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Research paper

The Finite-Difference Model of Fully Saturated Groundwater Contaminant Transport

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Abstract

Groundwater quality is one of water resource problem. This problem is driven by contaminant transport phenomena and can be described as a mathematical model. Contaminant transports equation usually is composed by advection and dispersion flux. In the porous medium or aquifer, contaminant meet tortuosity effect, therefore hydrodynamic dispersion must be considered as the development of dispersion flux. This paper explains the mathematical model of groundwater contaminant on fully saturated condition. It starts from governing equation of contaminant transport. Advection flux is based on groundwater velocity. In steady state condition, groundwater velocity can be determined as certain value. In another hand, in the transient condition, groundwater velocity must be determined based on the solution of groundwater flow model. Dispersion flux is calculated through first Fick's law and this component is distinguished into two parts follow mechanical dispersion and molecular diffusion. Mechanical dispersion affected by groundwater velocity and dispersivity. Contaminant transport equation is solved numerically using Finite Difference Method (FDM). This final model is validated theoretically and then this model is simulated into transient condition. The result of the simulation is described and explained graphically. Based on this research, the result of FDM model has similar physical behavior to FEM model from CTRAN example.

Keywords: *Alternating Direction Implicit, Finite-Difference Method, Groundwater Contaminant Transport, Numerical Modelling*

1. Introduction

Groundwater is valuable natural resources (Patil & Chore, 2014). The common problem of groundwater resources is not only about quantity problem but also quality problem. The quality problem of groundwater resources as important as to surface water quality problem. Usually, the quality problem of surface water is reported periodically, because it is easier to measure it than groundwater quality measurement(Freeze & Cherry, 1979). Contaminant is always on dynamic condition, it means that the contaminant interact to soil particles until equilibrium condition (Notodarmojo, 2005).

The mathematical model can solve this problem. It can describe the behavior of contaminant transport through porous medium. Generally, there are two types of mathematical model, follows analytical model and numerical model. Numerical model will be presented through this research. Numerical model allows more complex systems to be represented than analytical models, providing approximate solutions to the contaminant transport equation (Kumar, 2012). Many researchers have conducted mathematical modelling groundwater contaminant transport on various cases. Field case has been taken by (Rao et al., 2011)in the Basaltic Terrain, India. It provides an improved understanding of the contaminant migration in the regional aquifer system. The numerical method was not described in that research clearly. Other researches provide the information about the behavior of contaminant transport through porous media such as contaminant transport through layered soil (Sharma et al., 2014), contaminant transport on dual porosity (Corapcioglu & Wang, 1999), and the transport of nitrate and wastewater through groundwater flow system (Lalehzari et al., 2013).

The solution of numerical model commonly can be obtained through some techniques like as Finite-Difference method (FDM) or Finite-Element method (FEM). The FEM example of solution of groundwater contaminant transport can be taken from CTRAN Examples (Geo-Slope, n.d.). Figure 1 is the example of contaminant transport spreading through confined porous media using CTRAN (FEM model).

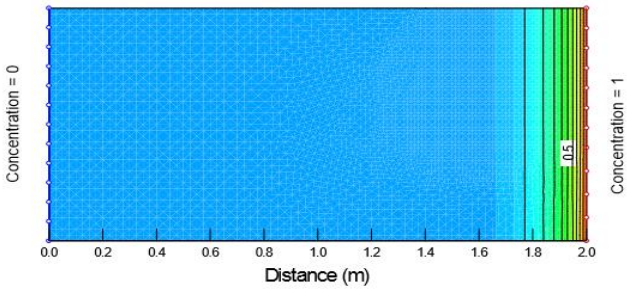


Fig. 1: The Example of CTRAN Result

The Finite-Difference model of groundwater equation as numerical solution has been developed by (Igboekwe & Achi, 2011). That research describes the application of FDM to solve steady-state condition of groundwater flow equation. Other research is presented by (Okiro et al., 2013)who describes the numerical treatment of confined aquifer boundary or no flow boundary.

The objective of this paper is to describe the mechanism of groundwater contaminant transport under saturated condition by

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mathematical model. Governing equation of groundwater flow and contaminant transport equations are conducted to make a mathematical model statement. The Finite-Difference Method is chosen to solve mathematical model numerically through Alternating Direction Implicit (ADI) scheme. Then, the result is compared and validated through another numerical method which is FEM.

2. Research Methodology

The concept of this model is simply described as flowchart on Figure 2. This figure describes the steps of this research which start from mathematical formulations, numerical solution by using FDM, simulation modelling and stability criteria of simulation. Each step will be discussed in the next sections.

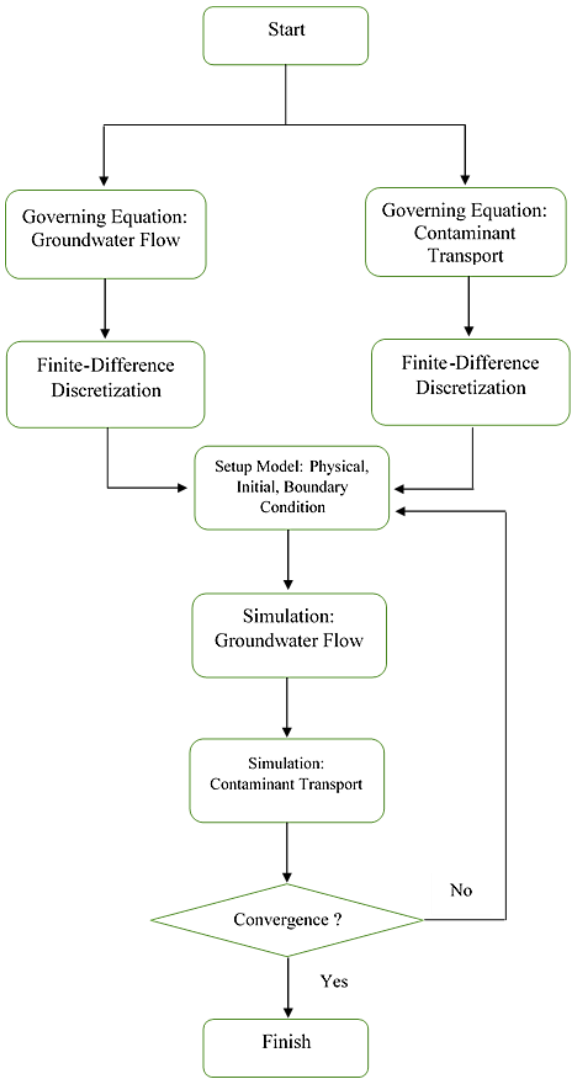


Fig. 2: The Flowchart of Research

3. Model Formulation

Contaminant transport equation is arranged of advection flux and hydrodynamic dispersion. Governing equation of groundwater contaminant transport is starts from mass conservation law for contaminant transport (Fischer et al., 1979).

$$\int_{CV} \frac{\partial}{\partial t} C d\forall + \int_{CS} q dA = 0 \tag{1}$$

Using the calculus rules, equation (1) is stated as

$$n\frac{\partial C}{\partial t} dxdydz = -\left[\frac{\partial q_x}{\partial x} + \frac{\partial q_y}{\partial y} + \frac{\partial q_z}{\partial z}\right] dxdydz \tag{2}$$

where n is porosity parameter. In the porous medium, the volume of the water depends on porosity(Bear & Cheng, 2010). If the both of $dxdydz$ on left and right-side are eliminated, equation (2) will transform as

$$n\frac{\partial C}{\partial t} = -\left[\frac{\partial q_x}{\partial x} + \frac{\partial q_y}{\partial y} + \frac{\partial q_z}{\partial z}\right] \tag{3}$$

Equation (3) is the final basic equation of contaminant transport in the porous medium. The term of flux (q) have to be expanded as advection-dispersion flux.

Advection flux

Advection is physical mechanism which the water as medium moving on and the contaminant carried in it. The flux advection is driven by fluid velocity (v). in the porous medium, the advection term is written as (Bear & Cheng, 2010)

$$q_{adv} = nvC \tag{4}$$

In the porous media, fluid velocity (v) is influenced by the groundwater potential head. By considering Darcian Approach, fluid velocity can be stated as (Notodarmojo, 2005)

$$v = -\frac{K}{n}\frac{\partial h}{\partial l} \tag{5}$$

K is hydraulic conductivity which depends on the type of the soil. Substitute equation (5) into equation (4), the equation becomes

$$q_{adv} = -n\frac{K}{n}\frac{\partial h}{\partial l}C \tag{6}$$

Where, C is the contaminant concentration. Equation (6) is the final term of advection flux in the porous medium.

Hydrodynamic Dispersion

Hydrodynamic dispersion is mechanism of contaminant particles spreading, caused by mechanics of dispersion and molecular diffusion(Bear, 1979). Hydrodynamic dispersion can be formulated as

$$D_h = D + D_m \tag{7}$$

The term of D is mechanics of dispersion and then Dm is molecular diffusion coefficient which depends on chemical element of contaminant. Mechanics of dispersion occurs caused by turbulence of groundwater motion and can be simply stated as longitudinal dispersion D_L and transversal dispersion D_T(Rubin & Atkinson, 2001)

$$D_L = \alpha_L v \tag{8}$$

$$D_T = \alpha_T v \tag{9}$$

Hydrodynamic dispersion flux is composed based on first fick law and can be written as (Bear & Cheng, 2010)

$$q_{disp} = -nD_h\frac{\partial C}{\partial l} \tag{10}$$

The final equation of advection-dispersion flux is arranged from equation (6) and equation (10), hence

$$q = -n\frac{K}{n}\frac{\partial h}{\partial l}C + \left(-nD_h\frac{\partial C}{\partial l}\right) \tag{11}$$

or if it is desired to distinguish contaminant transport term and groundwater flow term, the equation can be written as

$$q = -nvC + \left(-nD_h\frac{\partial C}{\partial l}\right) \tag{12}$$

Substitute equation (12) into the term of q on the equation (3), the groundwater contaminant transport model can be written as

$$\frac{\partial C}{\partial t} = -\left(v_x\frac{\partial C}{\partial x} + v_y\frac{\partial C}{\partial y} + v_z\frac{\partial C}{\partial z}\right) + \left(D_{hx}\frac{\partial^2 C}{\partial x^2} + D_{hy}\frac{\partial^2 C}{\partial y^2} + D_{hz}\frac{\partial^2 C}{\partial z^2}\right) \pm \frac{q_{s/o}}{n}C \tag{13}$$

Due on the equation (12) there is ∂h/∂l term (expanded by equation 5), it will be combined to groundwater flow model. The groundwater flow model has been derivate by (Harbaugh, 2005) and written as

$$\frac{\partial}{\partial x}\left(K_{xx}\frac{\partial h}{\partial x}\right) + \frac{\partial}{\partial y}\left(K_{yy}\frac{\partial h}{\partial y}\right) + \frac{\partial}{\partial z}\left(K_{zz}\frac{\partial h}{\partial z}\right) \pm W = S_s\frac{\partial h}{\partial t} \tag{14}$$

By considering the porous medium is in isotropic condition, equation (14) will be simply stated as

$$S_S\frac{\partial h}{\partial t} = K\left[\frac{\partial^2 h}{\partial x^2} + \frac{\partial^2 h}{\partial y^2} + \frac{\partial^2 h}{\partial z^2}\right] \pm W \tag{15}$$

Where S_s is specific storage and W is the term of sink and sources.

4. The Finite-Difference Discretization

The form of equation (13) and equation (15) are partial differential equations (PDE). The solution of these equations will be conducted numerically. The Finite Difference Method (FDM) is employed by this research. Alternating Direction Implicit scheme (ADI) was chosen to obtain the solution of PDE.

ADI scheme was shown in Figure3. ADI scheme is arranged into two steps in every one time step (Δt). On the first step, all of the x-direction components are analysed at time *l*, otherwise all of the y-direction components are analysed at time *l+1/2*. On the second step, all of the y-direction components are analysed like as first step and then all of the x-direction components are analysed at time *l+1*. Special case for time domain component, will be analysed by forward difference technique.

The component of PDEs are governed through Taylor Series. For two dimensional PDE, the Taylor Series can be written as (Triatmodjo, 2002) :

$$f(x_{i+1}, y_{j+1}) = f(x_i, y_j) + f'(x_i)\frac{\Delta x}{1!} + f'(y_j)\frac{\Delta y}{1!} + f''(x_i)\frac{\Delta x^2}{2!} + f''(y_j)\frac{\Delta y^2}{2!} + \ldots \tag{16}$$

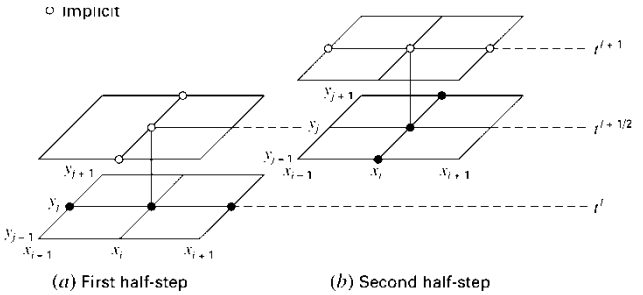


Fig.3: ADI Scheme (Chapra & Canale, 2015)

Using the ADI scheme and Taylor Series, the components of PDE can be expanded as

$$\frac{\partial f}{\partial t} = \frac{f_{i,j}^{l+1/2} - f_{i,j}^{l}}{\Delta t/2}, \tag{17}$$

$$\frac{\partial f}{\partial x} = \frac{f_{i+1,j}^{l} - f_{i-1,j}^{l}}{2\Delta x}, \tag{18}$$

$$\frac{\partial f}{\partial y} = \frac{f_{i,j+1}^{l+1/2} - f_{i,j-1}^{l+1/2}}{2\Delta y}, \tag{19}$$

$$\frac{\partial^2 f}{\partial x^2} = \frac{f_{i+1,j}^{l} - 2f_{i,j}^{l} + f_{i-1,j}^{l}}{(\Delta x)^2}, \tag{20}$$

$$\frac{\partial^2 f}{\partial y^2} = \frac{f_{i,j+1}^{l+1/2} - 2f_{i,j}^{l+1/2} + f_{i,j-1}^{l+1/2}}{(\Delta y)^2}. \tag{21}$$

for the first step and then

$$\frac{\partial f}{\partial t} = \frac{f_{i,j}^{l+1} - f_{i,j}^{l+1/2}}{\Delta t/2}, \tag{22}$$

$$\frac{\partial f}{\partial x} = \frac{f_{i+1,j}^{l+1} - f_{i-1,j}^{l+1}}{2\Delta x}, \tag{23}$$

$$\frac{\partial f}{\partial y} = \frac{f_{i,j+1}^{l+1/2} - f_{i,j-1}^{l+1/2}}{2\Delta y}, \tag{24}$$

$$\frac{\partial^2 f}{\partial x^2} = \frac{f_{i+1,j}^{l+1} - 2f_{i,j}^{l+1} + f_{i-1,j}^{l+1}}{(\Delta x)^2}, \tag{25}$$

$$\frac{\partial^2 f}{\partial y^2} = \frac{f_{i,j+1}^{l+1/2} - 2f_{i,j}^{l+1/2} + f_{i,j-1}^{l+1/2}}{(\Delta y)^2}. \tag{26}$$

for the second step.

Using equation (17) until equation (26), the solution of PDE (groundwater flow model and contaminant transport model) can be conducted. The first step solution of groundwater flow model and contaminant transport completely can be written as

$$2S_S\left[\frac{h_{i,j}^{l+1/2}-h_{i,j}^{l}}{\Delta t}\right]=K\left[\frac{h_{i+1,j}^{l}-2h_{i,j}^{l}+h_{i-1,j}^{l}}{(\Delta x)^2}+\frac{h_{i,j+1}^{l+1/2}-2h_{i,j}^{l+1/2}+h_{i,j-1}^{l+1/2}}{(\Delta y)^2}\right]\pm W \quad (27)$$

$$\frac{2\left(C_{i,j}^{l+1/2}-C_{i,j}^{l}\right)}{\Delta t}=-\frac{1}{2}\left(v_x\frac{C_{i+1,j}^{l}-C_{i-1,j}^{l}}{\Delta x}+v_y\frac{C_{i,j+1}^{l+1/2}-C_{i,j-1}^{l+1/2}}{\Delta y}\right)$$
$$+\left(D_{hx}\frac{C_{i+1,j}^{l}-2C_{i,j}^{l}+C_{i-1,j}^{l}}{(\Delta x)^2}+D_{hy}\frac{C_{i,j+1}^{l+1/2}-2C_{i,j}^{l+1/2}+C_{i,j-1}^{l+1/2}}{(\Delta y)^2}\right)\pm\frac{q_{s/o}}{n}C \quad (28)$$

From equation (28), the term of v_x and v_y are expanded as

$$v_x=-\frac{K}{n}\frac{\partial h}{\partial x}=-\frac{K}{n}\frac{h_{i+1,j}^{l}-h_{i-1,j}^{l}}{2\Delta x} \quad (29)$$

$$v_y=-\frac{K}{n}\frac{\partial h}{\partial y}=-\frac{K}{n}\frac{h_{i,j+1}^{l+1/2}-h_{i,j-1}^{l+1/2}}{2\Delta y} \quad (30)$$

The next step for dizcretization of PDE is the second step of ADI scheme. For the second step, the solution of groundwater flow model and contaminant transport sequentially can be written as

$$2S_S\left[\frac{h_{i,j}^{l+1}-h_{i,j}^{l+1/2}}{\Delta t}\right]=K\left[\frac{h_{i+1,j}^{l+1}-2h_{i,j}^{l+1}+h_{i-1,j}^{l+1}}{(\Delta x)^2}+\frac{h_{i,j+1}^{l+1/2}-2h_{i,j}^{l+1/2}+h_{i,j-1}^{l+1/2}}{(\Delta y)^2}\right]\pm W \quad (31)$$

$$\frac{2\left(C_{i,j}^{l+1}-C_{i,j}^{l+1/2}\right)}{\Delta t}=-\frac{1}{2}\left(v_x\frac{C_{i+1,j}^{l+1}-C_{i-1,j}^{l+1}}{\Delta x}+v_y\frac{C_{i,j+1}^{l+1/2}-C_{i,j-1}^{l+1/2}}{\Delta y}\right)$$
$$+\left(D_{hx}\frac{C_{i+1,j}^{l+1}-2C_{i,j}^{l+1}+C_{i-1,j}^{l+1}}{(\Delta x)^2}+D_{hy}\frac{C_{i,j+1}^{l+1/2}-2C_{i,j}^{l+1/2}+C_{i,j-1}^{l+1/2}}{(\Delta y)^2}\right)\pm\frac{q_{s/o}}{n}C \quad (32)$$

Equation (32) has v_x and v_y term like as the first step result. Therefore, based on the second step rule of ADI scheme, the term of v_x and v_y can be expanded as

$$v_x=-\frac{K}{n}\frac{\partial h}{\partial x}=-\frac{K}{n}\frac{h_{i+1,j}^{l+1}-h_{i-1,j}^{l+1}}{2\Delta x}, \quad (33)$$

$$v_y=-\frac{K}{n}\frac{\partial h}{\partial y}=-\frac{K}{n}\frac{h_{i,j+1}^{l+1/2}-h_{i,j-1}^{l+1/2}}{2\Delta y}. \quad (34)$$

5. Stability Criteria

Due this model will be simulated numerically, the numerical stability is become an important issue. To obtain convergence result from the simulation, hence determining stability criteria is necessary. There are three kinds of stability criteria will be used in this research follows Courant Condition, Neumann Criteria and Peclet Number (*Pe*). The first criteria is Courant Condition where the result of the multiply of fluid velocity *v* and Δt is equal to or less than Δx. Courant Condition can be formulated mathematically as (Notodarmojo, 2005)

$$C_{ox}=\left|\frac{\Delta t.v_x}{\Delta x}\right|\le 1 \quad \text{for ground water flow along x-direction} \quad (35)$$

$$C_{oy}=\left|\frac{\Delta t.v_y}{\Delta y}\right|\le 1 \quad \text{for ground water flow along y-direction} \quad (36)$$

The second criteria is Neumann criteria, in which this criteria describes the relationship between hydrodynamics dispersion with spatial component. The Neumann Criteria is written as (Notodarmojo, 2005)

$$\frac{D_{hx}.\Delta t}{(\Delta x)^2}+\frac{D_{hy}.\Delta t}{(\Delta y)^2}\le 0{,}5 \quad (37)$$

The last criteria is Peclet Number (Pe). The Peclet Number is ratio between advection to hydrodynamics dispersion and can be formulated as (Notodarmojo, 2005)

$$Pe_x=\frac{v_x.\Delta x}{D_{hx}}\le 2 \quad \text{for ground water flow along x-direction,} \quad (38)$$

$$Pe_y=\frac{v_y.\Delta y}{D_{hy}}\le 2 \quad \text{for ground water flow along y-direction.} \quad (39)$$

6. Model Setup

After the groundwater flow model and the contaminant transport model have been transformed to discrete equations, hence the next step is model setup. In this step, physical parameters have to be determined especially porous media properties and model configuration. This model is designed as simply rectangular form and confined condition. The boundary condition and initial condition of model are explained as follows:

1. Dirichlet boundary. It means that the value of primary variables are constant along the model boundary (Guo & Langevin, 2002). Based on this case, the variables which have a constant value are piezometric head (*h*) and contaminant concentration (*C*).
2. Neumann boundary. This boundary condition represents the condition of variables on the perpendicular model boundary (Guo & Langevin, 2002). This boundary is related to groundwater and contaminant flux which across model boundary. There are no flux boundary on the impermeable side. Due this model will be simulated into confined condition, hence on the top and bottom sides (impermeable side) have to fulfil conditions as follows

$$\frac{\partial h}{\partial y}=0 \quad (40)$$

$$\frac{\partial C}{\partial y}=0 \quad (41)$$

The boundary condition and initial condition can be described as shown in Figure 4.

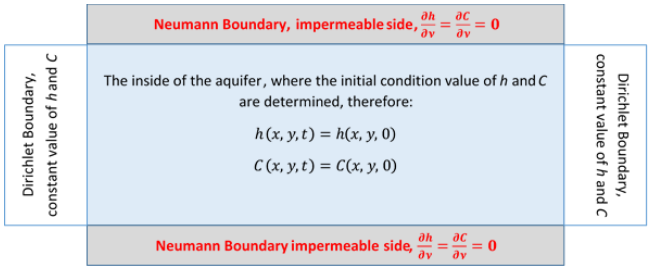


Fig. 4: The Boundary Condition and Initial Condition

The simulation of groundwater contaminant will be conducted through the simple scenario of sources. The scenario is continuous sources scenario. The continuous sources were chosen as boundary condition. Figure 5 describes the scenario of continuous sources.

The final discussion from this part is to determine the physical parameters and configuration of the studied model. This simulation taking assumption that the porous media is sandy. The physical parameters and configuration hypothetically can be shown in Table 1.

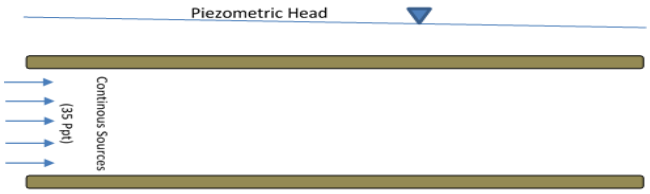


Fig. 5: The Term of Continuous Sources

Table 1: The Physical Parameters of Model

Num	Parameters	Unit	Values
1	The model width (x-direction)	m	100
2	The model height (y-direction)	m	30
3	Δx	m	5
4	Δy	m	3
5	Δt	day	1
6	Longitudinal dispersivity, α_L	m	25
7	Transversal dispersivity, α_T	m	4.17
8	Molecular diffusion coefficient, Dm	m^2/s	10^{-8}
9	Porosity		0.35
10	Hydraulic Conductivity, K	m/s	10^{-4}
11	Groundwater density, ρ	Kg/m^3	1000
12	Gravitational acceleration, g	m/s^2	9.81
13	Piezometric head (upstream)	m	2
14	Piezometric head (downstream)	m	1
15	Initial contaminant concentration, C	ppt	35

Determination of Δx, Δy and Δt depends on the value of *K*, piezometric head and molecular diffusion due the stability criteria.

7. Result and Discussion

The model is simulated up to 30 days as described in Figure 5. Simulation is conducted by developing computer program. Visual Basic for Application (VBA) is chosen in this research. Figure 6 shows the contour of contaminant concentration along the model domain. By evaluating one of point in the upstream of Figure 6, the change of contaminant concentration by time domain will be obtained. Figure 7 describes that the steady condition of concentration in the upstream will occurs after 30 days simulation. To reach 30 days simulation, it needs approximately 15 minutes in real time.

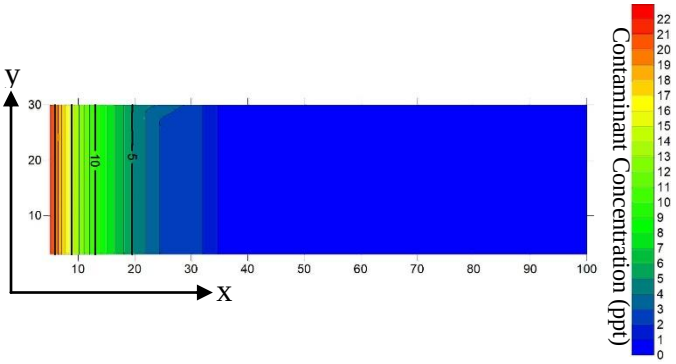


Fig. 6: The Contour of Contaminant Concentration at t = 30 days

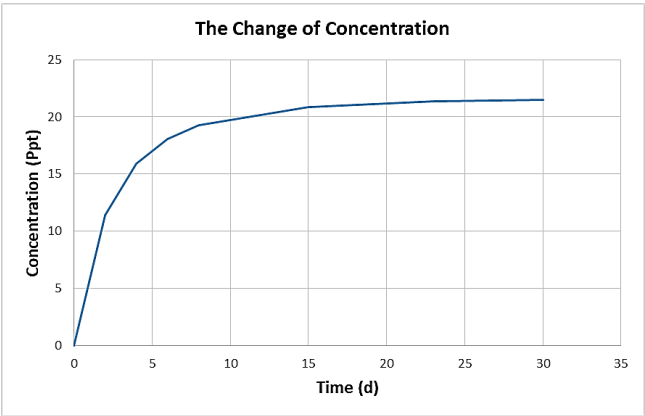


Fig. 7: The Change of Concentration by Time

The enhancement of contaminant concentration can be calculated based on Figure 7. Table 2 presents the tabulation of contaminant concentration at certain time and its enhancement.

To state that the model has a correct physical result, validation is necessary. For numerical simulation, despite conduct validation through physical model, it can be verified by comparing with the theoretical behaviour. One of the contaminant transport behaviour in the porous media can be shown in Figure 8 (Wang & Anderson, 1982).

The model on this research is simulation with dispersion effect. To obtain the behaviour of model with dispersion, results in Figure 7 have to be transformed into relative concentration graph. The relative result of concentration (C/Co) is presented in Figure 8, where C_o is initial concentration (35 ppt) and *C* is the concentration in each time step.

Based on Figure 9, the relative concentration of simulation has similar behaviour as theoretical behaviour (Figure 8). It can be stated that the simulation with dispersion has a correct physical result.

Table 2: Enhancement of Contaminant Concentration in the Upstream

Time (days)	Contaminant Concentration (ppt)	Enhancement (ppt)
0	0	
		11.43
2	11.43	
		4.50
4	15.92	
		2.16
6	18.08	
		1.19
8	19.27	
		1.60
15	20.87	
		0.47
23	21.34	
		0.13
30	21.47	

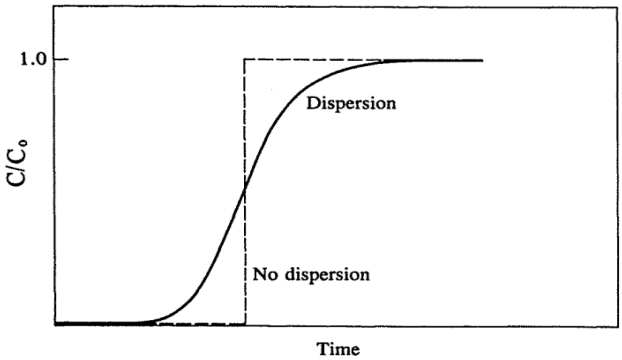


Fig. 8: The Theoretical Behaviour of Groundwater Contaminant Transport

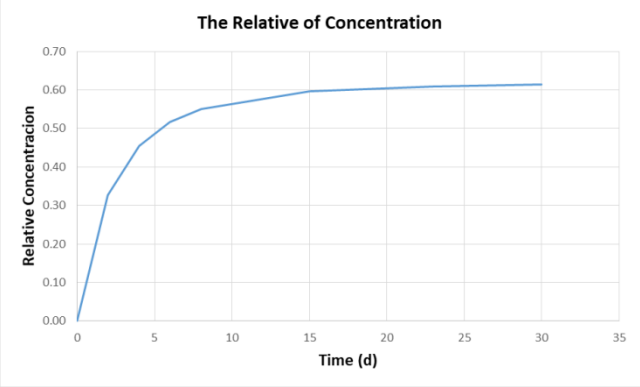


Fig. 9: Relative Contaminant Transport with Dispersion

After compared the numerical result with theoretical behaviour, the next qualitative validation was undertaken. The numerical result obtained by FDM model (Figure 6) has similar behaviour with the one obtained by FEM model (Figure 1). It can be concluded that the simulation has a correct physical result.

8. Conclusion

From this research, it can be concluded that groundwater contaminant transport can be simulated using Finite Difference Method especially through Alternating Direction Implicit scheme.
The most important parameter of groundwater contaminant modelling is the flux of advection based on groundwater flow model. Here, the change of contaminant concentration can be determined during the simulation. After simulation along certain time, the concentration will arrive to the steady state condition. The simulation of model has a correct physical result due the behaviour of model similar with theoretical behaviour and another numerical model using Finite Element Method.

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