Alternating direction implicit scheme as Finite-Difference method to solve coupled groundwater flow and contaminant transport model in the coastal aquifer

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Abstract. The simulation of coupled groundwater flow-contaminant transport equation can be conducted numerically. The Finite-Difference Method (FDM) through Alternating Direction Implicit (ADI) Scheme will be applied in this research. The ADI scheme is chosen because the FDM in two-dimensional form. The ADI scheme recognized to solve two-dimensional PDE (Partial Differential Equation) due the Crank-Nicholson has matrix dimension problem and other problem from another scheme of FDM. This research will use ADI scheme to transform the groundwater flow and contaminant transport equation become the discrete form. The model algorithm translated into VBA (Visual Basic Algorithm) code and the physical parameter determined hypothetically. The result of model simulation describes that the ADI scheme can be applied to solve coupled groundwater flow-contaminant transport equation. The result can be stated as stable because it reached the steady condition after 60 days of simulation.

1. Introduction

Many engineering problems can be stated as mathematical model on Partial Differential Equation (PDE) development. To solve PDE, there are two options to achieve it. The first option is analytical solution and second option is numerical solution. On PDE solving process, the analytical solution usually is very difficult, and then numerical solution is chosen to solve this problem. The Finite-Difference Method (FDM) is one of numerical methods which can be applied to solve the PDE.

Groundwater contaminant transport is one of engineering problems that can be stated as PDE. This model is arranged by groundwater flow model and contaminant transport model. The groundwater flow model simulation using FDM has been conducted [1]. This research describes the groundwater flow simulation under steady-state condition. Then, many cases for groundwater contaminant transport simulation has been conducted to trace the behaviour caused different condition such as contaminant transport through layered soil [2], dual porosity condition [3] and the transport of nitrate [4]. Literally, the main problem of groundwater contaminant transport simulation is the linkage of groundwater flow model and contaminant transport model. In the porous media, the fluid velocity is driven by the piezometric head of groundwater [5], hence the result of groundwater model simulation will be used along contaminant transport simulation. The advection flux of contaminant transport is calculated based on the value of piezometric head of groundwater [6].
Recently, many researchers have developed the groundwater flow model that can accommodate the effect of contaminant. This model called as dependent-density groundwater flow model such as SUTRA Model [7], Seawat Model [8]. Coupling this model to contaminant transport model is the pathway to solve this problem. The objective of this research to apply the FDM to solve the coupled groundwater flow-contaminant transport equation. Two dimensional PDE will be governed and the Alternating Direction Implicit (ADI) scheme used to solve it.

2. Groundwater flow and contaminant transport equations
This research involves two partial differential equations (PDE) follows groundwater flow equation and groundwater contaminant equation. The both of PDEs will coupled each other. The first PDE is dependent-density groundwater flow equation which written as [9]:

\[ \rho_f^2 g (n \beta + \alpha) \frac{\partial h}{\partial t} + nE \frac{\partial C}{\partial t} = \rho_f K \left( \frac{\partial^2 h}{\partial x^2} + \frac{\partial^2 h}{\partial y^2} \right) + KE \left( \frac{\partial h}{\partial x} \frac{\partial C}{\partial x} + \frac{\partial h}{\partial y} \frac{\partial C}{\partial y} \right) \pm q_{s,o} \]  

(1)

From equation (1) there are some physical parameters which have constant value. They are follows \( \rho_f \) as constant freshwater density, \( g \) as gravitational acceleration, \( n \) as porosity, \( K \) as hydraulic conductivity, \( \alpha \) as porous media compressibility, \( \beta \) as fluid compressibility and the term of \( q_{s,o} \) as sink and source. For \( K \) and \( n \), both of them are based on type of soil. The term of \( E \) is defined as the gradient of the changes of groundwater density to the changes of contaminant concentration. That values will be varying depends on the type of contaminant. In this research, NaCl will take role as contaminant and the value of \( E \) can state as 0.7143 [8].

As the second PDE, the groundwater contaminant transport equation governed using conservative advection-dispersion theories and can be written as [9]:

\[ \frac{\partial C}{\partial t} = - \left( v_x \frac{\partial C}{\partial x} + v_y \frac{\partial C}{\partial y} \right) + \left( D_{hx} \frac{\partial^2 C}{\partial x^2} + D_{hy} \frac{\partial^2 C}{\partial y^2} \right) \pm q_{s,o} \frac{n}{C_s} \]  

(2)

where \( v \) is the term of groundwater velocity. It is analysed by the numerical solution of equation (1) using groundwater velocity equation [6]:

\[ v_i = - \frac{K}{n} \frac{\partial h}{\partial i} \]  

(3)

\( D_{hx} \) and \( D_{hy} \) are hydrodynamic dispersion of porous media. The hydrodynamic dispersion of porous media is the summation of molecular diffusion coefficient \( (D_m) \) and mechanics of dispersion \( (D) \), then written as [10]:

\[ D_h = D + D_m \]  

(4)

The mechanics of dispersion \( (D) \) occurs on the two directions (longitudinal and transversal). The longitudinal and transversal mechanics of dispersion will be written sequentially as [11]:

\[ D_L = a_L v \]  

(5)

\[ D_T = a_T v \]  

(6)

where, \( a_L \) and \( a_T \) defined as longitudinal and transversal dispersivity.
3. Alternating Direction Implicit (ADI) discretization

Equation (1) and equation (2) will be transformed to discrete form as the numerical solution. This research applies the FDM to obtain the discrete form of PDE. Explicit scheme is one of the common techniques of FDM, where all of spatial variables component will be evaluated at current time \( t \) [12]. Unfortunately, the stability of simulation is an important issue due it very depends on the small value of \( \Delta t \) and it will take long time for the simulation.

Alternatively, there are some schemes as explicit scheme replacement, for examples are implicit scheme and Crank-Nicholson scheme. By the implicit scheme, the spatial variables component will be evaluated at next time step \((t+1)\), which is the value still unknown [12]. Although this scheme is recognized better than the explicit scheme, all of the solution of implicit scheme literally very depends on another unknown values around the reviewed point [12]. That is the main limitation of implicit scheme. In the other hand, Crank-Nicholson scheme use both of explicit and implicit scheme. By Crank-Nicholson scheme, weighting system is used on the explicit and implicit scheme. This scheme can be applied on two dimensional PDE, but the matrix form is very large [13]. The ADI is one of solution to solve this problem.

The ADI scheme is a FDM technique where every simulation at \( \Delta t \) divided into two steps. At the first step, the first spatial component (says as \( x \)-direction) is evaluated at time step \( t \), otherwise the second spatial component (says as \( y \)-direction) is evaluated at time step \( t+1/2 \). At the second step, the first spatial component is evaluated at time step \( t+1 \), then the second spatial component still evaluated at time step \( t+1/2 \). Figure 1 explains the ADI scheme [13].

![Figure 1. Illustration of ADI Scheme](image)

The ADI component arranged from two dimensional Taylor Series. The basic component for first step of ADI scheme can be written follows

\[
\frac{\partial f}{\partial t} = \frac{f_{i,j}^{t+1/2} - f_{i,j}^t}{\Delta t/2}, \\
\frac{\partial f}{\partial x} = \frac{2f_{i+1,j}^t - f_{i-1,j}^t}{2\Delta x}, \\
\frac{\partial f}{\partial y} = \frac{2f_{i,j+1/2}^t - f_{i,j-1/2}^t}{2\Delta y}, \\
\frac{\partial^2 f}{\partial x^2} = \frac{f_{i+1,j}^t - 2f_{i,j}^t + f_{i-1,j}^t}{(\Delta x)^2}, \\
\frac{\partial^2 f}{\partial y^2} = \frac{f_{i,j+1/2}^t - 2f_{i,j}^t + f_{i,j-1/2}^t}{(\Delta y)^2}.
\]
For the second step, equation (9) and (11) still applied for y-direction. Otherwise, for the second step, the term of $l$ on the equation (8) and (10) must be changed to $l+1$. The final term of second step is equation (7) which changed as

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

(12)

Use the ADI term and equation (7) to equation (12), the PDE which written as equation (1) and equation (2) will transformed become discrete equation as the PDE solution. The solution of groundwater flow equation written as

$$
2A \left[ \frac{h_{i,j}^{l+1} - h_{i,j}^l}{\Delta t} + 2nE \frac{c_{i,j}^{l+1/2} - c_{i,j}^l}{\Delta t} \right] = B \left[ \frac{h_{i,j+1}^{l+1} - 2h_{i,j}^{l+1} + h_{i,j-1}^l}{(\Delta x)^2} + \frac{h_{i+1,j}^{l+1} - 2h_{i,j}^{l+1} + h_{i-1,j}^l}{(\Delta y)^2} \right] + \frac{1}{4} \frac{KE}{\Delta t} \left[ \frac{\left( c_{i,j+1}^{l+1/2} - c_{i,j}^{l+1/2} \right) - \left( c_{i,j-1}^{l+1/2} - c_{i,j}^{l+1/2} \right)}{\Delta x} \right] + \frac{1}{4} \frac{KE}{\Delta t} \left[ \frac{\left( c_{i+1,j}^{l+1/2} - c_{i,j}^{l+1/2} \right) - \left( c_{i-1,j}^{l+1/2} - c_{i,j}^{l+1/2} \right)}{\Delta y} \right] \pm q_{s,0},
$$

(13)

for the first step of ADI, and the second step discretization will be written as

$$
2A \left[ \frac{h_{i,j}^{l+1} - h_{i,j}^l}{\Delta t} + 2nE \frac{c_{i,j}^{l+1} - c_{i,j}^l}{\Delta t} \right] = B \left[ \frac{h_{i,j+1}^{l+1} - 2h_{i,j}^{l+1} + h_{i,j-1}^l}{(\Delta x)^2} + \frac{h_{i+1,j}^{l+1} - 2h_{i,j}^{l+1} + h_{i-1,j}^l}{(\Delta y)^2} \right] + \frac{1}{4} \frac{KE}{\Delta t} \left[ \frac{\left( c_{i,j+1}^{l+1} - c_{i,j}^{l+1} \right) - \left( c_{i,j-1}^{l+1} - c_{i,j}^{l+1} \right)}{\Delta x} \right] + \frac{1}{4} \frac{KE}{\Delta t} \left[ \frac{\left( c_{i+1,j}^{l+1} - c_{i,j}^{l+1} \right) - \left( c_{i-1,j}^{l+1} - c_{i,j}^{l+1} \right)}{\Delta y} \right] \pm q_{s,0}.
$$

(14)

The term of $A$ and $B$ are defined in sequence

$$
\rho f^2 g(n\beta + \alpha) = A,
$$

(15)

$$
\rho f K = B.
$$

(16)

Similar to the groundwater flow equation, the groundwater contaminant transport equation is formed as discrete. The final discrete for groundwater contaminant transport equation are written as

$$
2 \frac{c_{i,j}^{l+1} - c_{i,j}^l}{\Delta t} = - \frac{1}{2} \left( v_x c_{i+1,j}^{l-1} - c_{i-1,j}^{l-1} \right) + v_y c_{i,j+1}^{l-1} - c_{i,j-1}^{l-1} \right) + \left( D_{hx} \frac{c_{i+1,j}^{l+1} - 2c_{i,j}^{l+1} + c_{i-1,j}^{l+1}}{(\Delta x)^2} \right) \pm \frac{q_{s,0}}{n} C, \quad (D_{hy} \frac{c_{i,j+1}^{l+1} - 2c_{i,j}^{l+1} + c_{i,j-1}^{l+1}}{(\Delta y)^2})
$$

(17)

for the first step and the second step written as

$$
2 \frac{c_{i,j}^{l+1} - c_{i,j}^{l+1/2}}{\Delta t} = - \frac{1}{2} \left( v_x c_{i+1,j}^{l+1/2} - c_{i-1,j}^{l+1/2} \right) + v_y c_{i,j+1}^{l+1/2} - c_{i,j-1}^{l+1/2} \right) \left( + \left( D_{hx} \frac{c_{i+1,j}^{l+1} - 2c_{i,j}^{l+1} + c_{i-1,j}^{l+1}}{(\Delta x)^2} \right) \pm \frac{q_{s,0}}{n} C, \quad (D_{hy} \frac{c_{i,j+1}^{l+1} - 2c_{i,j}^{l+1} + c_{i,j-1}^{l+1}}{(\Delta y)^2})
$$

(18)

Discretization process of PDEs has finished.

4. Model algorithm

Equation (13) and equation (14) are the discrete equations of groundwater flow. Otherwise, equation (7) and equation (18) are the discrete equations of groundwater contaminant transport. The finite difference
The simulation is conducted start from develop the two dimensional mesh grid. Figure 2 describes the two dimensional Cartesian coordinate (x-direction and y-direction), which the x-direction as the length of model (aquifer) and then the y-direction as the depth of model (aquifer). The red and blue arrow lines on the Figure 2 state the first step and the second step of ADI scheme. Based on that figure, along each time step simulation, the first step must be finished for entire of the mesh, after that the second step is conducted. The next step time level $t$ or $t+1$ on the simulation will be conducted after the second step of previous time step or $t-1$ finish.

![Figure 2. The ADI Pathway Step](image)

The simulation is conducted based on the pathway which explained before. On the every ADI step, the groundwater flow discrete equation will be analysed first and the second analysis is groundwater contaminant transport. The model algorithm can be described as the flowchart on the Figure 3 and Figure 4.

![Figure 3. The General Model Algorithm](image)

![Figure 4. The Subroutine of A](image)
5. Model simulation
To examine whether this model can simulate the mixing between freshwater-seawater in the coastal aquifer, the simple simulation will be conducted. The model algorithm translated as VBA code. The physical parameters listed on Table 1.

| Num | Parameters                              | Unit   | Values     |
|-----|-----------------------------------------|--------|------------|
| 1   | The model width (x-direction)           | m      | 50         |
| 2   | The model height (y-direction)          | m      | 25         |
| 3   | Δx                                      | m      | 2.5        |
| 4   | Δy                                      | m      | 2.5        |
| 5   | Δt                                      | day    | 1          |
| 6   | Longitudinal dispersivity, $a_L$        | m      | 2.5        |
| 7   | Transversal dispersivity, $a_T$         | m      | 0.42       |
| 8   | Molecular diffusion coefficient, $D_m$  | m$^2$/s| 10$^{-5}$  |
| 9   | Porosity                                |        | 0.35       |
| 10  | Hydraulic Conductivity, $K$             | m/s    | 10$^{-6}$  |
| 11  | Groundwater density, $\rho$             | Kg/m$^3$| 1000       |
| 12  | Gravitational acceleration, $g$         | m/s$^2$| 9.81       |
| 13  | Piezometric head (upstream)             | m      | 121.05     |
| 14  | Piezometric head (downstream)           | m      | 120        |
| 15  | Relative concentration, $C$             | ppt    | 35         |

Table 1. Physical Parameters of Model

Figure 5 and Figure 6 describe the initial condition and boundary condition of piezometric head $h$ and contaminant transport $C$. The light blue area informs boundary condition and other area informs initial condition.

**Figure 5. Boundary Condition and Initial Condition of $h$**

Based on Figure 5, the piezometric head $h$ along the aquifer are assumed linear due the value of $h$ in the upstream and downstream. The source of contaminant is origins from downstream of Figure 6 (right side picture) and the concentration $C$ will increase due the depth of aquifer [14].
The simulation is conducted based on flowchart model (Figure 3 and Figure 4). Taking 1 day simulation until steady condition achieved, the result of simulation described on Figure 7. Figure 7 presents the concentration contour in the aquifer. Based on that figure, the miscible condition was achieved. The concentration of contaminant can be determined in the entire of model as shown Figure 7.

Figure 6. Boundary Condition and Initial Condition of Contaminant Concentration C

Figure 7. Simulation Result

Figure 7 describes the steady condition achievement. To view the steps of the concentration rate changes, Figure 8 accommodates it as A-A selection on the Figure 7. In the Figure 8, the change of concentration rate will occurs in 0,10 d, 0,20 d, and 0,40 d. From Figure 8 we can also state that the change of concentration is very stable.
6. Conclusion
This research showed that ADI scheme can be used to simulate coupled groundwater flow-contaminant transport in the coastal aquifer. On the coupling process, iteration method can be applied. Based on the result of this research, this model can be simulated the seawater intrusion condition and its mitigation involving the sink/source term. The stability of simulation become the main issue in FDM simulation. If the simulation gets the unstable result, the physical parameter related to Courant Condition, Neumann Criteria and the Peclet (Pe) Number must be changed.

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Figure 8. A-A Selection
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