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Simulation–optimization model for groundwater contamination remediation using meshfree point collocation method and particle swarm optimization

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Abstract. Remediation of the groundwater contamination problem is a tedious, time consuming and expensive process. Pump and treat (PAT) is one of the commonly used techniques for groundwater remediation in which the contaminated groundwater is pumped, treated and put back to the aquifer system or other sources. Developing simulation-optimization (S/O) model proved to be very useful in the design process of an effective PAT system. Simulation models help in predicting the spatial and temporal variation of the contamination plume while optimization models help in minimizing the cost of pumping. Generally, grid or mesh based models such as Finite Difference Method (FDM) or Finite Element Methods (FEM) is used for the groundwater flow and transport simulation. But it is found that grid/mesh generation is a time consuming process. Therefore, recently Meshfree (MFree) based numerical models are developed to avoid this difficulty of meshing and remeshing. MFree Point Collocation Method (PCM) is a simple meshfree method used for the simulation of coupled groundwater flow and contaminant transport. For groundwater optimization problems, even though number of methods such as linear programming, nonlinear programming, etc. are available, evolutionary algorithm based techniques such as genetic algorithm (GA) and particle swarm optimization (PSO) are found to be very effective.

In this paper, a simulation model using MFree PCM for confined groundwater flow and transport and a PSO based single objective optimization model are developed and coupled to get an effective S/O model for groundwater remediation using PAT. The S/O model based on PCM and PSO is applied for a polluted hypothetical confined aquifer and its performance is compared with Finite Element Method–Binary Coded Genetic Algorithm (FEM–GA) model. It is found that both the models are in good agreement with each other showing the applicability of the present approach. The PCM–PSO based S/O model is simple and more effective in groundwater contamination remediation design using PAT.

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Keywords. Groundwater contamination; remediation, pump and treat; meshfree method; point collocation method; particle swarm optimization; simulation–optimization.

1. Introduction

The goal of a groundwater remediation effort includes a range of objectives such as limiting the migration of plume off-sites, isolating and containing a source area from further leaking or treating the affected groundwater aquifer down to some drinking water standard. Several physical, chemical and biological remedial techniques are nowadays available for treating contaminated groundwater, with each method having its own merits and demerits. Pump and treat (PAT) is one of the established techniques (Guan & Aral 1999) for restoring the contaminated aquifers. The technique involves locating adequate number of pumping wells in a polluted aquifer where contaminants are removed from the aquifers with the pumped out groundwater. For designing such a system, it is required to know how to minimize the cost, cleanup time to reach the maximum contaminant mass removal from the aquifer and at the same time, meeting the water quality requirement of the maximum contaminant level.

In the past decade, groundwater flow and transport models embedded in an optimization model are used in the design of remediation systems as an effort to produce an effective system at low cost and high performance (Eugene *et al* 2005). Simulation models along with the optimization models for the effective remediation of groundwater pollution give the complete solution for the complex groundwater contamination problem. For the simulation of coupled groundwater flow and transport, researchers developed models based on grid based methods like finite difference method (FDM) or finite element method (FEM). But the pre-processing part like meshing, remeshing in these methods is tedious and time consuming. MFree method uses a set of nodes scattered within the problem domain and on the boundaries of the domain to represent the problem domain and its boundaries, regardless of the connectivity information between them. Since there is no grid, it can lead to substantial cost and time savings (Liu & Gu 2005).

PSO shares many similarities with evolutionary computational techniques such as GA. The system is initialized with a population of random solutions and searches for optima by updating generations. However, unlike GA, PSO has no evolution operators such as crossover and mutation. In PSO, the potential solutions, called particles, fly through the problem space by following the current optimum particles (Kennedy & Eberhart 1995). Parsopoulas & Vrahatis (2002) also concluded that PSO is a very useful and simple technique for solving complex problems.

If simulation model is embedded in an optimization model using advanced optimization tools like particle swarm optimization (PSO) or genetic algorithm (GA), it may prove to be effective for groundwater contamination remediation (Wang & Zheng 1997). A number of researchers applied S/O models to the groundwater management and contamination remediation in the recent past, for example: Gill *et al* (1984), Ahlfeld *et al* (1988), Chang *et al* (1992), Huang & Mayer (1997), Wang & Zheng (1997), Prasad & Rastogi (2001) and Mondal *et al* (2010) to name a few. Shawn *et al* (2006) identified AEM–PSO model as an effective algorithm for solving pump-and-treat optimization problems.

In the present study, an attempt is made to develop S/O model using MFree point collocation method (PCM) for coupled flow and contaminant transport simulation and then it is coupled with particle swarm optimization (PSO) for more efficient and optimal groundwater pollution remediation using pump and treat method. The developed PCM–PSO model is compared with another S/O model based on FEM–GA and the results are found to be satisfactory.

2. Governing equations and boundary conditions

The governing equation describing the flow in a non-homogeneous confined aquifer in two-dimensions (2D) is given as (Bear 1979):

$$\frac{\partial}{\partial x}\left(T_x\frac{\partial h}{\partial x}\right)+\frac{\partial}{\partial y}\left(T_y\frac{\partial h}{\partial y}\right)=S\frac{\partial h}{\partial t}+Q_w\delta\left(x-x_i\right)\left(y-y_i\right)-q_s, \tag{1}$$

where, T_x and T_y are the transmissivities (m^2/d) in x and y directions; $h(x,\ y,\ t)$ is the piezometric head (m); S is the storage coefficient; $x,\ y$ are the horizontal space variables (m); Q_w is source or sink function ($-Q_w$ is Source, $+Q_w$ is Sink) (m^3/d/m^2) and $q_s(x,\ y,\ t)$ is the known inflow rate (m^3/d/m) and t is the time in days.

The initial conditions are

$$h\left(x,y,0\right)=h_0\left(x,y\right)\quad x,y\in\Omega, \tag{2}$$

where, $h_0(x,\ y)$ is the initial head in flow domain (m);Ω is the flow region. Generally, the boundary conditions are of two types, the prescribed head or flux. It can be written as

$$h\left(x,y,t\right)=h_1\left(x,y,t\right)\qquad x,y\in\partial\Omega_1;\ T\frac{\partial h}{\partial n}=q_1\left(x,y,t\right)\qquad x,y\in\partial\Omega_2, \tag{3a, 3b}$$

where, $\partial\Omega$ is the boundary region ($\partial\Omega_1\cup\partial\Omega_2=\partial\Omega$); $\partial/\partial n$ is the normal derivative; $h_1(x,y,t)$ is the known head value of the boundary head (m).

The partial differential equation for transport of a single chemical constituent in groundwater in 2D, considering the advection dispersion and fluid sources/sinks (Freeze & Cherry 1979; Wang & Anderson 1982) is given by

$$R\frac{\partial c}{\partial t}=\frac{\partial}{\partial x}\left(D_{xx}\frac{\partial c}{\partial x}\right)+\frac{\partial}{\partial y}\left(D_{yy}\frac{\partial c}{\partial y}\right)-\frac{\partial}{\partial x}(v_xc)-\frac{\partial}{\partial y}\left(v_yc\right)-\frac{c'W}{n_eb}-R\lambda c, \tag{4}$$

where v_x and v_y are seepage velocities in x and y directions (m/day); D_{xx}, D_{yy} are the components of dispersion coefficient tensor [L^{2}T^{-1}], which are calculated from the longitudinal and transverse dispersivities and Darcy's velocities; c is the dissolved concentration [ML^{-3}]; λ is the reaction rate constant [T^{-1}]; W is the rate of recharge of contaminated groundwater per unit volume; c' is the concentration of the solute from the source; n_e is the local porosity; t is the time; b is the aquifer thickness; R is the retardation factor. The initial conditions are

$$c\left(x,y,0\right)=f\qquad x,y\in\Omega. \tag{5}$$

The boundary conditions are

$$c\left(x,y,t\right)=g_1\qquad x,y\in\Gamma_1;\qquad \frac{\partial}{\partial x}\left(D_{xx}\frac{\partial c}{\partial x}\right)n_x+\frac{\partial}{\partial y}\left(D_{yy}\frac{\partial c}{\partial y}\right)n_y=g_2\qquad x,y\in\Gamma_2\ , \tag{6a, 6b}$$

where n_x and n_y are the components of the unit outward normal vector to the given boundary Γ and g_1 and g_2 are known concentration and concentration gradient.

3. Model development

In this study, PCM with standard multi quadric radial basis function (MQ-RBF) (Kansa 1990) is used to develop the groundwater flow and contaminant transport model. PSO is used to develop an optimization model. PCM formulation for flow and transport models as well as PSO algorithm is discussed in the following section.

3.1 *PCM formulation for 2D groundwater flow*

For transient groundwater flow in homogeneous confined isotropic media in 2D, Eq. (1) is written as (Bear 1979):

$$\frac{\partial^2 h}{\partial x^2} + \frac{\partial^2 h}{\partial y^2} = \frac{S}{T}\frac{\partial h}{\partial t}. \tag{7}$$

In PCM, the trial solution $\hat{h}(x, y, t)$ is defined as (Liu & Gu 2005)

$$\hat{h}\,(x, y, t) = \sum_{i=1}^{n} h_i\,(t)\,R_i\,(x, y). \tag{8}$$

Here, shape function used is MQ-RBF (Kansa 1990) and can be written as (Liu & Gu 2005; Mategaonkar & Eldho 2011)

$$R_i\,(x, y) = \sqrt{(x - x_i)^2 + (y - y_i)^2 + Cs^2}, \tag{9}$$

where, x, y are the co-ordinates of the point of interest in the support domain; x_i, y_i are the co-ordinates of ith node in the support domain; Cs=$\alpha_C d_c$. Here, α_C is the shape parameter and d_c is the nodal spacing in the support domain.

In PCM, every node in the problem domain is surrounded by few nodes for the collocation purpose called as support domain. For simplicity, rectangular support domain is used in this study. Figure 1 shows the schematic representation of a typical rectangular support domain. Using rectangular support domain, the dimension of support domain is determined by $d_{sx} = \alpha_{Cx} d_{cx}$; $d_{sy} = \alpha_{Cy} d_{cy}$; where, $d_{c(x,y)} = \sqrt{A_s}/\sqrt{n_{A_s}} - 1$; A_s is the area of the estimated support domain; n_{A_s} is the number of nodes covered by the estimated domain with the area of A_s; α_{Cx} and α_{Cy} are the dimensionless sizes of the support domain in x and y directions. For simplicity, one often uses $\alpha_{Cx} = \alpha_{Cy} = \alpha_C$ and d_{cx}, d_{cy} are nodal spacing in x and y direction. If the nodes are uniformly distributed, d_{cx} is simply the distance in x direction between two neighbouring nodes and d_{cy} is the distance in y direction between two neighbouring nodes. The discrete equations of PCM can be formulated using the shape functions. The schematic representation of support domain is given in figure 1.

The first and second derivatives of shape function with respect to x and y can be written as

$$\frac{\partial R_i\,(x, y)}{\partial x} = \frac{(x - x_i)}{R_i\,(x, y)};\quad \frac{\partial R_i\,(x, y)}{\partial y} = \frac{(y - y_i)}{R_i\,(x, y)}, \tag{10a, b}$$

$$\frac{\partial^2 R_i\,(x, y)}{\partial x^2} = \frac{\left((y - y_i)^2 + Cs^2\right)}{R_i^3\,(x, y)};\quad \frac{\partial^2 R_i\,(x, y)}{\partial y^2} = \frac{(x - x_i)^2 + Cs^2}{R_i^3\,(x, y)}. \tag{11a, b}$$

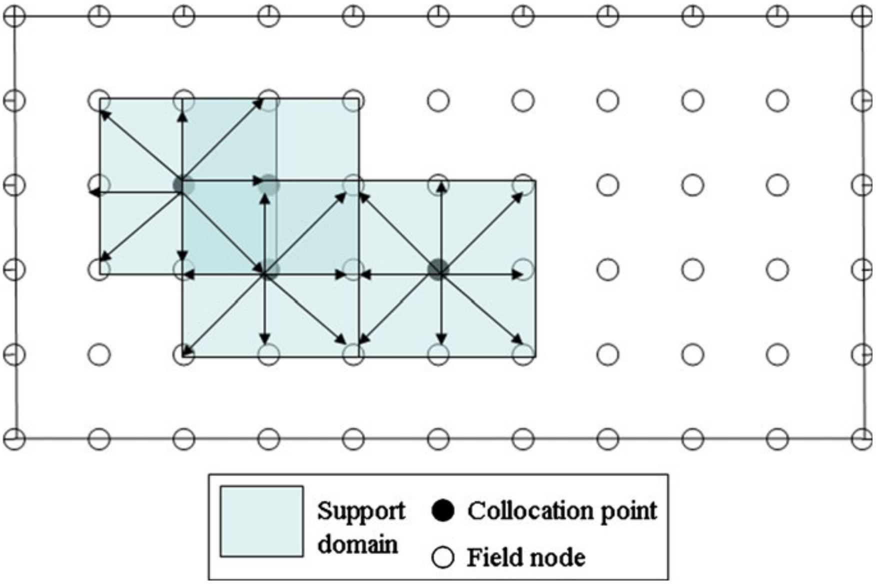

Figure 1. Schematic representation of support domain.

For time discretization, fully implicit finite difference approximation is used (Freeze & Cherry 1979; Wang & Anderson 1982). Therefore, Eq. (7) can be written as

$$R_i\,(x,y)\,h_i^{t+\Delta t}-\frac{T\,\Delta t}{S}\left(\left(\frac{\partial^2 R_i\,(x,y)}{\partial x^2}\right)+\left(\frac{\partial^2 R_i\,(x,y)}{\partial x^2}\right)\right)h_i^{t+\Delta t}=R_i\,(x,y)\,h_i^t, \qquad (12)$$

where, $R_i\,(x,y)$, $\left(\frac{\partial^2 R_i(x,y)}{\partial x^2}\right)$ and $\left(\frac{\partial^2 R_i(x,y)}{\partial y^2}\right)$ values are to be calculated for each support domain and they are incorporated in the global matrix for whole problem domain. Therefore, finally, Eq. (12) can be written in the matrix form as

$$\left([K_1]-\left(\left(\frac{T\,\Delta t}{S}\right)[K_2]+[K_3]\right)\right)\{h_i\}^{(t+\Delta t)}=[K_1]\,\{h_i\}^{(t)}\,, \qquad (13)$$

where, $[K_1]$ is the global matrix of shape function; $[K_2]$ is the global matrix of second derivative of shape functions with respect to x; $[K_3]$ is the global matrix of second derivative of shape functions with respect to y. Once the unknown head values are found, the velocities at nodes are found by using Darcy's law. The global matrix will be asymmetric sparse matrix due to the use of support domain (Liu & Gu 2005). The system of equation, after applying boundary conditions, can be solved by direct approach or iterative technique. In the present study, the system of equations is solved by Gauss Jordan method. When source or sink terms are to be considered, then Eq. (13) can be written as

$$\left([K_1]-\left(\frac{T\,\Delta t}{S}\right)([K_2]+[K_3])\,\{h_i\}^{(t+\Delta t)}\right)=[K_1]\,\{h_i\}^{(t)}\pm\left(\left(\frac{\Delta t}{S}\right)[K_1]\,\{Q_w\}\right), \qquad (14)$$

where, a_1 is the area of support domain in which the pumping well or recharge well lies and $\{Q_w\}$ is the global matrix of the entire source and sink terms. For the heterogeneous media, the domain is divided into zones and the transmissivity of that zone is considered for all the nodes lying in that particular zone. Once the head distribution in the aquifer is found, velocities in x and y directions, respectively (v_x and v_y), are calculated from Darcy's law (Bear 1979) as

$$v_x = -K_x \frac{\partial h}{\partial x}; \qquad v_y = -K_y \frac{\partial h}{\partial y}, \tag{15}$$

where, K_x and K_y are the hydraulic conductivities in x and y directions, respectively.

3.2 *PCM formulation for 2D transport equation*

The transport equation for a single constituent contamination in 2D can be written as (Freeze & Cherry 1979; Wang & Anderson 1982)

$$D_{xx} \frac{\partial^2 c}{\partial x^2} + D_{yy} \frac{\partial^2 c}{\partial y^2} - v_x \frac{\partial c}{\partial x} - v_y \frac{\partial c}{\partial y} = \frac{\partial c}{\partial t}. \tag{16}$$

In PCM, the trial solution $\hat{c}\,(x, y, t)$ is defined as (Liu & Gu 2005; Mategaonkar & Eldho 2011)

$$\hat{c}\,(x, y, t) = \sum_{i=1}^{n} c_i\,(t)\, R_i\,(x, y). \tag{17}$$

The shape function is given by Eq. (9). For time discretization, fully implicit finite difference approximation is used. From Eqs. (16) and (17),

$$\begin{aligned} R_i\,(x, y)\, c_i^{t+\Delta t} - \Delta t \left(D_{xx} \left(\frac{\partial^2 R_i\,(x, y)}{\partial x^2} \right) + D_{yy} \left(\frac{\partial^2 R_i\,(x, y)}{\partial x^2} \right) \right) c_i^{t+\Delta t}, \\ = R_i\,(x, y)\, c_i^t - \Delta t \left(v_x \left(\frac{\partial R_i\,(x, y)}{\partial x} \right) c_i^t + v_y \left(\frac{\partial R_i\,(x, y)}{\partial y} \right) c_i^t \right). \end{aligned} \tag{18}$$

Here, $R_i(x, y)$, $\left(\frac{\partial^2 R_i(x,y)}{\partial x^2}\right)$ and $\left(\frac{\partial^2 R_i(x,y)}{\partial y^2}\right)$values are to be calculated as per Eqs. (10a, b) and (11a, b) for each support domain and they are incorporated in the global matrix for whole problem domain after applying the boundary conditions. Therefore, Eq. (18) can be written in the matrix form as

$$\left([K_1] - \Delta t \left((D_{xx})\,[K_2] + \left(D_{yy}\right)[K_3]\right)\right)\{c_i\}^{(t+\Delta t)} = \left([K_1] - \Delta t \left((v_x)\,[K_4] + \left(v_y\right)[K_5]\right)\right)\{c_i\}^{(t)}, \tag{19}$$

where, $[K_4]$ is the global matrix of first derivative of shape function with respect to x; $[K_5]$ is the global matrix of first derivative of shape functions with respect to y. When the source of contamination is from an ash pond, a dump site, an industrial site or a well, then the Eq. (19) can be written as

$$\begin{aligned} &\left([K_1] - \Delta t \left((D_{xx})\,[K_2] + \left(D_{yy}\right)[K_3]\right)\right)\{c_i\}^{(t+\Delta t)} \\ &\quad = \left([K_1] - \Delta t \left((v_x)\,[K_4] + \left(v_y\right)[K_5]\right)\right)\{c_i\}^{(t)} + (\Delta t\,[K_1])\,\{c_2\}, \end{aligned} \tag{20}$$

where, $\{c_2\}$ is the global matrix of the contamination from ponds or recharge wells.

3.3 *PSO algorithm*

PSO is a population based stochastic optimization technique developed by Kennedy & Eberhart (1995), inspired by social behaviour of bird flocking or fish schooling. There are two variants of PSO: in first approach, global neighbourhood is considered and in second approach, local neighbourhood is considered. In global neighbourhood approach, each particle moves towards its best previous position and towards the best particle in the whole swarm. On the other hand, in second approach, each particle moves towards its best previous position and toward best particle in its restricted neighbourhood (Eberhart *et al* 1996). In the present study, the model is developed based on the global neighbourhood approach. The algorithm for PSO is as given below:

Position of individual particles updated as follows (Kennedy & Eberhart 2001; Parsopoulos *et al* 2001):

$$x^i_{k+1} = x^i_k + v^i_{k+1}, \tag{21}$$

where, velocity is calculated as

$$v^i_{k+1} = wv^i_k + c_1 r_1 \left(p^i_k - x^i_k\right) + c_2 r_2 \left(p^g_k - x^i_k\right), \tag{22}$$

where x^i_k is the particle position; v^i_k is the particle velocity; x^i_{k+1} is the updated position of the particle. p^i_k is the best 'remembered' individual particle position; p^g_k Best 'remembered' swarm position; v^i_{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; w is the inertia factor.

There are many advantages of PSO over GA such as algorithmic simplicity and easiness of implementation. The GA typically requires three major operators: selection, crossover, and mutation. There are several options of implementation for each of these operators. In the PSO, however, there is one simple operator: velocity calculation. The advantage of dealing with fewer operators is the reduction of computation time and elimination of the process to select the best operator for a given optimization. Also, the convergence time for PSO is less.

4. S/O model for groundwater contamination remediation

Based on the above formulation, PCM based simulation model for flow and transport is developed (PCM–GFTM). The flow model is verified with analytical solution given by Liggett & Liu (1983) and found to be satisfactory (Mategaonkar & Eldho 2011). The transport model is verified with analytical solution given by Marino (1974) and found to be in good agreement (Mategaonkar & Eldho 2012). Also, a PSO based model is developed for single objective function and verified with solution given by Deb (1995) and found to be satisfactory. Further, both the PCM based simulation model and PSO based optimization model are coupled to get a simulation–optimization model.

For PCM, the domain is discretized with number of nodes. Every node is having one support domain. The values of shape function, its first and second derivatives with respect to x and y are calculated for every support domain and these are incorporated in the global matrix for whole problem domain (Mategaonkar & Eldho 2012). The final equations are solved for head and contaminant concentration for the whole simulation period. The PCM model is embedded in the PSO model giving objective function with all constraints for remediation purpose.

In the single-objective remediation design, only minimization of the remediation cost is considered as an objective function. The cost function includes both capital and operational costs of extraction and treatment. The cost of extraction is proportional to the energy required to lift the water to ground level and the total time period of remediation, during which pumping is done, whereas, the cost of treatment depends only on the volume of water pumped. The initial cost of construction of well is not considered in the design, as it is fixed. The cost function is chosen as (Mondal *et al* 2010):

$$\text{Minimize cost} \quad f = t\left\{a_1 \sum_{i=1}^{N} \frac{\frac{Q_i \gamma (\Delta t) g}{\eta}\left[h_i^{gl} - h_i\right]}{864{*}10^5} + a_2 \sum_{i=1}^{N} Q_i\right\}, \tag{23}$$

where, f is objective function for minimization of the system cost; Q_i is the pumping rate of the well (m^3/day); η is the efficiency of pumping system; h_i^{gl} is the ground level at well i(assumed to be constant throughout the aquifer); h_i is the piezometric head at well i(m); 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 $\frac{Q_i \gamma (\Delta t) g}{\eta}\left[h_i^{gl} - h_i\right] \Big/ \left(864{*}10^5\right)$ converted to KWH. Considering the cost of electricity in India, INR 5.0/KWH, the cost coefficient for energy, $a_1 =$ INR 5*24/KW/day; a_2 is the cost coefficient for treatment (TDS pollution only), INR 3.0 per m^3 of water pumped; γ is the unit weight of water (1000 kg/m^3); $\left(h_i^{gl} - h_i\right)$ is the groundwater lift at well i; t is the fixed time for remediation.

The constraints to the problem are specified as

$$c_{\max} < c^*, \tag{24}$$

$$h_{\min} \geq h^*, \tag{25}$$

$$Q_{i,\min} \leq Q_i \leq Q_{i\max} \qquad i = 1....NP, \tag{26}$$

where i is the node number; *NP* is the total number of pumping nodes of flow domain; c^* is the specified limit of concentration in the region; Q_i is the pumping rate at well; $c_{\max}$ is the maximum concentration anywhere in the aquifer; $h_{\min}$ is the minimum head anywhere in the aquifer and h^* is the specified minimum groundwater head anywhere in the aquifer.

The optimal remediation of contaminated groundwater by pump and treat method is designed in two steps. In the first step, the simulation model is developed and calibrated to match the conditions of groundwater system. In the second step, an optimization methodology is used to solve values for decision variables. In any optimization problem, there are two sets of variables: decision variables and state variables. For PAT remediation system, decision variables include the pumping or injection rates for wells. The purpose of the design process is to identify the best combination of those decision variables. The state variables are hydraulic heads in the flow equation and the solute concentration in the transport equation. For any remediation design model, there are two major components to be considered: the simulation model that updates the state variables and the optimization model that selects the optimal values for the decision variables.

The step-by-step procedure for the S/O model is as given below

(i) Provide input parameters for PCM–GFTM model like transmissivity, storage coefficient, dispersivity, porosity, time steps and *Cs* value.
(ii) Generate initial population of particles (pumping rates) and initialize the PSO algorithm constants: w, c_1 and c_2.

(iii) Evaluate the objective function. If objective is achieved (reaching minimum cost), then stop else update the particles' positions and velocities of particles and again PCM–GFTM model is run for next time step.

(iv) Apply PCM–GFTM model to obtain the head and concentration distribution in the aquifer and check all the constraints.

(v) If the constraints are not satisfied, then the position and velocity of swarm particles is updated and the steps from 3rd to 4th are repeated till the difference between two iterations is less than 0.0001. Also, the solution is accepted when the maximum time is achieved.

(vi) The optimal pumping rates at the end of remediation time are noted down.

5. Case study

To see the applicability of the S/O model based on PCM–PSO, a hypothetical confined aquifer remediation problem is considered and its results are compared with FEM–GA model (Mondal 2007). For the case study, a hypothetical contaminated confined aquifer as shown in figure 2 is considered. The aquifer is confined, anisotropic and non-homogeneous with size of 1500 × 1400 m. The ground surface from the bottom of aquifer is assumed to be 40 m. The aquifer is divided into three zones with varying values of transsmitivities. Zone 2 is assumed to be recharged by an overlying clay aquitard at 0.0012 m/day. The direction of flow is towards the

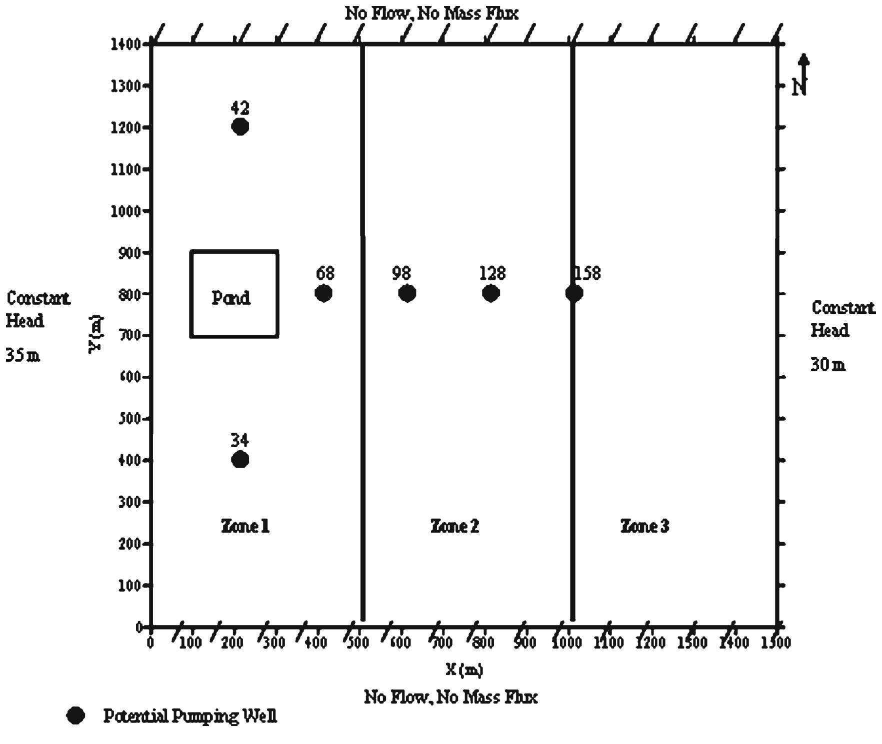

Figure 2. Diagrammatic representation of aquifer.

Table 1. Parameters for confined aquifer.

Aquifer property	Value
Hydraulic conductivity in x direction, K_x in Zone 1	40 m/day
Hydraulic conductivity in y direction, K_y in Zone 1	35 m/day
Hydraulic conductivity in x direction, K_x in Zone 2	50 m/day
Hydraulic conductivity in y direction, K_y in Zone 2	40 m/day
Hydraulic conductivity in x direction, K_x in Zone 3	60 m/day
Hydraulic conductivity in y direction, K_y in Zone 3	50 m/day
Thickness of aquifer	25 m
Average porosity in the aquifer	30%
Specific storage	0.004
Average depth of ground surface to datum	40 m
Longitudinal dispersivity	200 m
Transverse dispersivity	20 m

right boundary, which is maintained with a constant hydraulic head of 35.0 m on the Western boundary and a constant hydraulic head of 30.0 m on the Eastern boundary. The details of the aquifer parameters are given in table 1. For simulation of flow and transport, a PCM model is

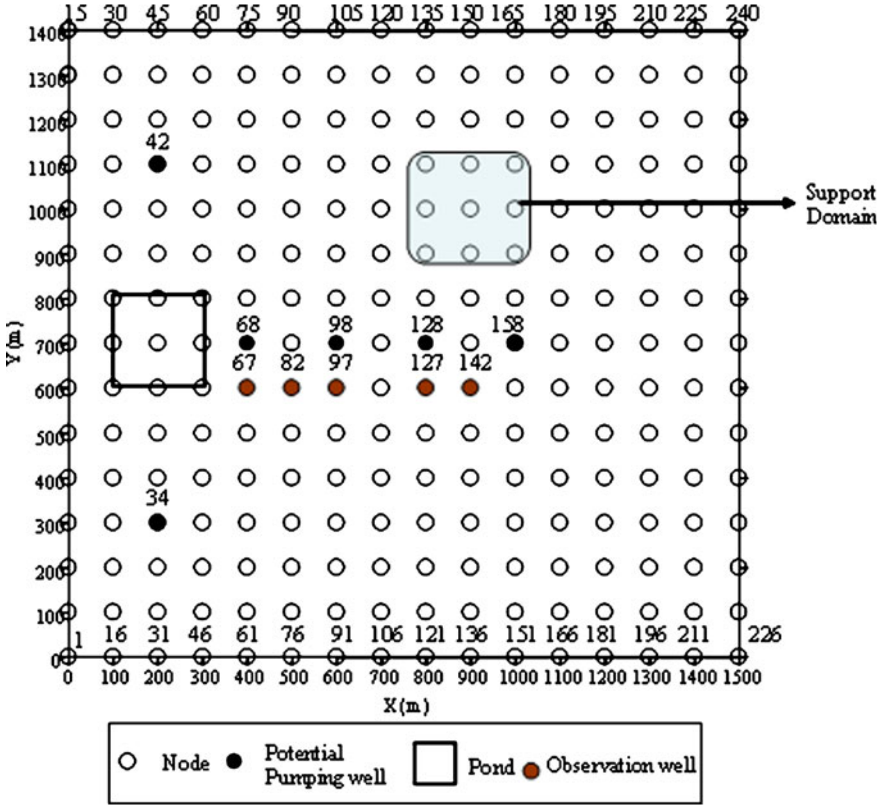

Figure 3. Nodal arrangement for aquifer.

developed with 240 equi-distant nodes having 9 nodes in every support domain (see figure 3). The time step of 1 day is considered and the value of *Cs* is taken as 300. The initial contaminant plume is generated assuming a source that is a disposal pond discharging total dissolved solids (TDS) at a rate of 3000 mg/l and 0.025 m/day for 5 years as shown in figure 2. The steady state head distribution is shown in the figure 4. The steady state heads are used as initial heads for the transient simulation. During the steady state, no pumping is assumed, while during disposal of contaminant for 5 years, pumping is assumed to take at a constant rate of 1000 m^3/day at the three wells at nodes 34, 42 and 158 as shown in figure 3.

The principal direction of dispersivity is assumed to be parallel to the flow direction. Along the left boundary, the contaminant concentration is assumed to be 0 mg/l, and concentration gradient is zero on the northern and southern directions. Since the area of the aquifer is relatively small, (2.1 km^2), any known concentration cannot be assumed on the Eastern boundary.

Initially, the entire aquifer domain is assumed to be uncontaminated ($c = 0$). The flow model takes into account the flux boundaries, known head boundaries and the areal recharge. The transport model can take known concentration boundaries, known mass flux boundaries and seepage from the disposal pond into account. The head distribution after 5 years is shown in figure 5 while the concentration distribution after 5 years is shown in the figure 6.

In the present work, the compliance requirement for the concentration level is considered to be lower than 750 ppm everywhere in the aquifer so that water quality will be fair for drinking

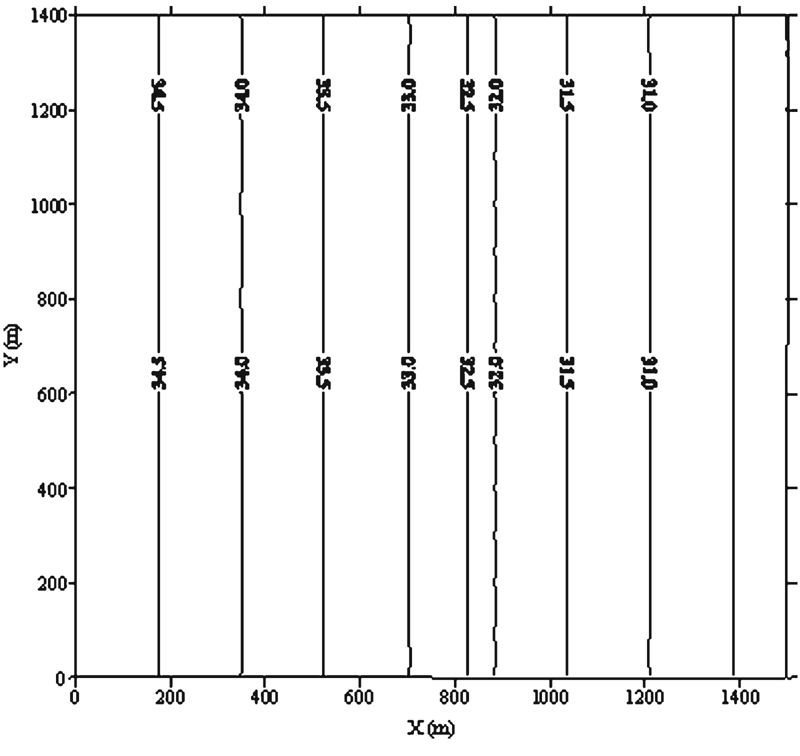

Figure 4. Steady state head distribution in m.

purpose (http://www.hc-sc.gc.ca), at the end of 5 years. After simulation for 5 years, the maximum concentration is found to be equal to 1475 ppm which is much higher than the allowable concentration of 750 ppm (c^*). At the end of 5 years, it is assumed that the contamination from the pond is stopped.

To remediate the contaminated groundwater in the aquifer system, PCM–PSO model is applied to find out the optimal pumping pattern for cleanup of the system within the specified time period of 2 years. Pump and treat (PAT) method is chosen for aquifer remediation. The optimization of PAT remediation design requires that the coupled flow and solute transport model is run repeatedly, in order to calculate the objective function associated with the possible design and to evaluate whether various hydraulic and concentration constraints are met.

The objective of the present study is to obtain optimal pumping rates for the wells to minimize the total lift cost of groundwater involved in definite volume of contaminated groundwater and treatment for the specified time period, which justifies the choice of the objective function (Mondal *et al* 2010). Concentration distribution in the system is analysed for different scenarios for the entire remediation period.

In the present problem, the minimum head anywhere in the aquifer should be greater than 25 m. The lower and upper bounds on the pumping rates are chosen as 0 and 1000 m^3/day. 85% of efficiency is considered for the pumping system.

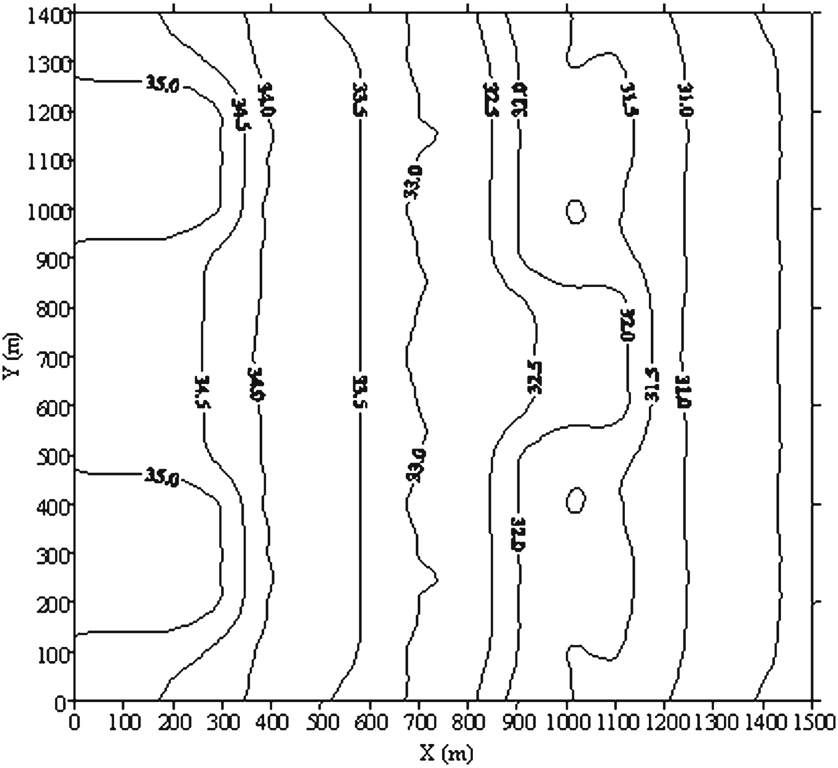

Figure 5. Head distribution after 5 years in m.

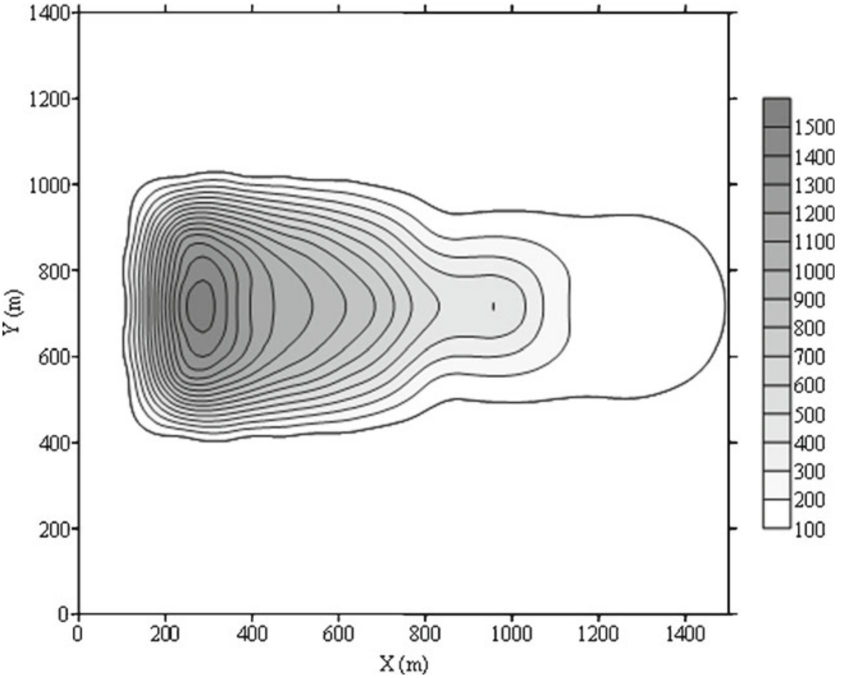

Figure 6. Concentration distribution after 5 years in ppm.

6. Results and discussion

The following section explains the results obtained from various scenarios using PCM–PSO and their comparison with FEM–GA model. Here for the remediation of the contamination, first one pumping well (at node 68) with flushing through the pond is considered and next, three pumping wells at node 68, 98 and 128 (see figure 3) with no flushing is considered. The wells are placed as near to the maximum concentration distribution as possible.

6.1 *One pumping well with flushing*

In this scenario, one pumping well, at node 68 (see figure 3), is considered for pumping out the contaminated groundwater, along with flushing pond. During the 2 years of remediation, the pond is assumed to recharge aquifer with treated water of TDS concentration of 750 mg/l at the rate of 0.025 m/day, thus acting like a flushing pond. Lower and upper bounds on the pumping capacity are chosen as 0 and 1000 m^3/day. For optimization by PSO, the dimension is taken as 2, $c_1 = c_2 = 0.5$ and $w = 1.2$. The solution is obtained for population size of 30, 50 and 100. The objective function v_s number of iterations is plotted and shown in figure 7. It is observed that the solution is almost same for population sizes of 50 and 100. For the two years of pumping and treating, the optimized pumping required is 256.51 m^3/day and the cost of remediation is Rs. 5,61,167/-. The concentration distribution at the end of remediation is shown in figure 8. The maximum concentration observed after remediation is 500.12 ppm. The result is compared with

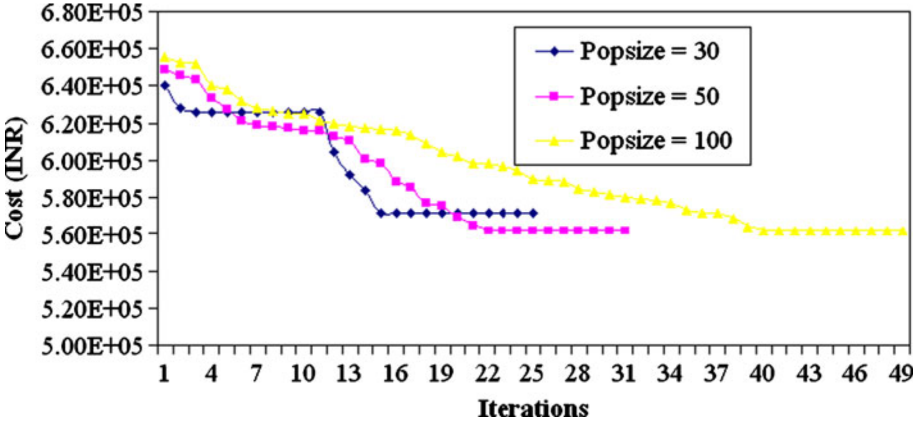

Figure 7. Objective function value variation with number of iterations for one well scenario.

FEM–GA model (Mondal 2007). For FEM simulation 240 nodes and 420 triangular elements are considered and the GA parameters considered are, 20 bit binary string for pumping rate, and size of population as 100, probability of crossover as 0.8 and lower mutation probability as 0.1.

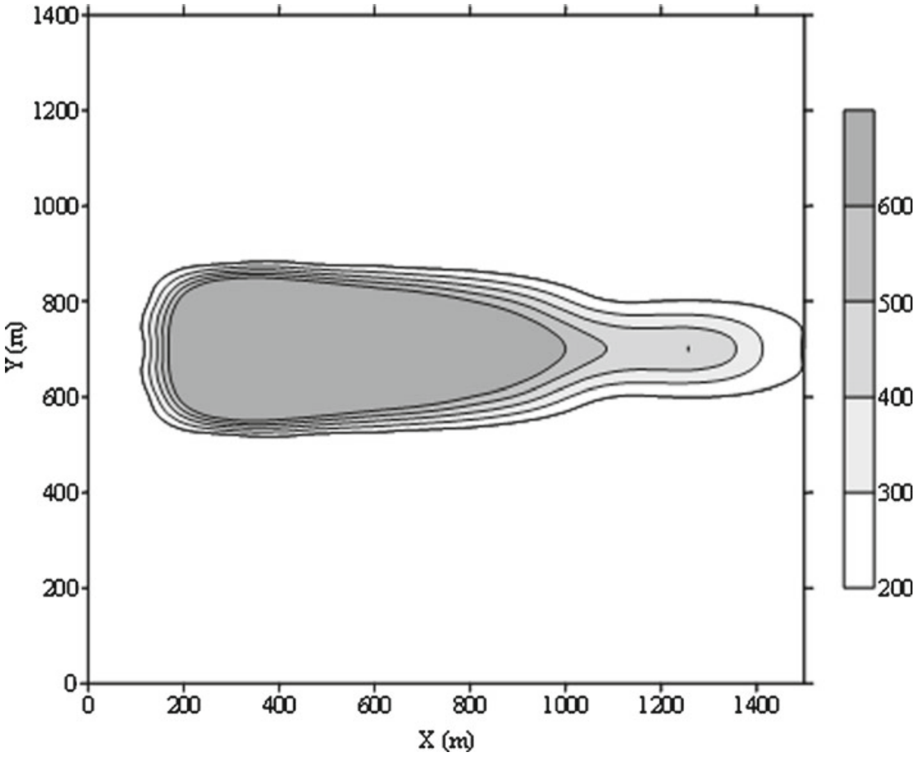

Figure 8. Concentration distribution after 2 years in ppm for one well pumping.

Table 2. Comparison of PCM–PSO model with FEM–GA model for one well scenario.

Parameters	PCM–PSO	FEM–GA
Cost (INR)	5,61,167	5,61,364
Pumping rate (m^3/day) at node 68	256.51	256.480

The comparison of results is given in the table 2. It is clear that the PCM–PSO model, results show good agreement with FEM–GA model showing the applicability of the present model.

6.2 *Three pumping wells*

In this scenario, three pumping wells, at node 68, 98 and 158 are considered (see figure 3) for pumping out the contaminated groundwater for 2 years of remediation period. Here the flushing/ recharge pond is considered as inactive. Lower and upper bounds on the pumping capacity are chosen as 0 and 1000 m^3/day. All other parameters for PSO and GA are kept same as for one well scenario. The objective function v_s number of iterations is plotted for this case also and shown in figure 9. Here also, it is observed that the solution is almost same for population sizes of 50 and 100. In this scenario, the pumping rates required are 59.439 m^3/day, 52.809 m^3/day and 34.596 m^3/day at the wells located at nodes 68, 98 and 158, respectively, giving the total cost of pumping and treating as Rs. 3,21,660/-. The maximum TDS concentration observed after remediation is 434.42 ppm. The results are compared with FEM–GA model and the comparison is given in the table 3. The concentration distribution is shown in figure 10.

The pumping rate for the one well scenario is 256.513 m^3/day for the well located at node 68 for the remediation period of 2 years. The model projected an optimal cost for pumping and treatment as Rs. 5,61,167/- while for three wells scenario it is 59.44 m^3/day, 52.81 m^3/day and 34.60 m^3/day at the wells located at nodes 68, 98 and 158, respectively, with the cost of Rs. 3,21,660/- which is much less than one well scenario. Hence the optimal pumping rate obtained

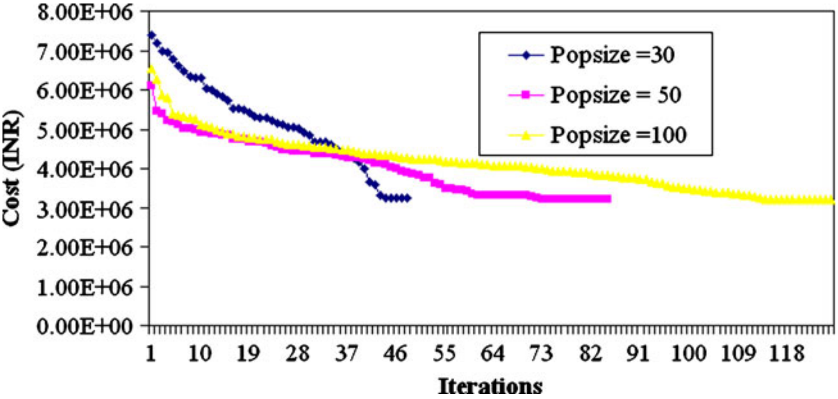

Figure 9. Objective function value variation with number of iterations for three wells scenario.

Table 3. Comparison of PCM–PSO model with FEM–GA model for three wells scenario.

Parameters	PCM–PSO	FEM–GA
Cost (INR)	3,21,660	3,21,657
Pumping rate (m^3/day) at node 68	59.44	59.43
Pumping rate (m^3/day) at node 98	52.81	52.87
Pumping rate (m^3/day) at node 158	34.60	34.57

in three wells scenario is the best pumping policy for the chosen problem to cleanup the aquifer within the specified time period.

From the results, it is clear that for the remediation of contaminated aquifer using three wells scenario, the concentration levels in the aquifer domain are much less than that the required value, everywhere in the system, whereas for one well scenario the maximum concentration level is marginally higher than the three wells scenarios in the system but less than the required value. This is due to the pumping well location which is placed in the highly polluted area, so that the removal of contaminant from these pumping wells is effective. However, the cost of one well scenario is much higher than the three wells scenario and hence the three wells scenario gives the optimal solution. In this study, the initial cost of construction of pumping wells is not considered. It is assumed that the pumping wells already exist in the system. These investigations

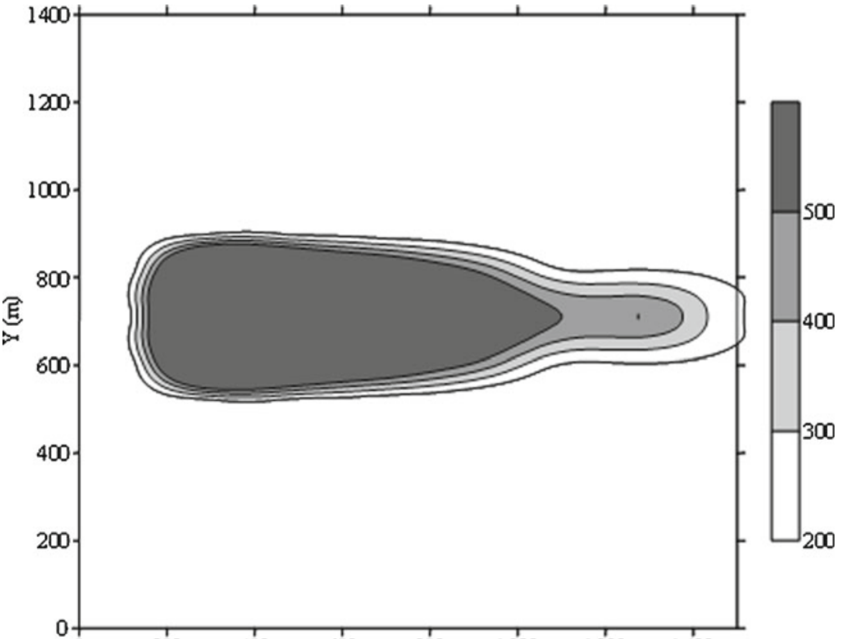

Figure 10. Concentration distribution after 2 years in ppm for three wells pumping.

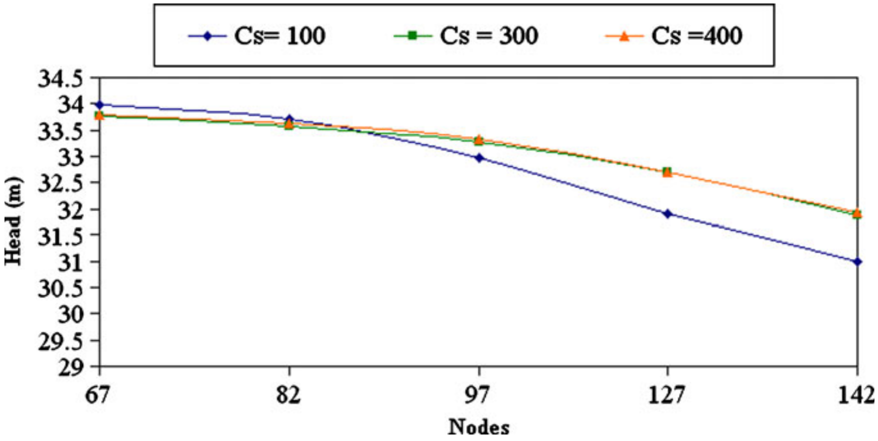

Figure 11. Sensitivity of *Cs* with the head (m) at some nodes.

have shown that an appropriately designed pump and treat system can have a significant effect on the decontamination of a polluted aquifer and preclude further spreading of contaminant plume.

For PCM model the value of *Cs* affects the accuracy of the results. Therefore, a sensitivity analysis is carried out with *Cs* value equal to 100, 300 and 400. It is found that the results obtained with *Cs* values more than or equal to 300 are almost similar but they diverge for values less than 300. It shows that the model gives good results for α_C value more than 3. The simulation results at some nodes (refer figure 3) for head (m) and solute concentration (ppm) are shown in figures 11 and 12, respectively. The CPU time required for PCM–PSO model is approximately 115 seconds (in PC AMD Athlon, 64 × 2 Dual Core Proceesor 4800+, 2.50 GHz) for three wells problem with population size of 100, maximum time of two years and time step of one day.

As shown in the present study, PCM–PSO is an effective S/O approach to design the complex pump and treat remediation strategy for groundwater decontamination. The pre-processing time

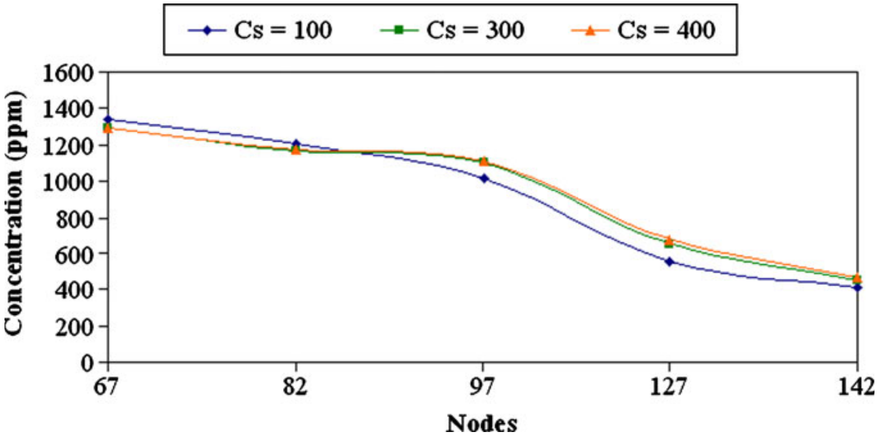

Figure 12. Sensitivity of *Cs* with the solute concentration (ppm) at some nodes.

required for grid-based numerical methods is saved in PCM. Also, using PSO, in comparison with GA, the computational burden is reduced due to fewer operators and lesser convergence time.

7. Conclusion

Groundwater contamination remediation is a very complex process. Pump and treat is one of the commonly used methods for groundwater remediation. S/O models can give effective solution for the remediation using pump and treat with the optimum cost. In this paper, S/O model based on meshfree PCM and PSO optimization model, PCM–PSO is developed for confined groundwater contamination remediation. The developed PCM–PSO model is applied for remediating contaminated hypothetical confined aquifer. Initially, the PCM model is used to simulate the flow and transport process in the aquifer system. Further, PCM–PSO model is used to design a remediation system using pump and treat with one well and flushing pond and only three wells scenario. The optimal results are obtained using the S/O model. The model results are further compared with FEM–GA model and found to be satisfactory, showing the applicability of the present approach. Compared to the grid based method such as FDM or FEM, PCM based meshfree model is much effective and flexible. Compared to optimization technique such as GA, PSO is simple and more effective. The coupled PCM–PSO model can be considered to be the result-oriented model for groundwater contamination remediation.

References

Ahlfeld D P, Mulvey M J, Pinder G F and Wood E F 1988 Contaminated groundwater remediation design using simulation, optimization, and sensitivity theory Model development. *Water Resour. Res.* 24(3): 431–441

Bear J 1979 *Hydraulics of groundwater*, New York: McGraw Hill Publishing

Chang L C, Shoemaker C A and Liu P L-F 1992 Optimal time varying pumping rates for groundwater remediation: application of a constrained optimal algorithm. *Water Resour. Res.* 28(12): 3157–3173

Deb K 1995 *Optimization for engineering design*, New Delhi: Prentice Hall of India

Eberhart R C, Simpson P and Dobbins R 1996 *Computational Intelligence PC Tools*, Academic Press

Eugene Agyei, Douglas Munch P G and Patrick Burger P E 2005 *Application of optimization modeling to water resource planning in East-Central Florida*, St. Johns River Water Management District, Technical Publication SJ2005–2, Palatka, Florida

Freeze R A and Cherry J A 1979 *Groundwater*, Englewood Cliffs, NJ: Prentice Hall-INC

Gill P E, Murray W, Saunders A, and Wright M H (1984) Aquifer reclamation design: The use of contaminant transport simulation combined with nonlinear programming. *Water Resour. Res.* 20(4): 415–427

Guan J and Aral M M 1999 Optimal remediation with well locations and pumping rates selected as continuous decision variables. *J. Hydrol.* 221: 20–42

Huang C and Mayer A S 1997 Pump-and-treat optimization using well locations and pumping rates as decision variables. *Water Resour. Res.* 33(5): 207–222

Kansa E J 1990 Multiquadrics-A scattered data approximation scheme with application to computational fluid dynamics II (Solutions to parabolic, hyperbolic and elliptic Partial Differential Equation). *J. Computers Mathematical Applications* 19(8/9): 147–161

Kennedy J and Eberhart R C 1995 Particle swarm optimization. *Proc. IEEE Int'l. Conf. on Neural Networks*, IV, 1942–1948. Piscataway, NJ: IEEE Service Center

Kennedy James and Eberhart R C 2001 *Swarm intelligence*, CA, USA: Academic press

Liggett J A and Liu P L-F 1983 *The boundary integral equation method for porous media flow*, London: George Allen and Unwin

Liu G R and Gu Y T 2005 *An introduction to meshfree methods and their programming*, Dordrecht, Berlin, Heidelberg, New York: Springer

Marino M A 1974 Longitudinal dispersion in saturated porous media. *J. Hydraulics Division, ASCE*, 100 (HY1), 151–157

Mategaonkar M and Eldho T I 2011 Simulation of groundwater flow in unconfined aquifer using meshfree polynomial point collocation method. *Eng. Analysis with Boundary Elements* 35: 700–707

Mategaonkar M and Eldho T I 2012 Two-dimensional contaminant transport modeling using meshfree point collocation method (PCM). *Eng. Analysis with Boundary Elements* 36: 551–561

Mondal Arpita 2007 *FEM-GA based simulation–optimization models for groundwater remediation*, M.Tech. Thesis, IIT, Bombay

Mondal Arpita, Eldho T I and Gurunadhrao V V S 2010 Multiobjective groundwater remediation system design using coupled finite element model and nondominated sorting genetic algorithm II. *J. Hydrologic Eng.* (ASCE) 15(5): 350–359

Parsopoulas K E and Vrahatis M N 2002 *Recent approaches to global optimization problems through particle swarm optimization. Natural computing* (1): 235–306, The Netherlands: Kluwer Academic Publishers

Parsopoulos K E, Plagianakos V P, Magoulas G D and Vrahatis M N 2001 Stretching technique for obtaining global minimizers through particle swarm optimization. *Proceedings of the Workshop on Particle Swarm Optimization*, Indianapolis, IN: Purdue School of Engineering and Technology, IUPUI (in press)

Prasad K L and Rastogi A K 2001 Estimating net aquifer recharge and zonal hydraulic conductivity values for Mahi right bank canal project Area, India by genetic algorithm. *J. Hydrol.* 243(3–4): 149–161

Shawn M L, Rabideau A J and Craig J R 2006 Pump-and-treat optimization using analytic element method flow models Advances in water resources. *J. Advances Water Resour.* 29(5): 760–775

Wang H and Anderson M P 1982 *Introduction to groundwater modeling finite difference and finite element methods*, New York: W H Freeman and Company. http://www.hc-sc.gc.ca/ewh-semt/pubs/water-eau/doc_sup-appui/tds-mdt/index_e.html

Wang M and Zheng C 1997 Optimal remediation policy selection under general conditions. *Groundwater* 35(5): 757–764