Groundwater remediation optimization using a point collocation method and particle swarm optimization

M. Mategaonkar, T.I. Eldho*

Department of Civil Engineering, Indian Institute of Technology Bombay, Mumbai 400076, India

Abstract

Groundwater contamination is a major problem in many parts of the world. Remediation of contaminated groundwater is a tedious, time consuming and expensive process. Pump and treat (PAT) is one of the commonly used techniques for groundwater remediation. Simulation-optimization (S/O) models are very useful in appropriate design of an effective PAT remediation system. Simulation models can be employed to predict the spatial and temporal variation of contaminant plumes. Optimization models, on the other hand, can be used to minimize the cost of pumping or recharge. Generally, grid or mesh based models using Finite Difference Methods (FDM) or Finite Element Methods (FEM) are used for groundwater flow and transport simulation. Recently, Meshfree (MFree) based numerical models have been developed due to the difficulty of meshing and remeshing in these methods. The MFree Point Collocation Method (PCM) is a simple MFree method to simulate coupled groundwater flow and contaminant transport. It saves time for pre-processing such as meshing or remeshing. Evolutionary algorithm based techniques such as for particle swarm optimization (PSO) and genetic algorithms (GA) have been found to be very effective for groundwater optimization problems. In this paper, a simulation model using MFree PCM for unconfined groundwater flow and transport and a PSO based optimization model are developed. These models are coupled to get an effective S/O model for the groundwater remediation design using PAT. The S/O model is applied to the remediation design of an unconfined field aquifer polluted by Total Dissolved Solids (TDS) by using pump and treat and flushing. The model provides an effective remediation design of pumping rate for the selected wells and costs of remediation.

1. Introduction

Groundwater remediation is often used to limit the migration of plume off-sites, to isolate and contain a source area from further leaking, or to treat an affected groundwater aquifer to bring it up to the drinking water standards. Several physical, chemical and biological remediation techniques are available for treatment of contaminated groundwater, with each method having its own merits and demerits. Remediation methods like pump and treat or pump and use have proven to be effective in several situations. Optimization models, on the other hand, are used to obtain remediation design for a particular remediation strategy, which best meets the design criteria (Eugene et al., 2005). Large scale groundwater remediation projects cannot be designed as a single step operation, due to many uncertainties associated with a system.

Design of such a system requires ways to minimize cost, maximize level of contaminant mass removal from the aquifer, while meeting various constraints like water quality requirement of the maximum concentration level.

Researchers have developed models for simulation of coupled groundwater flow and transport by using grid based methods such as finite difference methods (FDM) or finite element methods (FEM). However, the pre-processing part for these methods, like meshing or remeshing, is tedious and time consuming. The MFree method uses a set of nodes scattered within the problem domain and on the boundaries, regardless of connectivity information between them. Since there is no grid, it can lead to substantial cost and time savings (Liu and Gu, 2005). Apart from other engineering applications, several researchers and engineers have investigated groundwater problems with MFree methods (Lin and Atluri, 2000; Li et al., 2003; Liu, 2006; Zi and Xian-zhong, 2011; Ravazzani et al., 2011) and found that MFree methods perform well for complex groundwater problems.

Evolutionary algorithm based techniques such as genetic algorithms (GA) and particle swarm optimization (PSO) have been
found to be very effective for the groundwater optimization problems, even though a number of conventional methods such as linear programming, nonlinear programming etc are available. However PSO has no evolution operator such as crossover and mutation like GA. Further in PSO, the potential solutions called particles fly through the problem space by following the current optimum particles (Kennedy and Eberhart, 1995). Based on various studies, Parsopoulos and Vrahatis (2002) concluded that PSO is a very useful and simple technique for solving complex problems. Simulation models along with optimization model gives the complete solution for a complex field problem for an effective remediation design of groundwater pollution. Typical important works in the area of groundwater pollution remediation based on S/O models are now briefly reviewed here.

Gill et al. (1984) developed an S/O model based on FEM simulation combined with nonlinear optimization, which is capable of determining well locations and pumping/injection rates for quality control of groundwater. Allfeld et al. (1988) proposed two nonlinear optimization formulations along with FEM, which modeled the design process for location and pumping rates of injection/extraction wells in the aquifer cleanup system. Chang et al. (1992) presented a management model combining one pollutant transport FEM model with a constrained optimal control algorithm and concluded that the optimal constant pumping rates are 75% more expensive than the optimal time-varying pumping rates. Huang and Mayer (1997) combined a three-dimensional groundwater flow and solute transport model within a GA framework to solve a discrete-time, optimal control problem of pump-and-treat remediation management with multiple management periods. They showed that a nonlinear concentration term in the performance index contributes significantly to the remediation costs, and multiple management period strategies reduce the remediation cost but increase the computational cost. Wang and Zheng (1997) developed and demonstrated the application of an S/O model using GA, MODFLOW (McDonald and Harbaugh, 1988) and the MT3D 3D transport model (Zheng and Wang, 1998), for the optimal design of groundwater remediation systems under a variety of field conditions. Prasad and Rastogi (2001) developed an S/O model based on GA coupled with the Galerkin’s finite element flow simulation model and concluded that the developed algorithm is useful for successful estimation of aquifer parameters for large aquifer systems. Matott et al. (2006) used a multi-algorithmic optimization software package coupled with an Analytical Element Method (AEM) based flow model and explored usage of various pump and treat objectives and constraint formulations. They concluded that the AEM models coupled with PSO can be used to optimize the number, locations and pumping rates of wells. They also found that PSO is suitable for applications to problems that are computationally demanding and involve a large number of wells.

Mondal et al. (2010) developed a coupled FEM—NSGA II model for pump and treat remediation. They used the model for the optimal remediation of a field aquifer by combined use of flushing and pumping and demonstrated the effectiveness of the model for achieving the optimal pumping policy. Tian et al. (2011) used quantum-behaved particle swarm optimization (QPSO) to solve an inverse advection-dispersion problem of estimating strength of time-varying groundwater contaminant source from the knowledge of forensic observations, and concluded that the proposed method can be used efficiently to reconstruct the contaminant source history. Gaur et al. (2011) developed an AEM—PSO model and applied it to the Dore river basin in France, considering discharge and location of pumping wells as the decision variables, and concluded that the model is efficient in identifying the optimal locations and discharge of pumping wells.

An S/O model is developed in the present study by using the MFree point collocation method (PCM) for coupled flow and mass transport simulation. The PCM model is coupled with the optimization technique of particle swarm optimization (PSO) to get an efficient S/O model for groundwater pollution remediation using the pump and treat. The PCM—PSO model is applied to the optimal groundwater remediation design using the pump and treat of an unconfined field aquifer in Gujarat, India polluted by total dissolved solids (TDS). Results of the PCM—PSO model are found to be satisfactory.

2. Governing equations and boundary conditions

The governing equation describing flow in a two dimensional (2D) unconfined aquifer is given as (Bear, 1979):

\[ \nabla \cdot (K \nabla h) = -S \frac{\partial h}{\partial t} + P \]  

(1)

The following initial conditions are used:

\[ h(x, y, 0) = h_0(x, y) \quad x, y \in \Omega \]  

(2a)

On the other hand, boundary conditions

\[ h(x, y, t) = h_1(x, y, t) \quad x, y \in \partial \Omega_1 \]  

(2b)

\[ \nabla h \cdot \nu = q_1(x, y, t) \quad x, y \in \partial \Omega_2 \]  

(2c)

are used for the unconfined aquifer problems, where \( \vec{K} \), \( h(x, y, t) \), \( S \) represent the hydraulic conductivity [LT^{-1}] tensor, piezometric head (m) and specific yield, respectively, \( P = Q_w \delta(x-x_i)/(y-y_i) \) is the source or sink term [L^2T^{-1}L^{-1}] ; \( \nabla \) is the differential operator; \( x, y \) are the horizontal space variables (m); \( Q_w \) is the source or sink function (\( Q_w = \text{Source} \) , \( Q_w = \text{Sink} \) ) [L^2T^{-1}] ; \( t \) is the time in days [T] ; \( \delta \) is the Dirac delta function with the property that when \( x = x_i \) and \( y = y_i \), \( \delta = 1 \) otherwise = 0 else-where; \( \Omega \) is the flow region; \( \partial \Omega \) is the boundary region (\( \partial \Omega_1 \cup \partial \Omega_2 = \partial \Omega \) ); \( \nu \) is the normal derivative; \( h_0(x, y) \) is initial head in the flow domain [L]; \( h_1(x, y, t) \) is the known head value of the boundary head [L] and \( q_1(x, y, t) \) are the known inflow rates [L^2T^{-1}L^{-1}] through boundaries.

The governing equation for transport of a single chemical constituent in groundwater in 2D is given by

\[ \nabla \cdot (D \nabla c) - \nabla \cdot (v c) - R_f c = \frac{\partial c}{\partial t} \]  

(3)

by considering the advection, dispersion and fluid sources/sinks (Freeze and Cherry, 1979; Wang and Anderson, 1982).

An initial condition of \( c(x, y, 0) = f_1(x, y) \) for \( x, y \in \Omega \), for the transport problem is used.

Generally used boundary conditions are \( c(x, y, t) = g_1 \) for \( x, y \in \partial \Omega_1 \); \( \partial / \partial x D_{xx} \partial c / \partial x n_x + \partial / \partial y D_{yy} \partial c / \partial y n_y = g_2 \) for \( x, y \in \partial \Omega_2 \). Here, \( f_1 \) is known concentration value, \( n_x \) and \( n_y \) are the components of the unit outward normal vector to the given boundary \( \partial \Omega_1 \) and \( \partial \Omega_2 \), and \( g_1 \) and \( g_2 \) are known concentration and gradient boundary; \( \mathcal{B} \) is the dispersivity tensor; \( D_{xx}, D_{yy} \) are the components of dispersion coefficient tensor [L^2T^{-1}] in the x and y directions respectively; \( c \) is the dissolved concentration [ML^{-3}] ; \( v \) is the velocity tensor, \( v_x \) and \( v_y \) are components of velocity tensor [LT^{-1}] in the x and y directions respectively; \( R_f \) is the reaction rate constant [LT^{-1}] ; \( W \) is the rate of recharge of contaminated groundwater per unit volume; \( S \) is the concentration of the solute from the source; \( n_x \) is the local porosity; \( t \) is time; \( b \) is the aquifer thickness; \( R_f \) is the retardation factor (in the present study \( R_f \) is taken as 1).
3. Numerical formulation

PCM with a standard multi-quadric radial basis function (MQ-RBF) (Kansa, 1990) is used in this study to develop the groundwater flow and contaminant transport model (Mategaonkar and Eldho, 2011, 2012). A brief description of the PCM formulation for the flow and transport model is given in the sequel.

3.1. PCM formulation for 2D transient flow

An MFreqe formulation based on a point collocation method (PCM) with MQ-RBF is used in this paper to develop the flow model Eq. (1) can be written for transient groundwater flow in an unconfined aquifer in 2D without pumping or recharge, as (Bear, 1979),

$$\frac{\partial}{\partial x} \left( K_x \frac{\partial h}{\partial x} \right) + \frac{\partial}{\partial y} \left( K_y \frac{\partial h}{\partial y} \right) = S_y \frac{\partial h}{\partial t}$$

(4)

Here, $K_x$ and $K_y$ are the hydraulic conductivities (m/d) in $x$ and $y$ directions, respectively. By considering $K_x$ and $K_y$ to be constant for the particular zone considered, Eq. (4) can be written as

$$K_x \left( \frac{\partial^2 h}{\partial x^2} \right) + K_y \left( \frac{\partial^2 h}{\partial y^2} \right) + h \frac{\partial^2 h}{\partial x \partial y} = S_y \frac{\partial h}{\partial t}$$

(5)

after differentiation.

The first step in the PCM is to define the trial solution $h(x, y, t) = \sum_{i=1}^{n} h_i(t|R_i(x, y))$ (Liu and Gu, 2005). Here, $n$ is the number of nodes considered in the domain and $R_i(x, y)$ is the shape function. Further, the shape function is written as (Liu and Gu, 2005)

$$R_i(x, y) = \sqrt{(x-x_i)^2 + (y-y_i)^2 + C_s^2}; C_s = \frac{\alpha_c d_c}{\Delta t}$$

(6)

where $x$ and $y$ are the co-ordinates of the point of interest in the support domain; $x_i$ and $y_i$ are the co-ordinates of $i$th node in the support domain; $\alpha_c$ is the shape parameter and $d_c$ is the nodal spacing in the support domain. In PCM, the nodes are scattered in the domain and on the boundaries.

For collocation purposes, every node in the domain is surrounded by a support domain in PCM. The support domain for a point of interest can be of various shapes for a 2D domain. A circular or rectangular support domain is often used. A rectangular domain is simple to construct and easy to implement. Fig. 1 shows a schematic representation of a rectangular support domain. By using a rectangular support domain, the dimension of the support domain is determined by $d_{xx}$ and $d_{yy}$ in the $x$ and $y$ directions, respectively. Here, $d_{xx} = \alpha_c d_c x_i$; $d_{yy} = \alpha_c d_c y_i$; where, $d_{xx} = \sqrt{A_x/\pi A_c} - 1$: $A_c$ is the area of the estimated support domain; $n_A$ is the number of nodes covered by the estimated domain with the area of $A_c$; $\alpha_c x_i$ and $\alpha_c y_i$ are the dimensionless sizes of the support domain in the $x$ and $y$ directions and $d_{xx}$, $d_{yy}$ are nodal spacing in the $x$ and $y$ directions between two adjacent nodes. For simplicity, $\alpha_c x_i = \alpha_c y_i = \alpha_c$ is often used if the nodes are uniformly distributed. Discrete equations of PCM can be formulated using shape functions. These equations are often written in nodal matrix form and are assembled into the global system matrices for the entire problem domain. The discretized system of equations in PCM is similar to that of FEM in terms of bandness and sparseness, but it can be asymmetric depending on method used.

The first and second derivatives of the shape function in Eq. (6) with respect to $x$ and $y$ are calculated (Mategaonkar and Eldho, 2011). Fully implicit finite forward difference approximation is considered for the time discretization (Freeze and Cherry, 1979; Wang and Anderson, 1982).

By substituting the trial solution Eq. (6) in Eq. (5), Eq. (5) can be transformed as:

$$K_x \left( \frac{\partial R_i(x, y)}{\partial x} \right) h_i^t \left( \frac{\partial R_i(x, y)}{\partial x} \right) h_i^{t+\Delta t}$$

$$+ \left( R_i(x, y) h_i^t \right) \left( \frac{\partial^2 R_i(x, y)}{\partial x^2} \right) h_i^{t+\Delta t}$$

$$+ K_y \left( \frac{\partial R_i(x, y)}{\partial y} \right) h_i^t \left( \frac{\partial R_i(x, y)}{\partial y} \right) h_i^{t+\Delta t}$$

$$+ \left( R_i(x, y) h_i^t \right) \left( \frac{\partial^2 R_i(x, y)}{\partial y^2} \right) h_i^{t+\Delta t}$$

$$= S_y \frac{\Delta t}{\Delta t} \left( R_i(x, y) \left( h_i^{t+\Delta t} - h_i^t \right) \right)$$

(7)

where, $R_i(x, y)$, $(\partial R_i(x, y)/\partial x)$, $(\partial R_i(x, y)/\partial y)$, $(\partial^2 R_i(x, y)/\partial x^2)$ and $(\partial^2 R_i(x, y)/\partial y^2)$ values are to be calculated for each support domain (Mategaonkar and Eldho, 2011) and then they are incorporated in the global matrix for the whole problem domain. Further, Eq. (7) can be written in matrix form by considering the source and sink terms as

$$\left[ K_1 \right] - \left[ K_2 \right] \left[ h_i^t \right] \left[ K_3 \right]$$

$$+ \left[ K_4 \right] \left[ h_i^t \right] \left[ K_5 \right]$$

$$= \left( \frac{\Delta t}{\Delta t} \right) \left[ h_i^{t+\Delta t} \right]$$

(8)

Here, $[K_1]$ = Global matrix of shape function; $[K_2]$ = $[K_3]$ = $[K_4]$ = Matrix of Dirichlet or Neumann B.C.; $[K_5]$ = Related to the system PDE from Eq. (5). Therefore,

$$\left[ K \right] = \begin{pmatrix} K_{11} & K_{12} & \cdots & K_{1n} & K_{1w} \\ K_{12} & K_{22} & \cdots & K_{2n} & K_{2w} \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ K_{1n} & K_{2n} & \cdots & K_{nn} & K_{nw} \\ K_{1w} & K_{2w} & \cdots & K_{nw} & K_{ww} \end{pmatrix}$$

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\([K_x] = \) Global matrix of the first derivative of shape functions with respect to \(x\); \([K_y] = \) Global matrix of the second derivative of shape functions with respect to \(x\); \([K_v] = \) Global matrix of the first derivative of shape functions with respect to \(y\); \([K_u] = \) Global matrix of the second derivative of shape functions with respect to \(y\). \([K_{zi}], [K_z], [K_y] \) and \([K_v]\) are also created similar to \([K_1]\) as discussed above.

For incorporating the boundary conditions, nodes lying on boundaries should be assigned properties of boundary values depending on Dirichlet or derivative boundary. Here, \([h_i^1]\) and \([h_i^2]\) are nodal heads at time \(t\) and \((t + \Delta t)\) respectively; \(Q_w = q_w/\alpha_1\); \(q_w\) is the source or sink term \((\text{m}^3/\text{day})\), \(\alpha_1\) is the area of support domain in which pumping well or recharge wells lie \((\text{m}^2)\) and \([Q_w]\) is the global matrix of the entire source and sink terms.

The domain is divided into zones of different \(K\) values for a heterogeneous aquifer and the hydraulic conductivity of that zone is considered for all nodes lying in that particular zone. Once the head distribution in the aquifer is found, velocities in the \(x\) and \(y\) directions \((v_x\) and \(v_y\) respectively), are calculated from Darcy’s law (Bear, 1979) as \(v_x = -K_x \partial h/\partial x\) and \(v_y = -K_y \partial h/\partial y\).

### 3.2. 2D transport equation – PCM formulation

The transport equation for a single constituent contamination in 2D is written as (Freeze and Cherry, 1979; Wang and Anderson, 1982):

\[
D_{xx} \frac{\partial^2 c}{\partial x^2} + D_{yy} \frac{\partial^2 c}{\partial y^2} - v_x \frac{\partial c}{\partial x} - v_y \frac{\partial c}{\partial y} - \frac{\partial c}{\partial t} = 0
\]  

(9)

The trial solution in PCM is defined as \(c_i(x, y, t) = \sum_{i=1}^{m-1} c_i(t) R_i(x, y)\). Fully implicit finite difference approximation is used for discretizing time. Therefore, Eq. (9) can be written as

\[
c_i^{(t+\Delta t)} - \Delta t \left( D_{xx} \left( \frac{\partial^2 c_i}{\partial x^2} \right)^{(t+\Delta t)} + D_{yy} \left( \frac{\partial^2 c_i}{\partial y^2} \right)^{(t+\Delta t)} \right) = c_i^{(t)} - \Delta t \left( v_x \left( \frac{\partial c_i}{\partial x} \right)^{(t)} + v_y \left( \frac{\partial c_i}{\partial y} \right)^{(t)} \right)
\]

(10)

By using the trial solution in Eq. (10),

\[
R_i(x, y) c_i^{(t+\Delta t)} - \Delta t \left( D_{xx} \left( \frac{\partial^2 R_i(x, y)}{\partial x^2} \right) + D_{yy} \left( \frac{\partial^2 R_i(x, y)}{\partial y^2} \right) \right) c_i^{(t+\Delta t)} = R_i(x, y) c_i^{(t)} - \Delta t \left( v_x \left( \frac{\partial R_i(x, y)}{\partial x} \right) c_i^{(t)} + v_y \left( \frac{\partial R_i(x, y)}{\partial y} \right) c_i^{(t)} \right)
\]

(11)

Here, \(R_i(x, y)\), \(\frac{\partial R_i(x, y)}{\partial x}\), \(\frac{\partial R_i(x, y)}{\partial y}\), \(\frac{\partial^2 R_i(x, y)}{\partial x^2}\) and \(\frac{\partial^2 R_i(x, y)}{\partial y^2}\) values are calculated for each support domain (Mategaonkar and Eldho, 2011, 2012) and they are incorporated in the global matrices for the whole problem domain. Therefore, Eq. (11) is written in the matrix form as,

\[
([K_1] - \Delta t \left( (D_{xx})_i[K_x] + (D_{yy})_i[K_y] \right) [c_i]^{(t+\Delta t)} = ([K_1] - \Delta t \left( (v_x)_i[K_2] + (v_y)_i[K_4] \right) [c_i]^{(t)} \right)
\]

(12)

When source of contamination is an ash pond, a dump site, an industrial site or a well, Eq. (12) can be written as

\[
([K_1] - \Delta t \left( (D_{xx})_i[K_x] + (D_{yy})_i[K_y] \right) [c_i]^{(t+\Delta t)} = ([K_1] - \Delta t \left( (v_x)_i[K_2] + (v_y)_i[K_4] \right) [c_i]^{(t)} + (\Delta t[K_1]) [c_p] \right)
\]

(13)

Here, \([c_p]\) is the global matrix of the contamination from ponds or recharge wells and \([K_1], [K_2], [K_3], [K_4]\) and \([K_5]\) are the global matrices as defined earlier. Velocities \(v_x\) and \(v_y\) are obtained from the flow simulation using Darcy’s law. Eq. (13) is solved by the Gauss–Jordan method to find unknown concentration values.

### 3.3. PSO algorithm

PSO is a population based stochastic optimization technique developed by Kennedy and Eberhart in 1995, inspired by social behavior of bird flocking or fish schooling. It is based on mathematical constructs, having three main parameters: position, velocity and fitness. Position represents unknown variable of problem, velocity determines the rate of change of position (or change of variable) and fitness is a measure of how well the particle solves the objective function optimally. Initially, the swarm of particles is created. Each particle’s position consists of \(p\) variables where \(p\) is the number of unknowns in the optimization problem. Particles will search this \(p\)-dimensional space to find the optimum solution. A variable is initialized to a random value within the range [0, 1].

The flowchart of the PCM–PSO model is shown in Fig. 2.

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search space. Each particle will have a randomly determined initial velocity. The number of particles in a swarm is referred to as the population. An objective function is a measure of quality of a solution. Generally, swarm attempts to minimize the objective function. The particle swarm is a self-organizing system whose global dynamics emerge from local rules. Each individual trajectory is adjusted towards success of neighbors. Population converges or clusters in the optimal region of the search space. The search will fail if individuals did not influence one another. It may be possible that a particle cannot reach any point in the problem space in a single iteration, although this might be possible at some point of a new search with given sufficiently large velocity. However, any particle can eventually go anywhere when sufficient number of iterations and an appropriate set of parameters are chosen.

Each particle keeps track of its co-ordinates in the problem space which is associated with the best solution (fitness) it has achieved so far, while the fitness value is also stored. This value is called pbest. Another “best” value that is tracked by the particle swarm optimizer is obtained so far by any particle in the neighborhood of the particle. This location is called lbest. When a particle takes all the population as its topological neighbors, the best value is a global best and is called gbest. The algorithm for PSO is as given below.

Position of individual particles is updated as (Kennedy and Eberhart, 2001; Parsopoulos et al., 2001)

\[ x_{k+1} = x_k + u_{k+1} \]  
\[ u_{k+1} = wu_k + c_1 r_1 (p_k - x_k) + c_2 r_2 (g_k - x_k) \]

Here, \( x_{k+1} \) is the updated particle position; \( x_k \) is the particle position; \( u_k \) is the particle velocity; \( p_k \) is the best “remembered” individual particle position; \( g_k \) is the best “remembered” swarm position; \( u_{k+1} \) is the updated velocity of the particle; \( c_1, c_2 \) are the cognitive and social parameters; \( r_1, r_2 \) are the random numbers between 0 and 1 and \( w \) is the inertia factor.

4. S/O model for groundwater contamination remediation

Domain is discretized with number of nodes for the PCM models. Each node has one support domain. Values of shape function, its single and double derivatives with respect to \( x \) and \( y \) are calculated for every support domain and these are incorporated in the global matrix for the entire problem domain. Final equations are solved for head and mass concentration for the entire simulation period.

Based on the above formulation, PCM based simulation models for flow and transport are developed separately and coupled together to obtain the PCM-GFTMU model (Point Collocation Method Groundwater Flow and Transport Model – Unconfined). Further, the PCM model is embedded in the PSO model which solves the objective function with all constraints for the remediation purpose. A flow chart for the PCM-PSO model is presented in Fig. 2.

4.1. PCM model verification

The developed PCM flow model has been verified with an available analytical solution and details are available in Mategaonkar and Eldho (2011). The transport model has been verified with an analytical solution in one dimension (1D) given by
Marino (1974). Contaminant transport in a homogeneous and isotropic porous medium illustrated in Fig. 3 is considered (Marino, 1974). The transport equation in 1D is given as

$$\frac{\partial c}{\partial t} = D \frac{\partial^2 c}{\partial x^2} - v \frac{\partial c}{\partial x}$$

(16)

where $v$ is the seepage velocity; $D$ is the uniform dispersion coefficient; $x$ is the distance from the source and $t$ is the time. Here, a problem of domain length 1000 m is considered with boundary conditions, $c(0, t) = c_0 e^\gamma$; where $c_0 = 1$ is the input concentration, $\gamma$ is a constant taken as $-0.01$ day$^{-1}$. Also $c(1000, y, t) = 0$. The initial condition $c(x, 0) = 0$ is used. Other parameters are: $v = 1.0$ m/d, $D = 20$ m$^2$/d and $\Delta t = 1$ day. Contaminant transport simulation is performed by using the PCM transport model. Total time of simulation is 500 days and value of $C_s$ is taken as 350. The problem domain is divided into 21 equidistant nodes with biased 7 nodes in each support domain as shown in Fig. 3. Results of simulation using PCM are compared with the analytical solution (Marino, 1974) as shown in Fig. 4. The PCM simulation is found to be in good agreement with the analytical solution.

4.2. PSO model verification

The PSO based model for a single objective function is verified with solution for the Rosenbrock banana function. The objective is to minimize (Kennedy and Eberhart, 2001)

$$f(x_1, x_2) = 100 \left( x_2 - x_1^2 \right)^2 + (1 - x_1)^2$$

(17)

in the interval $-2 \leq x_1, x_2 \leq 1$. The swarm size is taken as 30 for the PSO model and the dimension is considered as 2. True solution of the problem is $(1.0, 1.0)$ having the function value equal to zero. The objective function value variation with number of iterations for 5 different test runs is shown in the Fig. 5. The PSO value obtained is in the range of $(0.9985, 0.9985)$ to $(0.9989, 0.9989)$ in 23–40 iterations, showing good agreement with the true solution.

4.3. S/O model for remediation

In groundwater pollution remediation using pump and treat, optimization is aimed at identification of cost-effective remediation...
designs, while satisfying the constraints on TDS concentration and hydraulic head values at all nodal points. Also, pumping rates at the pumping wells should not be more than a given specified rate. Only minimization of the remediation cost is considered as the objective function in this remediation design. The cost function includes both capital and operational costs of extraction and treatment. Because the capital cost of well construction and pump installation is constant, it is not considered in the design. Cost of extraction is proportional to the energy or power required to lift the water to ground level and to the total time period of remediation, during which pumping is done. On the other hand, cost of treatment depends only on volume of water pumped. The cost function is chosen as (Mondal et al., 2010)

\[
\text{Minimize Cost } f = t \left\{ a_1 \sum_{i=1}^{N} \frac{Q_i (\Delta t) g (h_i^{\text{eq}} - h_i)}{86400 \times 10^4} + a_2 \sum_{i=1}^{N} Q_i \right\}
\]  

(18)

Table 1
Parameters for the case study.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Area (km²)</td>
<td>150</td>
</tr>
<tr>
<td>Thickness of aquifer (m)</td>
<td>60</td>
</tr>
<tr>
<td>Specific yield</td>
<td>0.2</td>
</tr>
<tr>
<td>Longitudinal dispersivity (m)</td>
<td>500</td>
</tr>
<tr>
<td>Transverse dispersivity (m)</td>
<td>100</td>
</tr>
<tr>
<td>Average natural groundwater surface recharge</td>
<td>150 (million cubic meter per year (Mcm/yr).)</td>
</tr>
<tr>
<td>Lateral inflow from the Northern boundary (Mcm/yr)</td>
<td>0.03</td>
</tr>
<tr>
<td>Irrigation return flow (Mcm/yr)</td>
<td>0.64</td>
</tr>
<tr>
<td>Seepage from Meni Nadi (Mcm/yr)</td>
<td>1.2</td>
</tr>
<tr>
<td>Recharge from the refinery Mcm/yr</td>
<td>1.6</td>
</tr>
<tr>
<td>The average extraction rate from each pumping well (m³/day)</td>
<td>274</td>
</tr>
</tbody>
</table>

Fig. 7. Initial concentration distribution, zonation pattern and average hydraulic conductivity of the study area.

Fig. 8. Nodal arrangement for the study area (\(\Delta x = \Delta y = 750\)m).

Fig. 9. Head distribution after 12 years (in m).
Table 2
Comparison of head distribution (in m) and concentration distribution (in ppm) by FEM and PCM–GFTMU (at the end of 7 years).

<table>
<thead>
<tr>
<th>Node no.</th>
<th>Head in m (FEM)</th>
<th>Head in m (PCM–GFTMU)</th>
<th>% Diff.</th>
<th>Concentration in ppm (FEM)</th>
<th>Concentration in ppm (PCM–GFTMU)</th>
<th>% Diff.</th>
</tr>
</thead>
<tbody>
<tr>
<td>109</td>
<td>16</td>
<td>15.65</td>
<td>2.2117</td>
<td>1700</td>
<td>1599.98</td>
<td>6.0619</td>
</tr>
<tr>
<td>130</td>
<td>18</td>
<td>17.98</td>
<td>0.1111</td>
<td>1500</td>
<td>1400.01</td>
<td>6.8958</td>
</tr>
<tr>
<td>187</td>
<td>25</td>
<td>24.87</td>
<td>0.5213</td>
<td>450</td>
<td>425.98</td>
<td>4.0021</td>
</tr>
<tr>
<td>205</td>
<td>28</td>
<td>27.98</td>
<td>0.0714</td>
<td>400</td>
<td>389.76</td>
<td>2.1500</td>
</tr>
</tbody>
</table>

Here, $f$ is the objective function for the minimization of system cost; $Q_i$ is the pumping rate from the well (m$^3$/day); $\eta$ is the efficiency of the pumping system; $h_i^g$ is the ground level at the well $i$ (assumed to be constant throughout the aquifer, equal to the depth of ground surface datum = 40 m); $h_i$ is the piezometric head at well $i$ (m) and $g$ is the acceleration due to gravity (m/sec$^2$). The energy required to lift $Q_i$ m$^3$/day at the ith node to the ground level in joules per day is $(Q_i \gamma (\Delta t) g) / \eta [h_i^g - h_i] / (86400 \times 10^3)$ converted to KWh. Considering the cost of electricity in India, INR 5 per KWh, the cost coefficient for energy, $a_1 =$ INR 5/m$^3$/day; $a_2$ is the cost coefficient for treatment (assumed for TDS pollution only, INR 3.0 per m$^3$ of water pumped); $\gamma$ is the unit weight of water (1000 kg/m$^3$); $\Delta t$ is the time step; $(h_i^g - h_i)$ is the groundwater lift at well $i$; $t$ is the fixed total time of remediation.

Constraints to the problem are specified as $c_{\text{max}} < c^*$; $h_{\text{min}} \geq h^*$ and $Q_{\text{min}} \leq Q_i \leq Q_{\text{max}}$ for $i = 1,...,NP$; where $i$ is the node number; $NP$ is the total number of pumping nodes in the flow domain; $c^*$ is the specified limit of concentration in the region; $Q_i$ is the pumping rate at well; $c_{\text{max}}$ is the maximum concentration anywhere in the aquifer; $c_{\text{min}}$ is the minimum head anywhere in the aquifer and $h^*$ is the specified minimum groundwater head anywhere in the aquifer.

The steps followed in the S/O model are given below.

1. Input parameters for the PCM–GFTMU model i.e. hydraulic conductivity, specific yield, dispersivities, porosity, aquifer dimensions, time steps and $C_s$.
2. Calculate head and concentration distribution by the PCM–GFTMU model.
3. Generate the initial population of particles (pumping rates).
4. Initialize PSO algorithm constants: $w$, $c_1$ and $c_2$.
5. Check constraints and evaluate the objective function.
6. If the objective is achieved (reaching minimum cost), stop. Else update the particles’ positions and velocities and evaluate the objective function.
7. By using these pumping rates, apply the PCM–GFTMU model to obtain the head and concentration distribution in aquifer.
8. Check all the constraints. If all the constraints are satisfied, stop. Else repeat steps 3–8 and then proceed to the next time step.
9. Procedure is repeated till the end of the remediation time.
10. Note the optimal pumping rates at the end of remediation time.

5. Case study

Applicability of the developed PCM–PSO model is tested for a field unconfined aquifer near Vadodara, Gujarat, India (Fig. 6). Data required for this study are obtained from the literature (NGRI Report, 2001; Sharief, 2007; Mondal et al., 2010). The polluted unconfined aquifer region has an area of 150 sq km as shown in Fig. 6. Within the study area, there is a stream, Meni Nadi, flowing from the N–E boundary to the S–W boundary which joins the Mahi River. On the Western boundary of the aquifer, the Mahi River is flowing. Wastewater from a refinery established in 1965 (containing TDS) is considered as the main pollutant source. Unconfined aquifer flow is considered in the present study in two dimensions having five zones as shown in Fig. 7 (NGRI Report, 2001; Mondal et al., 2010). The gradient of the Mahi River is taken into consideration while assigning values at different river nodes and is considered as a constant head boundary. At the Northern part, it starts from 20 m varying linearly towards the Southern part and
ends at 4 m head. The North-Eastern boundary is considered as the constant head boundary (35 m), whereas the outflow towards the South-Eastern part is considered as the head gradient (the South-Eastern part starts from 8 m varying linearly and ending up with 4 m when it joins the Mahi River). On the Northern side, the flux enters the aquifer system. The omitted parts of the aquifer boundaries are treated as no flow boundaries. As shown in Fig. 7, 1–2, 4–5 and 6–1 are the constant head boundaries, 3–4 and 5–6 are no flow boundaries and 2–3 is a flux boundary. The TDS concentration of groundwater near the refinery area and its environs is high (above 2000 ppm) and unsafe for drinking. Concentration levels in the year 2000, measured by NGRI (2001), are considered as the initial TDS distribution in the study area for the present modeling purpose (Fig. 7). Data used in the model are given in Table 1.

It is observed that TDS concentration levels in the aquifer exceed safe value of 750 ppm (as prescribed in www.hc-sc.gc.ca) at different locations. Therefore, it is required to remediate groundwater. As the pump and treat method is one of the established methods of remediation, it is proposed in this study for remediation. The optimal remediation of contaminated groundwater by the pump and treat method is designed in two steps. In the first step, the simulation model is developed and calibrated to match conditions of the groundwater system. In the second step, the PSO model is used to solve values for decision variables.

5.1. PCM simulation

In this study, 246 nodes (Fig. 8) are considered with 9 nodes in every support domain. Cs is considered as 2000 and the time step for the numerical simulation is chosen as 1 day. The PCM model mentioned earlier is used to compute head and concentration distributions in the flow region. Based on the initial and boundary conditions, the steady state head distribution is computed prior to simulation with no pumping data. Further, thirty abstraction wells (Refer Fig. 8) are considered in the system during the simulation period of 12 years. Steady state head values are considered as initial heads in the system and the model is simulated for a period of 12 years with pumping wells operative in the system with an average pumping rate of 274 m³/day. Head distribution at the end of 12 years is presented in Fig. 9.

The concentration distribution given in Fig. 7 is considered as the initial concentration in the system and the model is simulated further for 12 years. The concentration distribution after 12 years is presented in Fig. 10. In the literature, results are available (Sharief, 2007) for FEM simulation with 238 nodes and 411 elements at the end of 7 years. Hence the head distribution and concentration distribution by the PCM–GFTMU model at the end of 7 years are compared at some selected nodes (109, 130, 187, and 205 in the Fig. 8). A comparison of results is given in Table 2. A good comparison is observed between the PCM and FEM results, showing applicability of the present approach.

Direction of the flow is towards the Mahi River and consequently the movement of concentration. The TDS concentration distribution in the study area after 12 years of simulation shows that there is a plume where the concentration distribution is nearly 2000 ppm at the N–E side.

5.2. PCM–PSO model

For pump and treat remediation system, decision variables include pumping or injection rates for the wells considered. The purpose of the design process is to identify the best combination of those decision variables. State variables are hydraulic head and solute concentration which are dependent variables in the flow and

Fig. 11. Objective function value variation with number of iterations by PCM–PSO.

Fig. 12. Concentration distribution after 15 years of remediation by PCM–PSO (in ppm).
transport equations, respectively. For the remediation design model, there are commonly two major components; the simulation model that updates state variables and the optimization model that selects the optimal values for the decision variables.

The objective of the present study is to obtain optimal pumping rates for wells to minimize the total lift cost of groundwater involved in a defined volume of contaminated groundwater and treatment for the specified time period, which justifies choice of the objective function (Mondal et al., 2010). Concentration distributions in the system are analyzed for two scenarios of only pump and treat and pump and treat with flushing for the entire remediation period.

In the present problem, minimum head anywhere in the aquifer is constrained to be greater than 4 m and concentration after remediation is constrained to be less than 750 ppm. The lower and upper bounds on pumping rates are chosen as 0 and 1000 m$^3$/day, respectively. An efficiency of 70% is considered for the pumping system. For the PSO model, values of the parameters are $c_1 = c_2 = 0.5$ and $w = 1.2$. Population size is taken as 100 while the dimension is considered to be 30.

Parameters $c_1$ and $c_2$ are not critical for PSO’s convergence. However, the role of the inertia weight $w$ is considered critical for the PSO’s convergence behavior. As default, $c_1 = c_2 = 2$ are used. However, a number of numerical experiments indicate that $c_1 = c_2 = 0.5$ provided even better results. Therefore, in this study, $c_1 = c_2 = 0.5$ are used. The suggested value of $w$ is between 0.6 and 1.2. A number of numerical studies were performed for $w$ in this range and found that $w = 1.2$ gave stable results. Hence, the inertia weight is kept constant as 1.2 in this study.

6. Results and discussion

Two scenarios are considered for remediation of the aquifer system. In the first case, 30 pumping wells are considered for pumping of contaminated water and treatment. In the second case with 30 pumping wells, two flushing ponds with size of 1500 m $\times$ 750 m each (see Fig. 8) are also considered. With only pump and treat, the maximum concentration in the aquifer after 15 years is found to be 956.33 ppm when flushing ponds are not considered. This is more than the allowable concentration of 750 ppm. Therefore, two flushing ponds, recharging at a rate of 0.2 m$^3$/day are considered as shown in Fig. 8. From the initial application of the PCM—PSO models, few considered pumping wells are found to be non-performing. Wells with pumping rates less than 10 m$^3$/day are considered as non-performing and discarded in the further model runs. Thus, the optimal pumping rates at 23 abstraction wells out of 30 are obtained and given in Table 3. The best objective function versus number of iterations plot for 5 different test runs with a population size of 200 is shown in Fig. 11. It is observed that the final minimized cost obtained from all the runs is nearly the same. Also, the model is run for a population size of 50, 100 and 200. It is observed that the final minimized cost obtained from the population size of 100 and 200 are almost similar. The concentration distribution after remediation of 15 years is shown in Fig. 12. The concentration distribution at some nodes in the domain (64, 86, 148, 167 and 186) is shown in Fig. 13. Further, the model was employed for 30 years study to understand the variation of optimum cost and maximum concentration after remediation. Results of the model for 30 years are plotted in Fig. 14. It is found that the optimum solution is achieved after 15 years of remediation with the maximum value of concentration at a hot spot as 743.22 ppm and the cost of remediation is found to be INR 196.54 $\times$ 10$^6$ (Rs. 196.54 million).

6.1. Model advantages and limitations

As demonstrated in this study, the PCM—PSO is a simple approach to design a strategy for groundwater contamination remediation. Though the pump and treat method is found to be time consuming for remediation purposes, it is one of the effective remediation technologies used in practice. The PCM is found to be a simple approach for simulation of coupled groundwater flow and transport. In the PCM model, only equidistant nodes are added to the aquifer. Therefore, pre-processing time for meshing and remeshing is saved and the algorithm is simple to implement. There are many advantages of PSO such as algorithmic simplicity over other evolutionary algorithms like GA. A GA typically requires three major operators; selection, crossover, and mutation. There are several options of implementation for each of these operators (Mondal et al., 2010). However, there is only one simple operator in PSO i.e. a velocity calculation. Advantages of dealing with fewer operators include reduction of computation efforts, elimination of the process to select the best operator for a given optimization and lesser convergence time.

However, there are some open issues with the PCM method such as shape parameter determination. Also, values of $c_1$, $c_2$ and $w$ were kept constant.
are required to be decided in the case of PSO, with number of numerical experiments. However, it is envisaged that it can be solved easily with experience.

7. Concluding remarks

Pump and treat is one of the commonly used methods for groundwater remediation. Simulation-optimization models give an effective solution for remediation by using pump and treat with the optimum cost. In this paper, a simulation model based on the MFree PCM and PSO optimization are developed and verified with available analytical solutions. Further, PCM and PSO models are coupled to get an effective S/O model, PCM-PSO, for groundwater contamination remediation design. The developed PCM-PSO model is applied for remediation of a contaminated unconfined aquifer near Vadodara, India. Initially, the PCM model is used to simulate flow and transport process in the aquifer system. Further, the PCM-PSO model is used to design a remediation system using pump and treat with pumping wells and two flushing ponds. Compared to grid based methods such as FDM or FEM, the PCM based MFree model is effective and flexible. Further, PSO is simple and more effective in comparison to the optimization technique such as GA.

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References


Further reading


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