Pollutant dispersion analysis in porous media
using dual reciprocity boundary element method

T.I. Eldho

Institute of Hydromechanics, University of Karlsruhe, D-76128, Karlsruhe, Germany

Abstract

Here dual reciprocity boundary element method is used for the analysis of pollutant dispersion in porous media. In the governing dispersion equation, the time dependent term and convective terms are approximated using dual reciprocity method and Green’s theorem is used to form boundary integral equations. Linear elements are used for boundary discretization. The model is verified with one dimensional analytical solution and found to be satisfactory. The model is applied for the solution of some two dimensional pollutant dispersion problems in homogeneous isotropic porous media.

Introduction

In any development and management of groundwater resource system, a major problem of interest is that of the quality of the water being extracted. For the assessment of groundwater quality, it is necessary to identify the source of pollution and predict the movement of the pollutants in the groundwater environment using effective tools. As very few analytical solutions are available, prediction of the movement of pollutants is done using numerical methods like finite difference (FDM), finite elements (FEM) and boundary elements (BEM) [1]. FDM and FEM are domain oriented methods and hence tedious in discretization and data preparation. BEM is more suitable since it is boundary oriented and hence very easier in discretization and data preparation for very large groundwater basins.

Here a BEM model based on dual reciprocity principle [2] is used in the prediction of pollutant dispersion in porous media. As the BEM reduces the computational dimension of the problem by one, two dimensional problems are solved in one dimension. The dual reciprocity BEM model is validated
with analytical solution and applied in the prediction of some two dimensional pollutant dispersion problems in porous media.

**Formulation of the problem**

**Governing equation and boundary conditions**

The basic differential equation in two dimensions, describing the process of solute transport in saturated porous media, considering the effects of convection and hydrodynamic dispersion and neglecting sources, decay etc., can be expressed as [1]:

\[
D_x \frac{\partial^2 C}{\partial x^2} + D_y \frac{\partial^2 C}{\partial y^2} = \frac{\partial C}{\partial t} + \frac{1}{n_e} \left( U_x \frac{\partial C}{\partial x} + U_y \frac{\partial C}{\partial y} \right)
\]  

(1)

where \( C \) is solute concentration, \( D \) is dispersion coefficient, \( U \) is Darcy’s velocity of flow in the porous media, \( n_e \) is the effective porosity of the media, and \( t \) is the time. A dimensionless form of eqn.(1) can be achieved by substituting,

\[
C = \frac{C_0 n_e}{C_0} ; X = \frac{x}{L'} ; Y = \frac{\beta y}{L'} ; u_x = \frac{U_x L'}{D_x} ; u_y = \frac{\beta U_y L'}{D_x} ; t' = \frac{D_x t}{L'^2}
\]

(2)

in which \( C_0 \) and \( L' \) are some reference concentration and length and \( \beta = (D_x/D_y)^{1/2} \).

For pollutant dispersion modelling, the appropriate initial and boundary conditions should be prescribed. The initial condition, usually concentration distribution at some initial time say \( t=0 \), is described throughout the considered domain \( \Omega \). Two boundary conditions are commonly used in the solution of solute transport problems. One is boundary of prescribed concentration and another one is boundary of prescribed flux (gradient of concentration) as given below:

\[
C(x,y,t) = g_1(x,y,t) \text{ on } \Gamma_1 ; C_n = \frac{\partial C}{\partial n} = g_2(x,y,t) \text{ on } \Gamma_2
\]

(3)

where \( n \) is the unit outward normal to the boundary.

**Boundary element formulation**

For a two dimensional dispersion problem, assuming \( D_x=D_y=D_T \), \( V_x = U_x/n_e \) and \( V_y=U_y/n_e \), then eqn.(1) can be written as:
In the dual reciprocity method, the time dependent term and convective terms are approximated [3] and eqn.(4) is represented as:

\[ \nabla^2 C = \frac{1}{D_T} \left( \frac{\partial C}{\partial x} + V_x \frac{\partial C}{\partial y} + \frac{\partial C}{\partial t} \right) = \frac{b}{D_T} \]  

where \( C_j \) is a series of particular solutions, \( N \) - number of boundary nodes, \( L \) - number of internal nodes, \( D_T \) - dispersion coefficient, \( \alpha_j \) - a set of initially unknown coefficients and \( f_j \) - approximating functions. Number of \( C_j \) is equal to total number of nodes \( N+L \). Here the right hand side of eqn.(4) has been replaced by a summation of products of coefficients \( \alpha_j \) and the Laplacian operating on the particular solution \( C_j \).

Now using reciprocity principle on both sides of eqn.(5), the boundary integral equations for each source node i can be written as [4],

\[ g_i \, C_i + \int_{\Gamma} \frac{\partial C^*}{\partial n} \, C \, d\Gamma - \int_{\Gamma} \, C^* \, \frac{\partial C}{\partial n} \, d\Gamma = \frac{1}{D_T} \sum_{j=1}^{N+L} \alpha_j \left( g_i \, \dot{C}_i + \int_{\Gamma} \frac{\partial C^*}{\partial n} \, \dot{C}_j \, d\Gamma - \int_{\Gamma} \, C^* \, \frac{\partial \dot{C}_j}{\partial n} \, d\Gamma \right) \]  

where \( C^* \) is the fundamental solution of Laplace equation (\( C^*=\frac{1}{2\pi \ln(1/r)} \)), where \( r \) is distance from the point i of application of the source or sink to any other point under consideration), \( n \) is the unit outward normal and \( g_i \) is Green's constant. \( g_i=1 \) for a point inside the domain \( \Omega \), \( g_i=0 \) for a point outside the domain and \( g_i=\theta/2\pi \) for a point on the boundary, in which \( \theta \) is the internal angle at point i in radians.

Matrix formulation and assembly of equations
From eqns.(4) and (5), by taking the value of \( b \) at \((N+L)\) different points, a set of equations in the following matrix form can be written:

\[ b = F \, \alpha \quad \alpha = F^{-1} \, b = F^{-1} \left( V_x \frac{\partial C}{\partial x} + V_y \frac{\partial C}{\partial y} + \frac{\partial C}{\partial t} \right) \]  

In eqn.(6), \( \dot{C} \) and \( \frac{\partial \dot{C}}{\partial n} \) are not necessarily be approximated over the boundary using interpolation functions as they are known once the ‘\( F \)’ function is chosen. But doing so will reduce the necessary boundary integration (eventhough the accuracy is slightly affected) and the same matrices may be used on both sides. Hence discretizing the boundary into \( N \) linear elements
and using L internal nodes, introducing the interpolation functions and integrating over each boundary elements, eqn.(6) can be written as:

\[ g_i C_i + \sum_{k=1}^{N} H_{ik} C_k - \sum_{k=1}^{2N} G_{ik} \frac{\partial C}{\partial n_k} = \]

\[ \frac{1}{D_T} \sum_{j=1}^{N+L} \alpha_j \left( g_i \hat{C}_{ij} + \sum_{k=1}^{N} H_{ik} \hat{C}_{kj} - \sum_{k=1}^{2N} G_{ik} \frac{\partial \hat{C}}{\partial n_{kj}} \right) \]  

(8)

Index k is used for the boundary nodes which are the field points. After application to all boundary nodes using a collocation technique and using eqn.(7), eqn.(8) can be represented as:

\[ HC - G \left( \frac{\partial C}{\partial n} \right) = \frac{1}{D_T} \left( H \hat{C} - G \left( \frac{\partial \hat{C}}{\partial n} \right) \right) F^{-1} \left( V_x \frac{\partial C}{\partial x} + V_y \frac{\partial C}{\partial y} + \frac{\partial C}{\partial t} \right) \]  

(9)

Here the approximating function ‘f’ can be a function of ‘r’ (r is the distance from the point i of application of the source or sink to any other point under consideration) and generally used ‘f’ function is ‘1+r’. Correspondingly [3]:

\[ \hat{C} = \frac{r^2}{4} + \frac{r^3}{9} ; \frac{\partial \hat{C}}{\partial n} = \left( r_x \frac{\partial x}{\partial n} + r_y \frac{\partial y}{\partial n} \right) \left( \frac{1}{2} + \frac{r}{3} \right) \]  

(10)

A mechanism must now be established to relate the nodal values of C to the nodal values of its derivatives \( \frac{\partial C}{\partial x} \) and \( \frac{\partial C}{\partial y} \). Similar to eqn.(7), putting \( C = F \beta \) (where \( \beta + \alpha \)) and differentiating,

\[ \frac{\partial C}{\partial x} = \frac{\partial F}{\partial x} \beta \ ; \frac{\partial C}{\partial y} = \frac{\partial F}{\partial y} \beta \]  

(11)

Rewriting \( \beta = F^{-1}C \), then

\[ \frac{\partial C}{\partial x} = \frac{\partial F}{\partial x} F^{-1} C \ ; \frac{\partial C}{\partial y} = \frac{\partial F}{\partial y} F^{-1} C \]  

(12)

Corresponding to the function ‘f=1+r’ [3]:

\[ \frac{\partial f}{\partial x} = \frac{\partial f}{\partial r} \frac{\partial r}{\partial x} = \frac{\partial f}{\partial r} r_x = r_x ; \frac{\partial f}{\partial y} = \frac{\partial f}{\partial r} \frac{\partial r}{\partial y} = \frac{\partial f}{\partial r} r_y = r_y \]  

(13)

Eqn.(9) can be now expressed as:
Therefore, eqn.(14) can be written as,

\[ P \frac{\partial C}{\partial t} + (H - R) C = G \left( \frac{\partial C}{\partial n} \right) \]  

where

\[ S = \left( H\dot{C} - G\frac{\partial C}{\partial n} \right) F^{-1} ; \quad P = -\frac{1}{D_T} S ; \quad R = S \frac{1}{D_T} \left( V_x \frac{\partial F}{\partial x} + V_y \frac{\partial F}{\partial y} \right) F^{-1} \]

For the sake of simplicity, a two level time integration scheme will be employed here. Within each time step, proposing a linear approximation for the variation of \( C \) and \( \partial C/\partial n \),

\[ C = (1 - \theta_u) C^m + \theta_u C^{m+1} \]

\[ \frac{\partial C}{\partial n} = (1 - \theta_q) \frac{\partial C^m}{\partial n} + \theta_q \frac{\partial C^{m+1}}{\partial n} \]

\[ \frac{\partial C}{\partial t} = \frac{1}{\Delta t} \left( C^{m+1} - C^m \right) \]  

where \( \theta_u \) and \( \theta_q \) are parameters which positions the values of \( C \) and \( \partial C/\partial n \), respectively between time levels \( m \) and \( m+1 \).

Substituting these approximations into eqn.(15) gives:

\[ \begin{bmatrix} \frac{1}{\Delta t} P + \theta_u (H - R) \end{bmatrix} C^{m+1} - \theta_q G \left( \frac{\partial C}{\partial n} \right)^{m+1} = \begin{bmatrix} \frac{1}{\Delta t} P - (1 - \theta_u) (H - R) \end{bmatrix} C^m + (1 - \theta_q) G \left( \frac{\partial C}{\partial n} \right)^m \]  

The right hand side of eqn.(17) is known at time \( (m+1)\Delta t \), since it involves values which have been specified as initial conditions or calculated at previous time step. Introducing the boundary conditions at time \( (m+1)\Delta t \), one can rearrange the left side of eqn.(17) and write as:
where $X$ is unknown matrix of $C$ and $\partial C/\partial n$, $F$ is a known matrix and $A$ is the coefficient matrix. Solution of eqn(18) give the unknown values of $C$ or $\partial C/\partial n$.

### Validation of the model

The DRBEM dispersion model is compared with some analytical solutions given by Marino [5] out of which one is presented here. The configuration of the porous media considered is shown in Fig.1. It is 600 m X 100 m size and is homogeneous, isotropic and fully saturated. The dispersion coefficient of the media ($D_T$) is assumed to be 7.616 m$^2$/day and seepage velocity is 1.219 m/day. The initial and boundary conditions are,

$$\begin{align*}
C(x,y,0) &= 0.0 \\
C(0,y,t) &= C_0 = 1.0 \ ; \ C(600,y,t) = 0.0 \\
\frac{\partial C}{\partial n} (x,0,t) &= \frac{\partial C}{\partial n} (x,100,t) = 0.0
\end{align*}$$

(19)

![Figure 1. Solution region for validation model](image)

The analytical solution to this problem, considering as a one dimensional problem given by Marino [5] is:

$$\frac{C}{C_0} (x,t) = \frac{1}{2} \left[ \text{erfc} \left( \frac{x-V_t t}{2\sqrt{D_T t}} \right) + \exp \left( \frac{V_x}{D_T} \right) \text{erfc} \left( \frac{x+V_t t}{2\sqrt{D_T t}} \right) \right]$$

(20)

In the dual reciprocity boundary element dispersion model, the boundary of the domain is discretized into 52 linear elements and 11 internal nodes are considered as in Fig.1. Time step $\Delta t = 1$ day; $\theta_u = 0.5$, $\theta_q = 1.0$ and $f = 1 + r$. The dispersion analysis is carried out for 300 time steps and concentration distribution is found out.

The concentration distributions along the domain at various times are plotted in Fig.2, using analytical solution and dual reciprocity BEM solution.
Good agreement is observed between both solutions.

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{figure2.png}
\caption{Concentration distribution: Model validation}
\end{figure}

**Case studies**

Here two case studies are presented to show the effectiveness of dual reciprocity BEM in the solution of pollutant dispersion problems.

**Case study 1**
Here the two dimensional dispersion in a homogeneous isotropic porous media of size 600 X 300 m, with a symmetric and uniform point source located at (0,150) with a relative concentration \((C/C_0)\) of one is considered. Due to symmetry in the input concentration, only one half of the full domain is considered as in Fig. 3. The flow is considered along the longitudinal direction.

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{figure3.png}
\caption{Solution region for Case study 1}
\end{figure}
with a seepage velocity of $1.219 \text{ m/day}$. The longitudinal dispersion coefficient ($D_T$) is $7.616 \text{ m}^2/\text{day}$ and lateral dispersion coefficient ($D_T$) is $0.7616 \text{ m}^2/\text{day}$. In the DRBEM model, $\theta_u=0.5$, $\theta_d=1.0$, $f=1+r$, time step $\Delta t=2 \text{ day}$ and analysis is done for 360 days. As in Fig. 3, 60 linear elements and 33 internal nodes are used for discretization. The contours of relative concentration distribution for the time instance of 360 days are shown in Fig. 4. The concentration movement with time at three nodes 7 (150,150), 13 (300,150) and 19 (450,150) are shown in Fig. 5.

**Figure 4. Contours of concentration distribution - 360 days**

**Figure 5. Concentration distribution with time: Case study 1**

**Case study 2**
Here the two dimensional dispersion in a homogeneous isotropic porous media of size $600 \times 300 \text{ m}$ with unsymmetric input concentration is considered. The input concentration varies along the $y$- axis by the following equation:
\[ C(0,y,t) = C_0 \exp \left[ \frac{-(y-125)^2}{3140} \right] \]  

where \( C_0 \) is the relative value of concentration and assumed to be unity. The dispersion is considered in unidirectional velocity field with a velocity of 1.22 m/day. The dispersion coefficient in x- direction (\( D_x \)) is 7.622 m²/day and in y- direction (\( D_y \)) is 0.4795 m²/day. As in Fig. 6, the boundary of the domain is discretized into 54 linear elements and 62 internal nodes are considered. In the DRBEM model, \( \theta_u = 0.5, \theta_q = 1.0, f = 1 + r \), time step \( \Delta t = 1 \) day and the analysis is carried out for 200 days. The contours of concentration distribution for 200 days are plotted in Fig. 7. The concentration movement with time at three nodes, 79 (100,125), 92 (200,150) and 83 (300,125) are shown in Fig. 8.
Conclusions

Here dual reciprocity BEM is used in the prediction of pollutant dispersion in porous media. The convective terms and time dependent term in the governing equation is approximated using dual reciprocity method so that a boundary only solution is achieved. Application of the model to various case studies demonstrates the effectiveness of the model in dispersion analysis in porous media. The model utilizes all basic advantages of BEM like reduction in computational dimension, easiness in data handling and less numerical dispersion compared to other numerical methods.

Index:

Pollutant Dispersion, Dual Reciprocity Method, Boundary Elements

References