A Dynamic Programming Solution to Solute Transport and Dispersion Equations in Groundwater

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ABSTRACT

The partial differential equations for water flow and solute transport in a two-dimensional saturated domain are rendered discrete using the finite difference technique; the resulting system of algebraic equations is solved using a dynamic programming (DP) method. The advantage of the DP algorithm is that the problem is converted from solving an algebraic system of order NC(NL-1) ×NC(NL-1) into one of solving a difference equation of order NC×NC over NL-1 steps and involving NL-1 matrix inversions of order NC×NC. The accuracy and precision of the solutions are shown by comparing the results with an analytical solution and calculation of mass the balance. In addition, the performance of the DP model was compared with the results of the MOC model developed by US Geological Survey. In all cases, the DP model showed good results with sufficient accuracy.

Keywords: Dynamic programming, Groundwater, Numerical model, Solute transport.

INTRODUCTION

In Iran, groundwater is an important source of irrigation water. In fact, it fulfills more than 50 percent of the country's total irrigation needs. Groundwater has played a major role in increasing food production and achieving food security. Groundwater, a renewable source of water, has the remarkable distinction of being a highly dependable and safe source of water supply for agriculture, domestic and industrial needs. Increased use of chemical fertilizers coupled with improper water management practices has resulted in the deterioration of groundwater quality in several parts of the country. Every year, almost 17.5 BCM of agricultural wastewater is returned to aquifers which account for almost 35% of groundwater extraction (1). This recycling of water causes secondary salinization in irrigated areas.

Solute transport models are being used to study groundwater quality and water pollution in the subsurface. Several methods have been used to generate a better and faster model, for example: Reddell and Sunada (20); Chatwal *et al.* (6); Cheng and Hodge (7); Gray and Pinder (11); Grove (12); Huyakorn *et al.* (13); Konikow and Bredehoeft (14); and Bouhroum and Bai (5). In addition, certain advances in analytical solutions have been made by some other researchers such as Basha and El Habel (2) and Sim and Chrysikopoulos (21). They have developed one-, two-, and three-dimensional analytical solutions for solute transport in saturated, homogeneous porous media. However, numerical algorithms are still the only solution to complex problems in the field of solute transport in groundwater.

In this paper, a numerical model to solve the solute transport and dispersion equation in groundwater is developed. The purpose of

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the simulation model is to compute the concentration of a non-reactive dissolved chemical species in an aquifer at any given time and place. The partial differential equations are made discrete using the finite difference technique and the resulting system of algebraic equations is solved using a dynamic programming (DP) method which is used here for the first time. Bellman (4), Collins (8) and Collins and Angel (9) applied this technique to the solution of parabolic and elliptic partial differential equations. A dynamic programming method was then used by Mirabzadeh (16, 17, 18, 19) to solve the flow equation in two and three dimensions for heterogeneous and anisotropic aquifers. The higher speed of this algorithm compared with the other matrix solutions such as Jacobi, Guass-Sidel, and Successive over Relaxation (SOR) has been the motivation for using the method in this research (9, 17).

Convective transport, hydrodynamic dispersion, and chemical reactions are the three main processes in solute transport. Among these, the first two phenomena are more important in most cases and those have been considered in this model. Because convective transport and hydrodynamic dispersion depend on the velocity of groundwater flow, the solute transport equation is a nonlinear equation and must be considered in conjunction with the groundwater flow equation. The computer program solves two simultaneous partial differential equations- one is the groundwater flow equation and the second one is the solute transport equation.

A solution to the solute transport equation in two dimensions has been obtained using a dynamic programming technique. In this paper, the analytical solution (2) and the method of characteristics were used to verify the developed algorithm. The method of characteristics was originally applied to transport in porous media by Garder *et al*. (11) in order to calculate miscible displacement in a reservoir simulation. This method was later implemented in a two-dimensional solute transport model by Konikow and Bredehoeft (14); their code is commonly

referred to as MOC. The method of characteristics uses a conventional particle tracking technique for solving the advection term. For more detail about this method, one can refer to Zheng and Bennett (22).

Theoretical Development

In a Cartesian coordinates, the governing equation for two dimensional fluid flow in a saturated porous medium by using the continuity equation and Darcy's low, is:

$$\frac{\partial}{\partial x}\left(T_{xx}\frac{\partial h}{\partial x}\right)+\frac{\partial}{\partial y}\left(T_{yy}\frac{\partial h}{\partial y}\right)=S\frac{\partial h}{\partial t}\pm q \qquad (1$$

where h is hydraulic head [L]; t is time [T]; q is source/sink term [L/T] with a positive sign for the source and negative for sink terms; S is storage coefficient; and T_{xx} and T_{yy} are transmisivity $[L^2/T]$ in x and y direction, respectively. Transmisivity is defined as follows:

$$[T_{ij}]=b[K_{ij}] \qquad (2$$

where b is the saturated thickness of the aquifer [L]; and $[K_{ij}]$ is the hydraulic conductivity tensor. It is assumed that the coordinate system is oriented with the conductivity tensor, so that $K_{ij}=0$ for $i\neq j$.

The solute transport equation describing convection and dispersion of a nonreactive dissolved chemical species in groundwater is as follows (14):

$$\left[\frac{\partial}{\partial x}\left(bn_eD_{xx}\frac{\partial C}{\partial x}\right)+\frac{\partial}{\partial y}\left(bn_eD_{yy}\frac{\partial C}{\partial y}\right)\right]$$
$$+\left[\frac{\partial}{\partial x}\left(bn_eD_{xy}\frac{\partial C}{\partial y}\right)+\frac{\partial}{\partial y}\left(bn_eD_{yx}\frac{\partial C}{\partial x}\right)\right] \qquad (3$$
$$=bn_e\frac{\partial C}{\partial t}+\left(bV_x\frac{\partial C}{\partial x}+bV_y\frac{\partial C}{\partial y}\right)+C(n_e\frac{\partial b}{\partial t}-S\frac{\partial h}{\partial t})$$
$$+q(C'-C)$$

where C is the concentration of the dissolved chemical species $[M/L^3]$; C' is the concentration of dissolved chemical in a source or sink fluid $[M/L^3]$; n_e is the effective porosity; V_x and V_y are Darcy's velocities in x and y directions, respectively [L/t]; and $D_{i,j}$ is the coefficient of the hydrodynamic dispersion $[L^2/T]$. The dispersion coefficient for

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two-dimensional flow in an isotropic aquifer may be written as (4):

$$D_{xx} = \alpha_L \frac{(V_x)^2}{|V|} + \alpha_T \frac{(V_y)^2}{|V|} \tag{4}$$

$$D_{yy} = \alpha_T \frac{(V_x)^2}{|V|} + \alpha_L \frac{(V_y)^2}{|V|} \tag{5}$$

$$D_{xy} = D_{yx} = (\alpha_L - \alpha_T)\frac{V_x V_y}{|V|} \tag{6}$$

where α_L and α_T are the longitudinal and transverse dispersivities of the aquifer, respectively [L]; and $|V|$ is the magnitude of the velocity [L/T].

Finite Difference Formulation

The two-dimensional model presented here is based on an implicit finite difference scheme using the dynamic programming solution.

Flow Equation

The compact finite difference form of equation (1) is given by:

$$Wx_{(i-1,j)}h_{(i-1,j)}^k + Wx_{(i,j)}h_{(i+1,j)}^k + Wy_{(i,j-1)}h_{(i,j-1)}^k$$
$$+ Wy_{(i,j)}h_{(i,j+1)}^k - Wc_{(i,j)}h_{(i,j)}^k = R_{(i,j)}^{k-1} \tag{7}$$

$i = 2,…,NL-1$

$j = JD(i),…, JF(i)$

where i, j, k are, respectively, the indices in the x, y, and time dimensions and JD(i), JF(i) are the column numbers at the beginning and the end of each row, respectively.

$$Wx_{(i,j)} = T_{xx(i+1/2,j)} \frac{\Delta y_{(j)}}{\Delta x_{(i)}} \tag{8a}$$

$$Wy_{(i,j)} = T_{yy(i+1/2,j)} \frac{\Delta x_{(i)}}{\Delta y_{(j)}} \tag{8b}$$

$$Wc_{(i,j)} = Wx_{(i-1,j)} + Wx_{(i,j)} + Wy_{(i,j)}$$
$$+ Wy_{(i,j-1)} + S_{(i,j)}\frac{\Delta x_{(i)}\Delta y_{(j)}}{\Delta t} \tag{8c}$$

$$R_{(i,j)}^{k-1} = \Delta x_{(i)}\Delta y_{(j)}\left(S_{(i,j)}\frac{h_{(i,j)}^{(k-1)}}{\Delta t} + q_{i,j}^{k-1/2}\right) \tag{8d}$$

Solute Transport Equation

Using the finite difference discretization approach, equation (3) can be written as:

$$\left[B_{xx(i-1,j)}C_{(i-1,j)} + B_{xx(i,j)}C_{(i+1,j)}\right.$$
$$\left. + B_{yy(i,j-1)}C_{(i,j-1)} + B_{yy(i,j)}C_{(i,j+1)} - B_{c(i,j)}C_{(i,j)}\right]^k$$
$$= R_{c(i,j)}^{k-1} \tag{9}$$

where

$$B_{xx(i,j)}^k = b_{(i+1/2,j)}^k n_{e(i,j)} D_{xx(i+1/2,j)}^k \tag{10a}$$

$$B_{yy(i,j)}^k = b_{(i,j+1/2)}^k n_{e(i,j)} D_{yy(i,j+1/2)}^k \tag{10b}$$

$$B_{c(i,j)}^k = \left[B_{xx(i-1,j)} + B_{xx(i,j)} + B_{yy(i,j-1)} + B_{yy(i,j)}\right.$$
$$\left. + \frac{\Delta x_{(i)}\Delta y_{(j)}}{\Delta t}n_{e(i,j)}b_{(i,j)}\right]^k \tag{10c}$$

$$R_{c(i,j)}^{k-1} = R_{2(i,j)}^{k-1} + R_{3(i,j)}^{k-1} - R_{1(i,j)}^{k-1} -$$
$$\frac{\Delta x_{(i)}\Delta y_{(j)}}{\Delta t}n_{e(i,j)}b_{(i,j)}^k C_{(i,j)}^{k-1} \tag{10d}$$

$$\frac{R_{1(i,j)}^{k-1}}{\Delta x_{(i)}\Delta y_{(j)}} = \left[\frac{\partial}{\partial x}\left(bn_e D_{xy}\frac{\partial C}{\partial y}\right) + \frac{\partial}{\partial y}\left(bn_e D_{yx}\frac{\partial C}{\partial x}\right)\right]^{k-1} =$$
$$\frac{1}{\Delta x_{(i)}\Delta y_{(j)}}\left\{B_{xy(i,j)}^k\left[C_{(i,j-1)} + C_{(i-1,j-1)} - C_{(i,j+1)} - C_{(i-1,j+1)}\right]^{k-1}\right.$$
$$+ B_{xy(i,j)}^k\left[C_{(i,j+1)} + C_{(i+1,j+1)} - C_{(i,j-1)} - C_{(i+1,j-1)}\right]^{k-1}$$
$$+ B_{yx(i,j)}^k\left[C_{(i-1,j-1)} + C_{(i-1,j)} - C_{(i+1,j-1)} - C_{(i+1,j)}\right]^{k-1}$$
$$\left. + B_{yx(i,j)}^k\left[C_{(i+1,j)} + C_{(i+1,j+1)} - C_{(i-1,j)} - C_{(i-1,j+1)}\right]^{k-1}\right\} \tag{10e}$$

$$B_{xy(i,j)}^k = b_{(i+1/2,j)}^k n_{e(i,j)} D_{xy(i+1/2,j)}^k \tag{10f}$$

$$B_{yy(i,j)}^k = b_{(i,j+1/2)}^k n_{e(i,j)} D_{yy(i,j+1/2)}^k \tag{10g}$$

$$\frac{R_{2(i,j)}^{k-1}}{\Delta x_{(i)}\Delta y_{(j)}} = \left[bV_x\frac{\partial C}{\partial x} + bV_y\frac{\partial C}{\partial y}\right] = \frac{1}{\Delta x_{(i)}\Delta y_{(j)}}\{\alpha_1 Wx_{(i-1,j)}$$
$$[h_{(i-1,j)} - h_{(i,j)}]^k[C_{(i-1,j)} - C_{(i,j)}]^{k-1} + \alpha_2 Wx_{(i,j)}$$
$$[h_{(i+1,j)} - h_{(i,j)}]^k[C_{(i+1,j)} - C_{(i,j)}]^{k-1} + \alpha_3 Wy_{(i,j-1)}[h_{(i,j-1)}$$
$$- h_{(i,j)}]^k[C_{(i,j-1)} - C_{(i,j)}]^{k-1} + \alpha_4 Wy_{(i,j)}[h_{(i,j+1)} - h_{(i,j)}]^k$$
$$[C_{(i,j+1)} - C_{(i,j)}]^{k-1} \tag{10h}$$

where $\alpha_1\begin{cases}=0 & [h_{(i-1,j)} - h_{(i,j)}]^k \le 0 \\ =1 & [h_{(i-1,j)} - h_{(i,j)}]^k > 0\end{cases}$ and

also the same thing for α_2, α_3, and α_4.

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$$\frac{R_{3(i,j)}^{k-1}}{\Delta x_{(i)} \Delta y_{(j)}} = \left[C \left(n_e \frac{\partial b}{\partial t} - S \frac{\partial h}{\partial t} \right) + q \left(C' - C \right) \right] =$$

$$C_{(i,j)}^{k-1} \left[n_{e(i,j)} \frac{b_{(i,j)}^k - b_{(i,j)}^{k-1}}{\Delta t} - S_{(i,j)} \frac{h_{(i,j)}^k - h_{(i,j)}^{k-1}}{\Delta t} \right] \quad (10i$$

$$+ q \left[C'_{(i,j)} - C_{(i,j)}^{k-1} \right]$$

Dynamic Programming Solution

In this section, the proposed relationships for solving the resulting algebraic equations are presented. In order to solve equation (7) subject to the boundary conditions, we define the vectors H_i, W_i, and R_i^* with the dimension of $N(i) = NC-2$ for each row:

$$H_i = h_{(i,j)}^{k+1} \qquad W_i = \left[W_{x(i,j)} h_{(i,j)}^k \right]$$

$$R_i^* = R_{(i,j)}^k$$

$$i = 2, NL - 1 \qquad j = JD(i)...JF(i)$$

Using the above definitions, equation (7) may be rewritten as follows:

$$F_{(i-1)} H_{(i-1)} + F_{(i)} H_{(i+1)} - G_{(i)} H_{(i)} + W_i = R_{(i)}^*$$

$$i = 2, 3, ..., NL - 1$$

$$(11$$

Vectors $H_{(1)}$, $H_{(NL)}$, and W_i are known from the boundary conditions, $F_{(i)}$ and $F_{(i-1)}$ are the diagonal matrices, and $G_{(i)}$ is a tridiagonal matrix with the components defined by the coefficients of the system of equations (7) as follows:

$$F_{(i)} = diag(f) \qquad f = Wx_{(i,j+1)}$$

$$G_{(i)} = \left[g_{(i,j)} \right] \quad g_{(i,j)} = \begin{cases} Wc_{(i,j+1)} & i = j \\ -Wy_{(i,j+1)} & i - j = 1 \\ -Wy_{(i,j)} & j - i = 1 \\ 0 & otherwise \end{cases}$$

Using dynamic programming, equation (11) may be cast in the following form:

$$H_{(i)} = A_{(i-1)} H_{(i-1)} + B_{(i-1)} \qquad (12$$

Solving (11) for $H_{(i)}$ and using $H_{(i+1)} = A_{(i)} H_{(i)} + B_{(i)}$ gives the following equation:

$$H_{(i)} = F_{(i-1)} \left(G_{(i)} - F_{(i)} A_{(i)} \right)^{-1} H_{(i-1)}$$

$$+ \left(G_{(i)} - F_{(i)} A_{(i)} \right)^{-1} \left(F_{(i)} B_{(i)} + W_i - R_{(i)}^* \right)$$

$$(13$$

Comparing (12) and (13) yield the following recurrence relations:

$$A_{(i-1)} = F_{(i-1)} \left(G_{(i)} - F_{(i)} A_{(i)} \right)^{-1} \qquad (14$$

$$B_{(i-1)} = A_{(i-1)} F_{i-1}^{-1} \left(F_{(i)} B_{(i)} + W_i - R_{(i)}^* \right) \qquad (15$$

The initial conditions for (14) and (15) are derived from (12) setting i = NL

$$A_{(NL-1)} = 0 \qquad\qquad B_{(NL-1)} = H_{(NL-1)}$$

Then, the backward solution of (14) and (15) will give the matrices $A_{(i)}$ and the vectors $B_{(i)}$. Equation (12) may now be solved for $H_{(i)}$ by utilizing $A_{(i)}$ and $B_{(i)}$.

Equation (9) can be solved in the same way. In each time step, after calculating the dispersion coefficient tensor, matrices $Ac_{(i)}$ and vectors $Bc_{(i)}$ and $C_{(i)}$ will be computed in a similar procedure to $A_{(i)}$,(14), $B_{(i)}$,(15), and $H_{(i)}$,(12), respectively.

RESULTS AND DISCUSSION

In order to verify that the numerical model is solving the governing equations correctly, it is necessary to compare the results to known solutions or results from other models. The solution developed by Basha and El Habel (2) was used to verify the model against the analytical solution. A one-dimensional solute transport in saturated media in x direction was solved analytically. Table 1 shows the parameters that were used in this solution. Figure 1 shows the comparison between the analytical solution and DP model. The mean absolute error was 0.8 percent and the root mean square error between two methods was 0.03 percent which shows good agreement between results.

Table 1. Parameters used in the analytical solution.

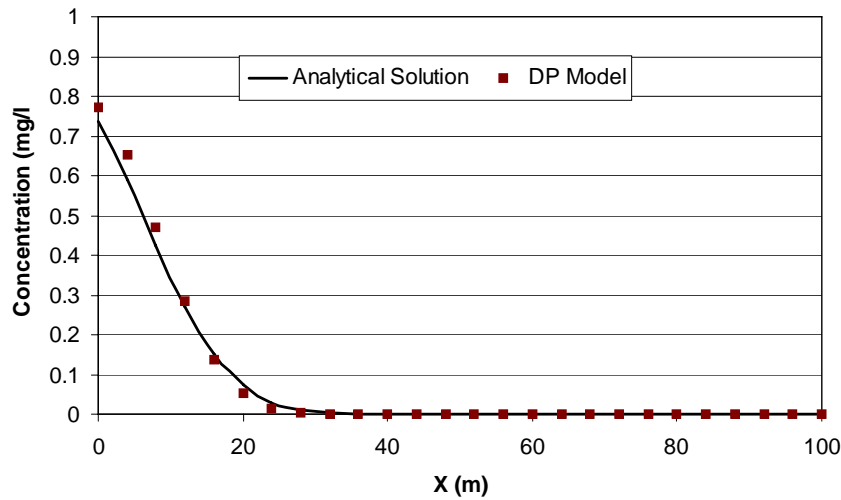| Parameter	Value
Δx	25 m
Length (L)	100 m
Initial Concentration (C_0)	0 mg/lit
Velocity (V_x)	0.25 m/s
Dispersivity (α_L)	10 m
Injected Mass (C')	1 mg/lit

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Figure 1. Comparison between the analytical solution and the DP model.

In addition, the model was compared to the results obtained from the MOC model (14). A mass balance test was used as a measure of the numerical accuracy of the solutions in DP and MOC comparisons. Here, the model uses, as the mass residual, M_r, a criterion compared with the difference between the initial mass, M_i, and the net mass flux, N_f.

$$Error = \frac{100M_r}{M_i - N_f} \qquad (16$$

where $M_r = \Delta M_s - N_f$ and ΔM_s is the change in mass stored in the aquifer [M].

One recharge well and one extraction well were considered in a 2192×2466 m domain. The left and right sides of the domain were impermeable and the northern and southern sides of the domain had constant head boundaries with a 22.5 m and 30 m water elevation, respectively. Figure 2 shows the result for test problem number 1 and the following parameters were used in the compu-
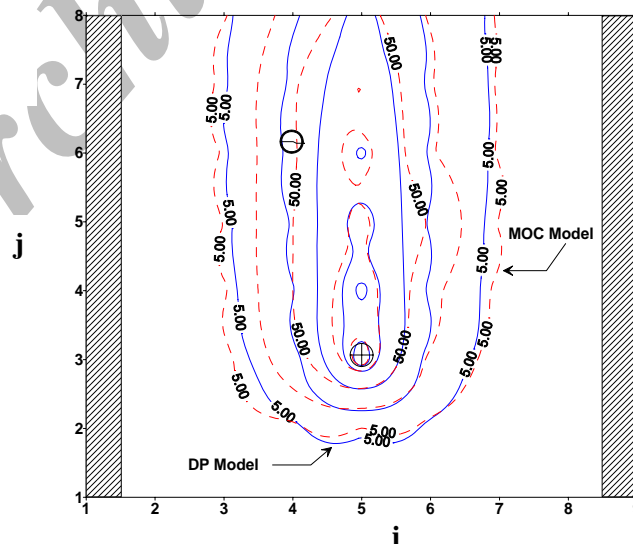

Figure 2. Comparison of the computed concentration between the DP and MOC models after 30 months for test problem number 1.
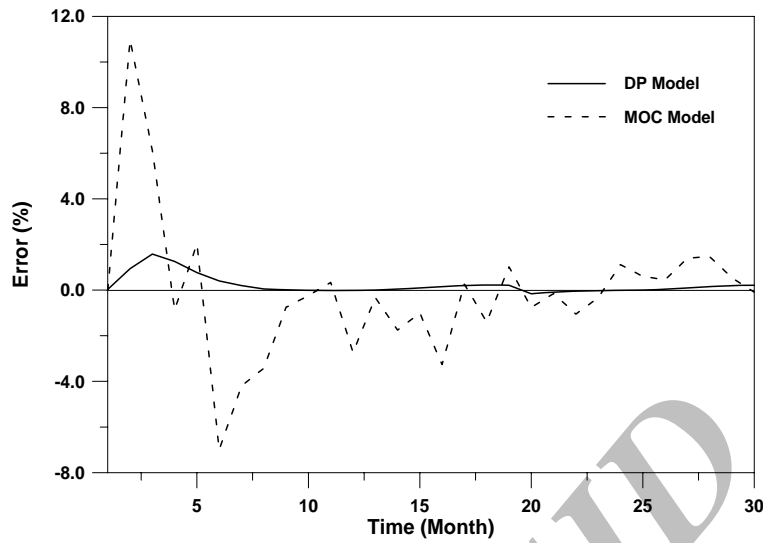
Figure 3. Mass balance error for test problem 1.

tations:

$K = 1.5 \times 10^{-3}$ m/s	$\Delta x = \Delta y = 274$ m
$b = 6.1$ m	$S = 0.3$
$\alpha_L = 30.5$ m	$C' = 220$ mg/lit
$\alpha_T / \alpha_L = 0.3$	$C_0 = 0.0$ mg/lit
$q(3, 5) = 0.028$ m^3/s	
$q(6, 4) = -0.028$ m^3/s	

Figure 3 presents the mass balance error for

the dynamic programming method and method of characteristic.

In test problem 2, the effect of dispersion was eliminated ($\alpha_L = 0.0$) and other parameters remained the same as in test problem number 1. Again, Figure 4 shows the results of the solute concentration after 2 1/2 years and Figure 5 shows the mass balance errors for this period.
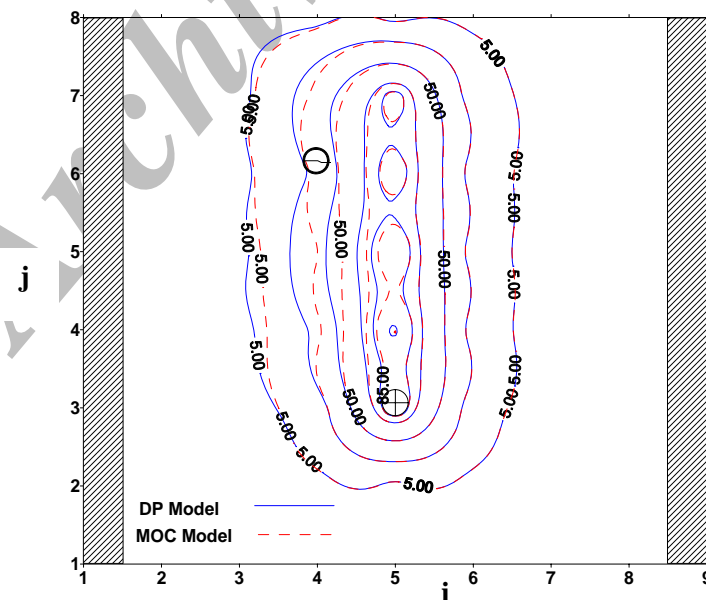

Figure 4. Comparison between the computed concentrations in test problem 2.
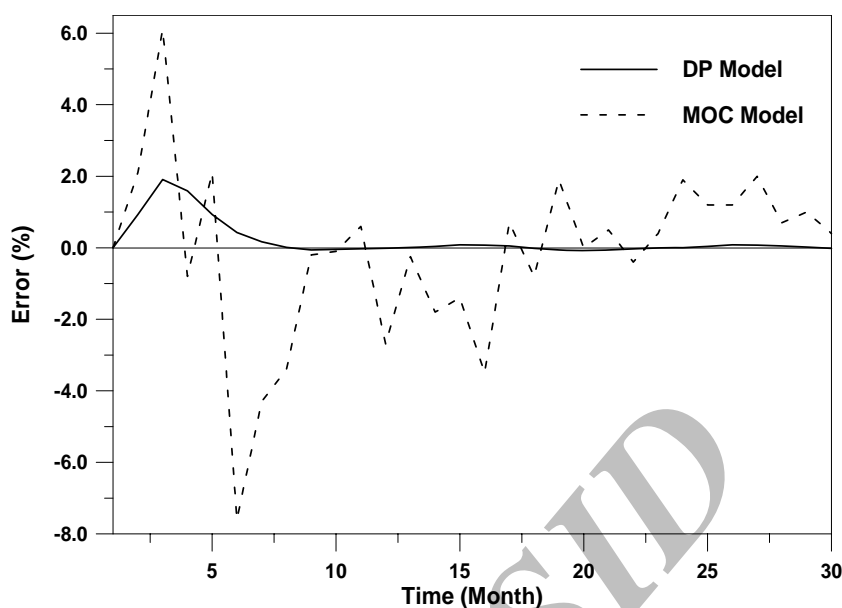
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Figure 5. Mass balance error in test problem 2.

CONCLUSION

A general two-dimensional model has been developed to simulate solute transport through heterogeneous porous media. The agreement between the results from the present model and the analytical solution and the MOC model are good and the mass balance error for the DP model is less than for the MOC model.

Using a dynamic programming method can reduce the time of computation and computer error due to inversion of the large matrices. The application of this method converts the problem from solving an algebraic system of order NC (NL-1)×NC(NL-1) into that of solving a difference equation of order NC×NC over NL-1 steps and involving NL-1 matrix inversions of order NC×NC. In addition, it reduces the storage requirements, since instead of having to store $(NL×NC)^2$, we need to store only (NC×NC) numbers at each step.

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حل برنامه ریزی پویای معادله انتقال و پخشیدگی املاح در آب زیرزمینی

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چکیده

معادلات دیفرانسیل با مشتقات جزئی برای جریان و انتقال املاح در محیط دو بعدی و اشباع آب زیرزمینی با روش تفاضل های محدود بصورت گسسته در آمده و دستگاه معادلات جبری بدست آمده به روش برنامه ریزی پویا و حل گردیدند. مزیت آلگوریتم برنامه ریزی پویا در این است که از حل یک دستگاه معادلات از مرتبه(1-NC(NL-1)×NC(NL را به حل یک دستگاه معادلات از مرتبه NC×NC در NL-1 گام تبدیل کرده که شامل NL-1 معکوس کردن ماتریس مرتبه NC×NC است. دقت روشهای حل با مقایسه نتایج با حل تحلیلی و محاسبه بیلان جرمی نشان داده شده است. مدل برنامه‌ریزی پویا همچنین با مدل MOC که توسط موسسه زمین شناسی آمریکا تهیه شده مقایسه گردید. در همه موارد مدل DP نشان داد که می تواند نتایجی با دقت خوب ارائه دهد.

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