contamination process, data must be provided on the groundwater velocity, coefficients of hydrodynamic dispersion , initial concentrations of solutes in the aquifer, configuration of the solute source, and boundary conditions along the physical boundaries of the groundwater flow system.

In this paper, the governing partial differential equation for one-dimensional solute diffusion equation is solved numerically by explicit finite difference method.

MATLAB code is developed to obtain the numerical solution by using explicit finite difference for solute transport in groundwater flow. The numerical solution model is validated along a data for several solute concentrations in the study area wells.

2 – Groundwater flow models

The solute transport and groundwater flow models are often derived for a small representative elemental volume where the properties of the medium are assumed to be effectively constant. A diffusion balance is obtained on the water flowing in and out of this small volume along with Darcy's law to arrive at the transient groundwater flow models. Groundwater models are used as tools for studying and management of a water resource system. It also be used to predict some future ground-water flow behavior and dissolved solute diffusion [9].

In a literature, the numerical solution techniques used for solving the governing equations of ground flow models are Finite Difference or Finite Element approximation or a combination of both provided that model parameters and initial and boundary conditions are properly specified [10].

3- Model Development

A solute transport in ground water flow can be described by One dimensional convection-dispersion parabolic second order partial differential equation model. The model derived from Darcy's law combined with a conservation of mass which defined mathematically as:

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

Where:

C [ML⁻³]: is a solute concentration, X [L]: is a spatial distance, T [T]: is a time, D [L²T⁻¹]: is a longitudinal dispersion, U [LT⁻¹]: is a seepage velocity, R[/]: is the dimensionless retardation factor.

The mathematical model of partial differential equation that represent a solute transport (PDE) can be simplified by introduce these assumptions:

1. solute transport through a homogenous aquifer , adsorbing, and semi-infinite long.
2. initially, initially at t=0, the contamination of solute is assumed to be low in the domain.
3. dispersion coefficient and seepage velocity are assumed to be constant over the entire range of a case study conditions.
4. the contamination is entered to the system from the left boundary i.e (x=0).
5. input concentration can be represented by a step function of time.
6. the aquifer is assumed to be semi-infinite porous media where usually represents the situation when the aquifer is quiet large and other ends of domain unaffected by input concentration in the time domain of study.

By applying these assumptions to equation (1), it can be rewritten as:

$$R \frac{\partial C}{\partial t} = D \frac{\partial^2 C}{\partial x^2} - u. \frac{\partial C}{\partial x}$$

4- Numerical Solution:

The numerical solution that applied in this work is a finite difference. The method is an approach based on Taylor's series approximation which is very affective in ground water flow modeling. Numerical models are used in groundwater modeling because it yields approximate solution to the governing equation through discretization of space and time. The basic idea of finite difference methods (FDM) in the study of groundwater flow problems includes three major steps. First, the flow region is divided by a grid and the time interval into time steps. Second the partial derivatives involved in the PDE are replaced by their finite difference approximations. As a result, the PDE is transformed into a system of

algebraic equations. Third, the algebraic system is solved and the nodal values of the unknown function are obtained. These discrete values approximately describe the time-space distribution of the unknown variable. The replacement of a particular derivative of a P.D.E by a finite difference approximation can be done by forward, backward, or central difference [9]

The derivatives in equation (2) can be replaced by their finite difference approximation that may be written as:

For a first derivative:

$$\frac{\partial C}{\partial t} = \frac{C_{i,j+1} - C_{i,j}}{\Delta t} \quad (3)$$

$$\frac{\partial C}{\partial x} = \frac{C_{i+1,j} - C_{i,j}}{\Delta x} \quad (4)$$

For a second derivative:

$$\frac{\partial^2 C}{\partial x^2} = \frac{C_{i+1,j} - 2C_{i,j} - C_{i-1,j}}{\Delta x^2} \quad (5)$$

By substituting equation's (3),(4), and (5) in equation (2), equation (2) rewritten as:

$$R \frac{C_{i,j+1} - C_{i,j}}{\Delta t} = D \left[\frac{C_{i+1,j} - 2C_{i,j} - C_{i-1,j}}{\Delta x^2} \right] - u \frac{C_{i+1,j} - C_{i,j}}{\Delta x} \quad (6) \quad \text{equation (6)}$$

rearranged as:

$$C_{i,j+1} - C_{i,j} = \frac{D\Delta t}{R\Delta x^2} [C_{i+1,j} - 2C_{i,j} - C_{i-1,j}] - \frac{\Delta t u}{R} [C_{i+1,j} - C_{i,j}] \quad (7)$$

To simplify equation (7), use new parameters v and q that can be defined as:

$$v = \frac{D\Delta t}{R\Delta x^2} \quad (8)$$

$$q = \frac{\Delta t u}{R} \quad (9)$$

Replace a relevant expressions from equations (8), (9) in equation (7), then , equation (7) rearranged as follows

$$C_{i,j+1} - C_{i,j} = v[C_{i+1,j} - 2C_{i,j} - C_{i-1,j}] - q[C_{i+1,j} - C_{i,j}] \quad (10)$$

Equation (10) rearranged as:

$$C_{i,j+1} = C_{i,j} [1 - 2v + q] + C_{i+1,j}[v - q] + v C_{i-1,j} \quad (11)$$

Equation (11) is the final equation that introduced to MATLAB code for solute concentration distribution in groundwater flow.

5- Computational Algorithm:

• MATLAB PROGRAM OVERVIEW:

MATLAB (Matrix Laboratory) is a generalized mathematical software program with many features such as numerical computations, Simulink and control analysis, visualization of results is available from Mathworks [12]

As with any software program, there are few ' rules' and 'codes' which must be followed. The structure of MATLAB consists of M-file or command file type, M-file, there are few general statements to be made about M-file or MATLAB code, is a collection of commands that are executed sequentially, commands can be mathematical operation, function call, flow control statement, and calls to the functions or scripts, the execution of m-file program can be controlled from command file windows or other m-file code. There are two types of m-files, functions and scripts. Function has variables that can passed into and out of the function. Any other variables used inside the function are not saved in memory when the execution of function is finished. Scripts on the other hand, save all their variables in the MATLAB work space. Functions and scripts should be nominated. The first line of a function must contain a function declaration, using a following format:

output Function name [y1, y2,] = input function name(x1, x2, ...)

Commented lines immediately following the function declaration and variables nomenclature [13]

- **Modelling and simulation in MATLAB**

For advanced techniques in modelling and simulation, identification, and control, MATLAB has a variety of tool boxes that are licensed individually. Relevant built in functions for Ordinary Differential Equation (ODE) solver include: several types that are use suitable numerical technique, Relevant tool boxes for process control include: control system, Fuzzy logic, neural networks, optimization [14]

- **Built-in ODE Solvers in MATLAB:**

As with most differential equation solvers, there a number of different numerical methods that can be used. Essentially, they are split non-stiff and stiff differential equations. A stiff differential equation is one that has a rapidly varying derivative. That is, the derivative changes rapidly and is therefore susceptible to relatively large errors in the numerical analysis. There are also choices within these two broad categories and these choices are based on the type of errors that can tolerated.

Table.1 shows several ode solvers in a MATLAB library .

Stiff ode solvers	Non-stiff ode solvers
Ode15s	Ode45
Ode23s	Ode23
Ode23t	Ode113

The numbers associated with the names indicates the "order" of the numerical method, the "s" indicates the stiff algorithm and the "t" indicates an implementation of the trapezoidal rule. The best bet is to initially try ode45, which utilizes a 4th -5th order Runge-Kutta algorithm. If this takes an unduly long time, then try one of the stiff solvers. If you find that you are having difficulty, the most likely reason is that you have not posed the problem correctly [15]

- **MATLAB Method of Lines:**

Method of lines is based on the concept of converting the partial differential equation (PDE) into a set of ordinary differential equations (ODE) by discretizing only the spatial derivatives using finite difference and leaving the time derivative unchanged [16]

The method of lines (MOL) is generally recognized as a comprehensive and powerful approach to the numerical solution of time-dependent partial differential equations (PDEs). This method proceeds in two separate steps:

- spatial derivatives are first replaced with finite difference, finite volume, finite element or other algebraic approximations.
- the resulting system of, usually stiff, semi-discrete (discrete in space – continuous in time) ordinary differential equations (ODEs) is integrated in time. [17]

- **Model Validation and visualization of Parameters**

It easy to visualize and display results in MATLAB graphically. The plot function is used to create simple plots. The command syntax is: plot(x1,y1,format1,x2,y2,format2,.....), x1 and x2 are independent variables (usually time), y1, y2 are dependent variables. The format1 and format2 arguments are short combination of characters containing the plot formatted commands. [18]

The essential processes for solving transport equations (7), (8) and (10) is a finite difference technique, maybe automated by functionality and matrix-based capabilities of MATLAB. the conceptual steps of initializing parameters, setting up the initial profile and the output steps are a common features of any numerical solution.

6- Groundwater model validation:

MATLAB algorithm is used to generate the solution for a solute concentration distribution over a time period and a spatial distance. Numerical solution of MATLAB Algorithm where obtained at several years over a spatial distance and a plots of $c(x, t)$ are shown in figures 1 and 2.

Tales 1 and 2 present a parameters considered for the numerical solution validation. In this case, the validation has been carried out for several years where a time step is one year and five kilometer of distance.

Table 1 Data used for model validation

Parameter (unit)	Value
Seepage velocity km/year	0.01
Length of the reach (km)	5
Longitudinal dispersivity (km^2/year)	0.1
Retardation factor	1.15
Total duration of simulation (years)	11
Time step (Δt) (year)	1
Number of divisions in length direction	10
Initial concentration mg/l	10

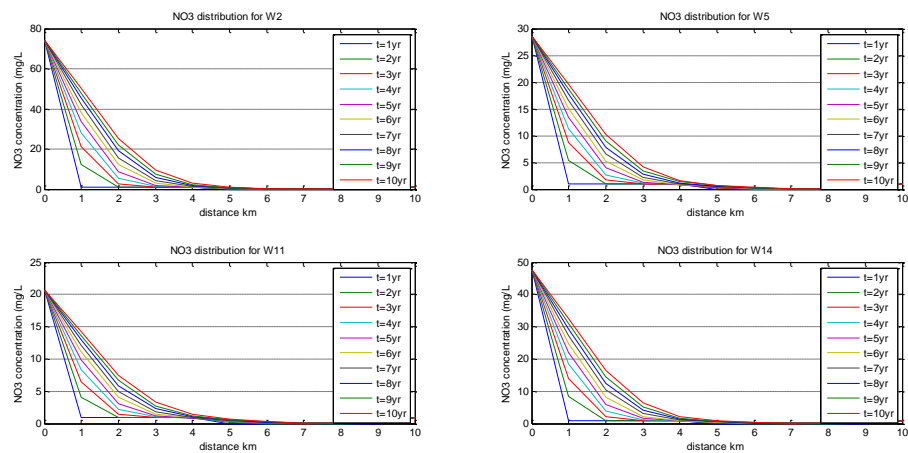
Table 2. solute concentrations used for model validation

Well no.	Chloride Concentration {mg/L}	Well no.	Nitrate Concentration {mg/L}
W3	1366.66	W2	74
W6	220	W5	28.6

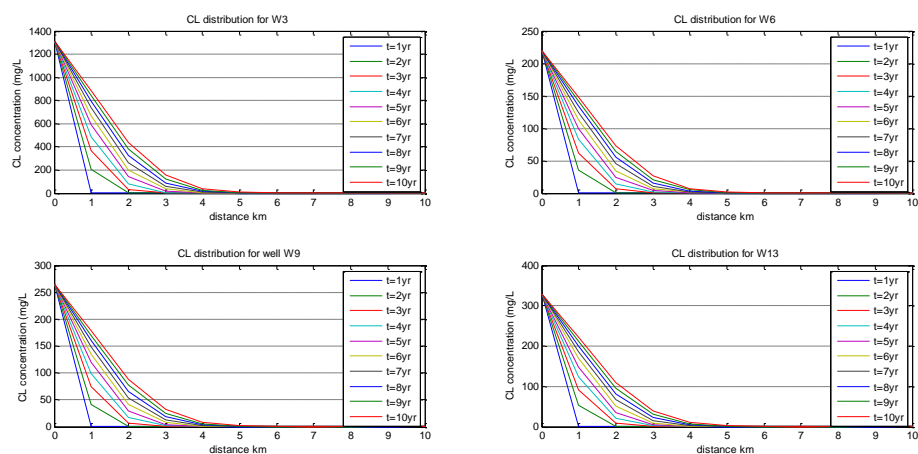
W9	264	W11	20.7
W13	329.26	W14	47.6

7- Results of model validation:

The proposed algorithm demonstrates the application of the numerical solution is a solute diffusion in groundwater, the numerical model is validated to find the concentration of a solute, as a function of time and space, in a finite, adsorbing, porous media subject to a step input function C_0 . The data that used in model validation are shown in Tables 1 and 2. The solute diffusion in terms of chlorides or nitrates are calculated for several time periods with a longitudinal distance. The results are presented in figures 1 and 2



Figure(1) ditribution of CL^- concentration



Figure(2) distribution of NO_3^- concentration

, the results showed th numerical solution with explicit finite difference is gradually along spatial distance in aquifer of ground water. The decreased numerical solution predicts the solute concentration as a function of time and space if a seepage velocity, adsorption rate, and dispersion coefficients are prescribed. They are useful for solving similar field problems

8- Conclusions:

In this paper, MATLAB has been used to solve the computational algorithm for finite difference, unsaturated flow problems within soil physics. These two problems demonstrate the versatility of the finite difference algorithm in handling one dimensional transport equation with source / sink terms and can be applied to other areas of science that involve convective and diffusion processes. In addition the MATLAB library a DQE and ODE approach to time integration that can be readily applied in MATLAB algorithms. These approaches could be used to gain better accuracy around steep wetting fronts and will explored in future work, finite difference discretization in explicit form provides a relatively easy approach to the numerical solution of transport equations.

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