

Prediction of Contaminant Transport in Pasangan Groundwater Aquifer, Using Control Volume Model

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Abstract: For investigating the solute transport in groundwater aquifers, the governing equation of fluid movement through porous media was solved by the three dimensional numerical control volume methods using the three diagonal matrix algorithm. To test the model, it was applied to the examples used for the analytical methods in horizontal direction, in vertical direction. Comparisons of the analytical results with the obtained results show a good agreement. Also, to compare the present model with the finite difference model, the modular finite difference ground water flow model (MODFLOW) software developed by the U. S. Geological Survey (USGS) was used; the results are close to each other. This model was applied to the Pasangan watershed in Ghom state, which is located in the center of Iran. The concentration of chloride (Cl^-) was taken as the investigating property of the fluid (water). The model result was compared with the actual data of this watershed, which are close to each other. So, it is concluded that the present model can be a good potential to predict the contamination transport in groundwater aquifers and control the groundwater pollution crisis.

Key words: Contamination transport, groundwater aquifer, control volume model, pasangan watershed

INTRODUCTION

Contamination of groundwater resources is a serious problem in many places. To investigate the problem both analytical and numerical methods have been used. Ogata and Banks^[1] considered the solute transport in groundwater aquifers using one-dimensional analytical model. They considered only longitudinal diffusion transport. Batu^[2] introduced an analytical solute transport model with unidirectional flow field from time and space dependent sources in a bounded homogeneous media using the flux-type (third-type or Cauchy) boundary condition at the inlet location of the medium. Shan and Javandel^[3] introduced an analytical solution for solute transport in vertical section under two different source conditions: (1) a constant concentration of known value at the source (type A) and (2) a constant flux rate of known value from the sources (type B). In both cases the source face is parallel to the groundwater flow direction.

Also, during the past decade, numerical models have been widely used to study solute transport in porous media. Sun and Yeh^[4] proposed an alternative upstream weighing numerical method to simulate the transport process in groundwater under variety of conditions. Noorishad and Mehran^[5], developed an upstream finite-element method using efficient two nodal point

elements. Grisak and Pickens^[6] used a finite element method to model solute transport for a case with upstream Dirichlet boundary conditions (fixed concentration) for both fracture and matrix. Putti *et al.*^[7] developed a finite volume scheme with reference to triangular control volumes, for the convective and depressive fluxes. Burnett and Frind^[8] by combining Galerkin finite elements with the alternating direction finite difference method developed a technique that provides the accuracy, efficiency and flexibility needed to make three dimensional transport simulations practical. Also, Burnett and Frind^[9] applied the three-dimensional alternating direction Galerkin technique to the simulation of advective dispersive transport in a generic field scaled system. Kennedy and Lennox^[10] demonstrated the application of a control volume method to problems of contaminant transport through fractured clay. They discretized the transport equations using a control volume technique and emphasis on two important characteristics of the method: (1), its inherent conservation of mass and (2), its correct interpretation of physical phenomena, such as diffusivity at the interface between two control volumes.

In the present study, using a control volume technique, the general equations of solute transport in unsteady condition were linearized. Then using the Three Dimensional Matrix Algorithm (TDMA), the coefficient

parameters of the model evaluated and a computer program was written to solve the model. The model results were compared with analytical models.

Finally, this model was applied on the Pasangan watershed in Ghom state located in the center of Iran to investigate the contamination transport in groundwater aquifer.

Governing equation: The governing equation of mass transport through groundwater aquifers, for conservative solute is:

$$\frac{\partial(\rho C)}{\partial t} + \frac{\partial(\rho V_x \cdot C)}{\partial x} + \frac{\partial(\rho V_y \cdot C)}{\partial y} + \frac{\partial(\rho V_z \cdot C)}{\partial z} = \frac{\partial}{\partial x}(D_x \frac{\partial C}{\partial x}) + \frac{\partial}{\partial y}(D_y \frac{\partial C}{\partial y}) + \frac{\partial}{\partial z}(D_z \frac{\partial C}{\partial z}) + S \quad (1)$$

Where:

D_i = Hydrodynamic diffusion coefficient in I direction, L^2T^{-1} ;

C = Concentration of solute, ML^{-3} ;

V_i = Darcy's velocity of flow in I direction, LT^{-1} ;

S = Source or Sink, $ML^{-3}T^{-1}$

ρ = Density of fluid, ML^{-3} ;

The initial and boundary conditions are

$$\begin{aligned} C(0, 0, 0, t) &= C_0 & t &\geq 0 \\ C(x, y, z, 0) &= 0 & x, y, z, &\geq 0 \\ C(\infty, \infty, \infty, t) &= 0 & t &\geq 0 \end{aligned} \quad (2)$$

To solve this equation, a three-dimensional control volume model is introduced (Fig. 1). Using this control volume model and integrating the above equation with respect to time and space (the control volume) results the linear equation as below:

$$a_p C_p = a_w C_w + a_s C_s + a_n C_n + a_b C_b + a_t C_t + a_p^0 C_p^0 \quad (3)$$

Where:

a = The coefficients;

C = The concentration of solute at each node I;

p = Unknown nodes;

0 = The time.

The coefficients a_i can be introduced as:

$$\begin{aligned} a_w &= \max [D_w + F_w, (D_w + F_w/2), D_w], \dots \\ a_e &= \max [D_e - F_e, (D_e - F_e/2), D_e] \\ a_s &= \max [D_s + F_s, (D_s + F_s/2), D_s], \dots \\ a_n &= \max [D_n - F_n, (D_n - F_n/2), D_n] \\ a_b &= \max [D_b + F_b, (D_b + F_b/2), D_b], \dots \\ a_t &= \max [D_t - F_t, (D_t - F_t/2), D_t] \\ a_p &= a_w + a_e + a_s + a_n + a_b + a_t + a_p^0 + \Delta F, \dots \\ \Delta F &= F_e - F_w + F_n - F_s + F_t - F_b \end{aligned} \quad (4)$$

Where:

$$\begin{aligned} a_p^0 &= \frac{\Delta V}{\Delta t} \\ F_i &= \rho_i C_i V_i \\ \Delta V &= \Delta X \cdot \Delta Y \cdot \Delta Z \end{aligned} \quad (5)$$

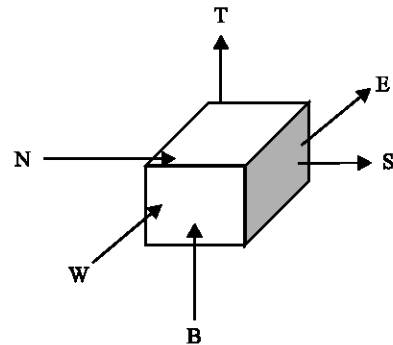


Fig. 1: A control volume model, which E, W, S, N, T and B represent directions in east, west, south, north, top and bottom, respectively

Table 1: Results of present model and analytical model in horizontal direction^[1]

Distance from contaminant source (m)	Analytical model results ^[1]	Present model results
0	10.000	10.00
10	9.610	9.59
20	8.850	8.81
30	7.740	7.65
40	6.280	6.22
50	4.730	4.72
60	3.220	3.34
70	2.020	2.21
80	1.140	1.37
90	0.830	0.79
100	0.280	0.44
110	0.068	0.23
120	0.023	0.11
130	0.007	0.05
140	0.002	0.02
150	0.000	0.01

Table 2: Results of present model and analytical model in vertical direction^[2]

Distance from contaminant source (m)	Analytical model results ^[2]	Present model results
2.5	2.420	1.88
7.5	1.610	1.46
12.5	0.710	0.66
19.5	0.210	0.22
24.5	0.040	0.06
29.5	0.006	0.01

Control volume method is used to solve the above-linearized equation. To test the model, it was applied on the examples used by Ogata and Banks^[1] in horizontal direction and Shan and Javandel^[3] in vertical direction. The model results in horizontal direction and the Ogata and Banks^[1] results are shown on Table 1, also the model

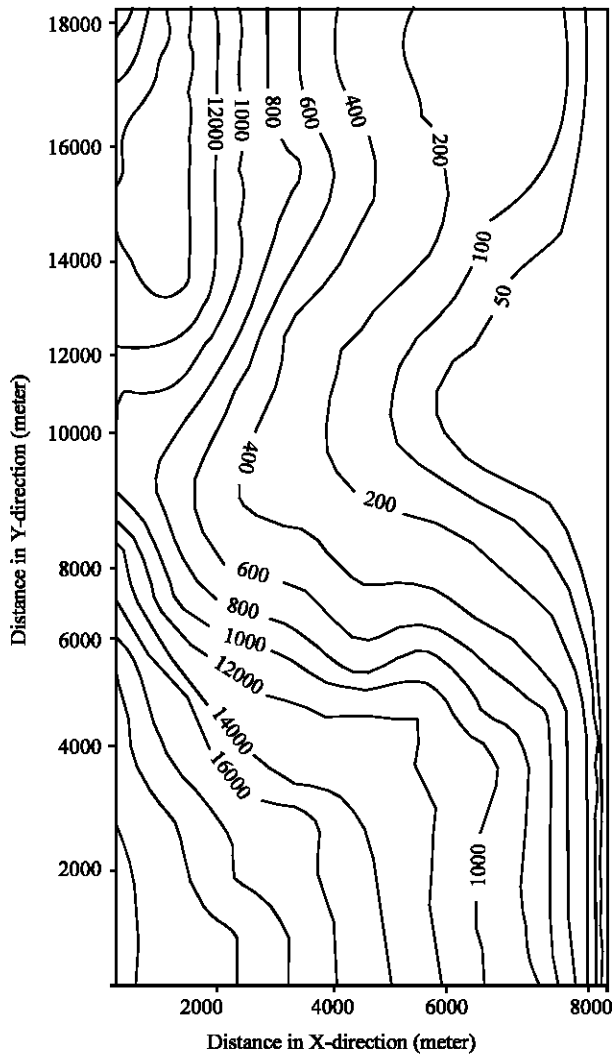


Fig. 2: Chloride concentration of the Pasangan watershed after 365 days

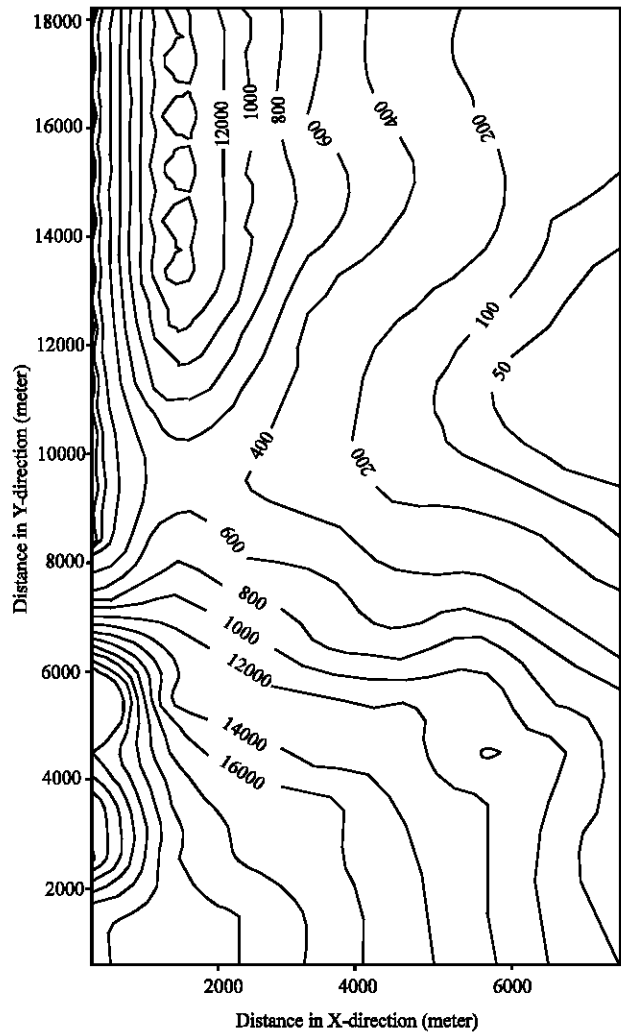


Fig. 3: Prediction of chloride concentration of the Pasangan watershed for the next 10 years

Table 3: Results of analytical model, present model and finite difference model (MT3D)

Distance from contaminant source (m)	Analytical model results ^[1]	Present model results	Finite difference model results (MT3D)
0	10.000	10.000	10.000
10	9.610	9.593	9.616
20	8.850	8.811	8.871
30	7.740	7.647	7.748
40	6.280	6.219	6.700
50	4.730	4.719	4.663
60	3.220	3.339	3.237
70	2.080	2.206	2.103
80	1.140	1.366	1.249
90	0.830	0.794	0.644
100	0.280	0.436	0.273
110	0.070	0.226	0.122
120	0.023	0.112	0.063
130	0.007	0.053	0.029
140	0.002	0.024	0.013
150	0.000	0.010	0.006
160	0.000	0.004	0.002

results in vertical direction and the Shan and Javandel^[3] results are shown on Table 2.

Also, to compare the present model with the finite difference model (MT3D), in the Modflow88 software, the Ogate and Banks example data were used. The results of the present model and the finite difference model with the Ogate and Banks^[1] analytical result are in a good agreement (Table 3).

To test the effect of nodes number on the control volume model behavior, the Ogate and Banks^[1] example data were used and the nodes number of the model were changed from 5 to 20-40-80 and 100. Results of the model for each nodes number were compared with the results of the analytical solution^[1] results are shown on Table 4. It is clear that by increasing the nodes number, the two model results become closer (Table 4).

Table 4: Nodes number effect on the model results

		Contaminant concentration (mg L ⁻¹)				
Distance from contaminant source (m)	Analytical model results ^[1]	Finite volume model results with different nodes number				
		5 nodes	20 nodes	40 nodes	80 nodes	100 nodes
0	10.000	10.00	10.000	10.000	10.000	10.000
10	9.610		9.593	9.598	9.599	9.599
20	8.855		8.811	8.840	8.846	8.847
30	7.743		7.647	7.706	7.720	7.721
40	6.277	6.36	6.219	6.289	6.307	6.309
50	4.734		4.719	4.771	4.786	4.787
60	3.218		3.339	3.351	3.359	3.357
70	2.017		2.206	2.177	2.171	2.171
80	1.144	2.73	1.366	1.310	1.296	1.294
90	0.835		0.794	0.731	0.714	0.712
100	0.280		0.436	0.380	0.365	0.363
110	0.068		0.226	0.184	0.173	0.171
120	0.023	0.87	0.112	0.084	0.076	0.075
130	0.007		0.053	0.036	0.032	0.031
140	0.002		0.024	0.014	0.012	0.012
150	0.000		0.010	0.006	0.004	0.004
160	0.000	0.00	0.004	0.002	0.002	0.001

Table 5: Effect of time intervals on the model results for a network with 20 nodes in each direction

		Contaminant concentration (mg/lit)						
Distance from contaminant source (m)	Analytical model results ^[1]	Finite volume model results with different time interval						
		0.01 days	0.05 days	0.1 days	0.5 days	1 days	5 days	10 days
0	10.000	10.000	10.000	10.000	10.000	10.000	10.000	10.000
10	9.610	9.598	9.598	9.596	9.596	9.593	9.576	9.560
20	8.855	8.818	8.817	8.814	8.814	8.811	8.794	8.792
30	7.743	7.640	7.640	7.640	7.643	7.647	7.692	7.766
40	6.277	6.174	6.176	6.178	6.196	6.219	6.396	6.600
50	4.734	4.624	4.627	4.632	4.671	4.710	5.062	5.415
60	3.218	3.198	3.204	3.211	3.269	3.339	3.826	4.377
70	2.017	2.044	2.049	2.058	2.125	2.206	2.772	3.332
80	1.144	1.206	1.213	1.221	1.286	1.366	1.933	2.516
90	0.835	0.660	0.665	0.672	0.727	0.794	1.303	1.860
100	0.280	0.336	0.340	0.345	0.385	0.436	0.851	1.349
110	0.068	0.159	0.162	0.165	0.192	0.226	0.540	0.962
120	0.023	0.071	0.072	0.074	0.900	0.112	0.334	0.676
130	0.007	0.029	0.030	0.031	0.040	0.053	0.202	0.467
140	0.002	0.012	0.012	0.012	0.017	0.024	0.128	0.321
150	0.000	0.004	0.004	0.005	0.007	0.010	0.070	0.217
160	0.000	0.001	0.002	0.002	0.002	0.004	0.040	0.145
170	0.000	0.000	0.001	0.001	0.001	0.0002	0.022	0.095

Also, to investigate the effect of the time intervals on the model results, it was used with 20 nodes in each direction (x, y, z) and different time intervals $\Delta t=0.01, 1, 2, \dots$ to $\Delta t = 10$ days. As shown on Table 5, reduction of the time interval (Δt), increases the accuracy of the model results. Therefore it can be concluded that by increasing the nodes number and reducing the time interval the precision of the model results increases.

Application of the model to the Pasangan watershed: The present model was applied to the Pasangan watershed in Ghom state, which is located in the center of Iran. This watershed has an area of 152 square kilometers with 11 piezometric wells. The thickness of the aquifer is about 200 m, with transmissibility of $T=800$ square m per days and porosity of 0.3. The chloride (Cl^-) concentration of

groundwater was measured at all wells during two years since 1999-2000. The first year chloride concentration data was used to calibrate the model for the Pasangan watershed. Then, the control volume model with time interval of one day was used to predict the chloride concentration of the wells for 365 days, (Fig. 2). The model results and the second year actual data of the wells were in a good agreement. So, it is concluded that, this control volume model can be used to predict the chloride concentration of the Pasangan watershed with the sufficient accuracy. Using this model, the chloride concentration of the Pasangan watershed is predicted for the next 10 years, results are shown on Fig. 3.

To investigate the contamination transport in groundwater resources, a finite volume model in unsteady condition was introduced. Results of this model were

compared with analytical models (both in horizontal and vertical directions) and the finite difference model (MT3D), in Modflow 88 software, which are in a good agreement. To increase the accuracy of this model, effect of nodes number and time steps on the model results were investigated. Results show that precision of the model increases by increasing nodes number and decreasing time steps.

This model was applied to Pasangan watershed in Ghom state, which is located in the center of Iran. This model was used to predict the Chloride (Cl^-) concentration of the groundwater in the watershed. Comparison of the model results with the actual data of this watershed shows a good agreement. So, the present model can be used to predict the contamination transport in groundwater aquifers and control the groundwater pollution crisis.

REFERENCES

1. Ogata, A. and R.B. Banks, 1961. A Solution of the Differential Equation of Longitudinal Dispersion in Porous Media. U. S. Geol. Surv. Prop. Paper, 411-418.
2. Batu, V., 1993. A Generalized Two-Dimensional Analytical Solute Transport Model in Bounded Media for Flux-Type Finite Multiple Sources. *Water Resources Res.*, 29: 2881-2892.
3. Shan, C. and I. Javandel, 1997. Analytical Solutions for Solute Transport in a Vertical Aquifer Section. *Contaminant Hydrol.*, 27: 63-82.
4. Sun, N.Z. and W.G. Yeh, 1983. A Proposed Upstream Weight Numerical Method for Simulating Pollutant Transport in Groundwater. *Water Resources Res.*, 19: 1489-1500.
5. Noorishad, J. and M. Mehran, 1982. An Upstream Finite Element Method for Solution of Transient Transport Equation in Fractured Porous Media. *Water Resources Res.*, 18: 588-596.
6. Grisak, G.E., J.F. Picken and J.A. Cherry, 1980. Solute Transport Through Fractured Media, 2. Column Study of Fractured Till. *Water Resources Res.*, 16: 731-739.
7. Putti, M., W.W. Yeh and W.A. Mulder, 1990. A Triangular Finite Volume Approach With High Resolution Upwind Terms for the Groundwater Transport Equations. *Water Resources Res.*, 26: 2865-2880.
8. Burnett, R.D. and E.O. Frind, 1987. Simulation of Contaminant Transport in Three Dimensional, 1. The Alternating Direction Galerkin Technique. *Water Resources Res.*, 23: 683-694.
9. Burnett, R.D. and E.O. Frind, 1987. Simulation of Contaminant Transport in Three Dimensional, 2. Dimensionality Effects. *Water Resources Res.*, 23: 683-694.
10. Kennedy, C.A. and C. Lennox, 1995. A Control Volume Model of Solute Transport in a Single Fracture. *Water Resources Res.*, 31: 313-322.