In-situ bioremediation of groundwater using a meshfree model and particle swarm optimization

Meenal Mategaonkar, T. I. Eldho and Sahajanand Kamat

ABSTRACT

Groundwater contamination due to contaminants like trichloroethylene (TCE), tetrachloroethylene, dichloroethylene, phenol, etc., is an alarming concern for most of the manufacturing areas. It is important to identify the type of pollutant, concentration, location, and direction of the contaminant plume for groundwater remediation. Bioremediation has been identified as one of the important remediation techniques for these types of contaminants. Bioremediation modeling comprises solutions to biodegradation equations and fixing the time of remediation and locating the oxygen injection wells. In this study, a simulation-optimization (S/O) model based on the coupled meshfree point collocation method (MFree-PCM) and particle swarm optimization (PSO) is proposed for *in-situ* bioremediation design. The *in-situ* bioremediation process of groundwater contamination is explored using the developed PCM-BIO-PSO multi-objective model with different strategies of minimization of cost, number of wells and time of remediation. The proposed model can be effectively used for the *in-situ* bioremediation design of contaminated sites.

Key words | groundwater pollution, *in-situ* bioremediation, meshfree point collocation method, particle swarm optimization, simulation-optimization model

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INTRODUCTION

The requirement of groundwater increases with the increase of population, industrialization, agriculture, and navigation. The groundwater quality has also become a major concern in terms of color, odor, taste, and hardness. The conservation of the quality and quantity of the groundwater requires supreme priority. Any groundwater contamination study involves identification of the source of contaminant, the movement of the pollutants in the groundwater environment once they are introduced, proper management of resource utilization, and preventive measures to ensure suitable development and remediation of polluted sites (Eldho 2001).

For the remediation of groundwater contaminated with pollutants such as trichloroethylene (TCE), dichloroethylene or phenol, conventional approaches such as pump and treat (PAT), pump and use are not effective. In such cases, *in-situ* bioremediation is one of the effective methods for remediation (Bedient *et al.* 1999).

In a typical *in-situ* bioremediation system, an aerobic environment is created by adding oxygenated fluid for the growth of microorganisms. Biological degradation is facilitated by oxygenated fluid. The process continues until the concentration of contaminants is reduced to the approved levels. The type of oxygenated fluid to be used is a further challenge for this method. The type of oxygenated fluid is preferably air, but pure oxygen, steam, water vapor, etc. are some other types used (Bedient *et al.* 1999).

The purpose of modeling bioremediation of groundwater is for the prediction of contaminant concentrations at receptor positions and the estimation of source control actions on remediation. Further, it also gives the point allocations of observation wells while the remedial study is

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carried out and evaluates the remedial functioning for different designs. Modeling of bioremediation of groundwater is an effective tool to predict the efficacy and clean-up time to stated levels (Bedient *et al.* 1999).

Numerical models are necessary for developing an efficient operative design and upkeep of an *in-situ* bioremediation arrangement. Simulation-optimization (S/O) models can give an efficient injection approach, suitable positions for remediation wells and time of remediation. The efficacy of S/O models for bioremediation is demonstrated by various studies (e.g., Minsker & Shoemaker 1998; Yoon & Shoemaker 2001; Prasad & Mathur 2008; Mategaonkar & Eldho 2012c).

Meshfree (MFree) methods have gained acceptance in many engineering applications owing to their mesh-free character. With the removal of grid, pre-processing time of simulation is reduced. With the ease in computing the distances in any number of spatial dimensions, working in higher dimensions does not increase the intricacy and computational cost of the method (Liu 2003, 2006; Liu & Gu 2005).

MFree methods have been applied successfully to groundwater flow and transport problems by many researchers (e.g., Li *et al.* 2003; Praveen Kumar & Dodagoudar 2008, 2010). Mategaonkar & Eldho (2012a; 2012b) developed a coupled flow and transport model for groundwater.

Simulation models along with optimization models for the effective remediation of groundwater pollution give the complete solution for the complex groundwater contamination problem. Shieh & Peralta (2005) presented a parallel recombinative simulated annealing (PRSA) model along with BIOPLUME II to optimize *in-situ* bioremediation system design with a two-stage management approach. The first-stage design goal is to minimize total system cost (pumping/treatment, well installation, and facility capital costs) and the second-stage goal is to minimize the cost of a time-varying pumping strategy using the optimal system chosen by the first-stage optimization.

Mategaonkar & Eldho (2012c) developed a S/O model for *in-situ* bioremediation using meshfree PCM and PSO (PCM-BIO-PSO). It is observed that the PCM-BIO-PSO model is an effective model for *in-situ* bioremediation of groundwater contamination. Mategaonkar & Eldho (2014) also developed a multi-objective model for PAT method for the remediation of total dissolved solids (TDS).

Luo *et al.* (2014) and Akbarnejad-Nesheli *et al.* (2016) developed a multi-objective S/O model to achieve the best *in-situ* bioremediation system design for groundwater with contaminated dissolved hydrocarbons and observed that the Pareto-optimal solution with low variability, high reliability is a potentially effective tool for optimizing multi-objective groundwater remediation problems under uncertainty.

Kumar *et al.* (2015) presented the use of a new hybrid algorithm to optimize a multi-objective function which includes the cost of remediation as the first objective and residual contaminant at the end of the remediation period as the second objective. The hybrid algorithm was formed by combining the methods of differential evolution (DE), genetic algorithms, and simulated annealing (SA). The results obtained from the hybrid algorithms were compared with DE, non-dominated sorting genetic algorithm (NSGA II) and SA. It is found that the proposed hybrid algorithm can provide the best solution. Ehsai *et al.* (2017) used a BIOPLUME III simulation model coupled with a NSGA-II-based model for optimal design of *in-situ* groundwater bioremediation system. The multi-objective optimization model tries to minimize: (1) cost; (2) sum of contaminant concentrations that violate standard; (3) contaminant plume fragmentation. The simulation period is divided into smaller time intervals for more efficient optimization aiming to minimize the contaminant plume fragmentation.

In this study, an S/O model is presented using MFree PCM for the simulation of coupled groundwater flow and transport and PSO for getting the optimal solution for efficient *in-situ* bioremediation. Two strategies of cost minimization with number of wells and cost minimization with time of remediation are considered with different population sizes. The proposed model is applied to a case study to demonstrate the applications of the developed model.

GOVERNING EQUATIONS AND BOUNDARY CONDITIONS

Oxygen and contaminants are assumed to be the only substrates necessary for development in aerobic biodegradation (Bedient *et al.* 1999). The following scheme of equations (Freeze & Cherry 1979; Borden & Bedient 1986;

Mategaonkar & Eldho 2012c) can be used in the simulation of biodegradation:

$$\frac{\partial}{\partial x}\left(k_x \frac{\partial h}{\partial x}\right) + \frac{\partial}{\partial y}\left(k_y \frac{\partial h}{\partial y}\right) = S_y \frac{\partial h}{\partial t} + Q_w \delta(x - x_i)(y - y_i) - q_s \tag{1}$$

According to Darcy's law:

$$v_x = -k_x \frac{\partial h}{\partial x}; \; v_y = -k_y \frac{\partial h}{\partial y} \tag{2}$$

$$\frac{\partial c}{\partial t} = \frac{1}{R_c}\left(\begin{array}{l} \frac{\partial}{\partial x}\left(D_{xx}\frac{\partial c}{\partial x}\right) + \frac{\partial}{\partial x}\left(D_{yy}\frac{\partial c}{\partial y}\right) - \frac{\partial}{\partial x}(V_x c) - \frac{\partial}{\partial y}(V_y c) - \\ M_t \frac{\mu_{\max}}{R_c}\left(\frac{c}{K_c + c}\right)\left(\frac{O}{K_o + O}\right) \end{array}\right) \tag{3}$$

$$\frac{\partial O}{\partial t} = \left(\begin{array}{l} \frac{\partial}{\partial x}\left(D_{xx}\frac{\partial O}{\partial x}\right) + \frac{\partial}{\partial x}\left(D_{yy}\frac{\partial O}{\partial y}\right) - \frac{\partial}{\partial x}(V_x O) - \frac{\partial}{\partial y}(V_y O) - \\ M_t \frac{\mu_{\max}}{R_c} F\left(\frac{c}{K_c + c}\right)\left(\frac{O}{K_o + O}\right) \end{array}\right) \tag{4}$$

Here, h is the piezometric head; S_y is the specific yield; t is time; v_x and v_y are the velocities in the x and y directions, respectively; K_x and K_y are the hydraulic conductivities in the x and y directions. respectively; Q_w is flow rate from the well and q_s is the volume rate of steady uniform recharge per unit area per unit thickness of the aquifer. Actual velocity is obtained as $V_x = v_x/n_e$ and $V_y = v_y/n_e$; n_e is the porosity; c is contaminant concentration; M_t is the total microbial concentration; $\mu_{\max}$ is maximum contaminant utilization rate per unit mass of microorganisms; K_c is the contaminant half saturation constant; O is oxygen concentration; K_o is oxygen half saturation constant; M_t is the concentration of microbes; Δt is the time interval being considered; F is the ratio of oxygen to contaminant consumed; R_c is the retardation coefficient for the contaminant; D_{xx}, D_{yy} are dispersion coefficient [L^2T^{-1}] in x and y directions, respectively.

For the above-mentioned equations, the initial conditions used are $h(x, y, 0) = h_0(x, y)$; $c(x, y, 0) = f_1$ and $O(x, y, 0) = f_2$. The generally used boundary conditions are:

$$\begin{aligned} h(x, y, t) &= h_1(x, y, t);\ c(x, y, t) = g_1 \text{ and } T\frac{\partial h}{\partial n} \\ &= q_1(x, y, t)\,\partial/\partial x\left(\frac{D_{xx}\partial O}{\partial x}\right)n_x + \partial/\partial y\left(\frac{D_{yy}\partial O}{\partial y}\right)n_y \\ &= g_2 \text{ for } x, y \in \Gamma \end{aligned}$$

where h_0 and h_1 are the known head values and q_1 is the known flux value. f_1 and f_2 are original strengths of contaminant and oxygen, respectively; n_x and n_y are the components of the unit outer normal vector to the given boundary Γ and g_1 is known concentration while g_2 is known flux.

MESHFREE FORMULATION FOR TWO-DIMENSIONAL TRANSPORT AND OXYGEN EQUATIONS

The trial solutions $\hat{h}(x, y, t)$, $\hat{c}(x, y, t)$ and $\hat{O}(x, y, t)$ need to be defined first as (Liu & Gu 2005; Mategaonkar & Eldho 2012c):

$$\hat{h}(x, y, t) = \sum_{i=1}^{n} h_i(t) Ri(x, y) \tag{5a}$$

$$\hat{c}(x, y, t) = \sum_{i=1}^{n} c_i(t) Ri(x, y) \tag{5b}$$

$$\hat{O}(x, y, t) = \sum_{i=1}^{n} O_i(t) Ri(x, y) \tag{5c}$$

Here, n is the number of nodes in the support domain and $R_i(x, y)$ is the multi-quadric–radial basis (MQ-RBF) shape function (Liu & Gu 2005). The shape function is given as:

$$R_i(x, y) = sqrt((x - x_i)^2 + (y - y_j)^2 + Cs^2) \tag{6}$$

where x and y are the co-ordinates of the point of interest in the support domain; x_i, y_i are the co-ordinates of i^{th} node in the support domain; $Cs = \alpha_c d_c$; α_c is the shape parameter and d_c is the nodal spacing in the support domain. The first and second derivatives of the shape function with respect to x and y are calculated as given in Mategaonkar & Eldho (2012a; 2012b). Forward finite difference scheme is adopted for time discretization. Therefore, from Equations (1), (3), and (4) we get (Mategaonkar & Eldho 2012c):

$$\left([K_1] - \left(\begin{array}{l}\dfrac{k_x \Delta t}{S_y}\left([K_2]\{h_i^t\}[K_2] + [K_1]\{h_i^t\}[K_3]\right) + \\ \dfrac{k_y \Delta t}{S_y}\left([K_4]\{h_i^t\}[K_4] + [K_1]h_i^t[K_5]\right)\end{array}\right)\right)$$

$$\left\{h_i^{(t+\Delta t)}\right\} = [K_1]\{h_i^t\} \pm \left(\frac{\Delta t}{S_y}\right)([K_1]\{Q_w\}) \tag{7a}$$

$$\left([K_1] - \frac{\Delta t}{R_c}\left((D_{xx})[K_3] + (D_{yy})[K_5]\right)\right)\{c_i\}^{(t+\Delta t)} = \left(\begin{array}{l}\left([K_1] - \dfrac{\Delta t}{R_c}\left((V_x)[K_2] + (V_y)[K_4]\right)\right)\{c_i\}^t - \\ \dfrac{\Delta t}{R_c}\left(M_t \mu_{\max}\left(\dfrac{[K_1]c_i^t}{K_c + [K_1]c_i^t}\right)\left(\dfrac{[K_1]O_i^t}{K_o + [K_1]O_i^t}\right)\right)\end{array}\right) \tag{7b}$$

$$\left([K_1] - \Delta t\left(\begin{array}{l}(D_{xx})[K_3] + \\ (D_{yy})[K_5]\end{array}\right)\right)\{O_i\}^{(t+\Delta t)} = \left(\begin{array}{l}\left([K_1] - \Delta t\left((V_x)[K_2] + (V_y)[K_4]\right)\right)\{O_i\}^{(t)} \\ -\dfrac{\Delta t}{R_c}\left(M_t \mu_{\max} F\left(\dfrac{[K_1]\{c_i\}^{(t)}}{K_c + [K_1]\{c_i\}^{(t)}}\right)\left(\dfrac{[K_1]\{O_i\}^{(t)}}{K_o + [K_1]\{O_i\}^{(t)}}\right)\right)\end{array}\right) \tag{7c}$$

where $[K_1]$ is global matrix of shape function; $[K_2]$ is global matrix of first derivative of shape functions with respect to x; $[K_3]$ is global matrix of second derivative of shape functions with respect to x; $[K_4]$ is global matrix of first derivative of shape functions with respect to y; and $[K_5]$ is global matrix of second derivative of shape functions with respect to y.

Here, a_1 is the area of support domain in which the pumping well or recharge well lies and (Q_w/a_1) is the global matrix of the entire source and sink terms. The basis function and its derivatives are calculated for each support domain following the Kronecker delta property and are assimilated in the global matrix for whole problem domain.

Based on the above formulation, a two-dimensional meshfree model for flow, transport, and bioremediation has been developed. The developed flow, transport, and bioremediation equations were verified using available analytical and numerical solutions (Mategaonkar & Eldho 2012a; 2012b; 2012c). Further, the flow models are coupled to get an efficient model with PCM-BIO model for bioremediation simulation. To simulate the transport of pollutant and oxygen in the subsurface in aerobic bioremediation, Equations (7b) and (7c) are solved simultaneously.

PSO-BASED OPTIMIZATION MODEL

PSO is an evolutionary optimization technique presented by Kennedy & Eberhart (2001). The 'particles' are the mathematical hypotheses, comprising three main factors: location, velocity, and fitness. Location denotes the unknown variable of the problem, velocity defines the rate of change of location, and fitness is a degree to solve the objective function optimally. The PSO concept involves acceleration of each particle toward its *pbest* and *lbest* positions. Acceleration is biased by a random term that splits random numbers being generated for acceleration to *pbest* and *lbest* locations (Parsopoulos *et al.* 2001). Position of individual particles is updated as follows (Kennedy & Eberhart 1995; Parsopoulos *et al.* 2001):

$$x_{k+1}^i = x_k^i + u_{k+1}^i \tag{8a}$$

with velocity calculated as:

$$u_{k+1}^i = w u_k^i + c_1 r_1 (p_k^i - x_k^i) + c_2 r_2 (p_k^g - x_k^i) \tag{8b}$$

where x_{k+1}^i is the updated position; x_k^i is the particle position; u_{k+1}^i is the updated velocity; u_k^i is the particle velocity; p_k^i is the best 'remembered' individual particle position; p_k^g is the best 'remembered' swarm position; 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 weight.

SIMULATION OPTIMIZATION (S/O) MODEL

For getting the optimal solution of *in-situ* bioremediation of groundwater, simulation model PCM-BIO is coupled with the PSO model (PCM-BIO-PSO-MO). The flow chart for

PCM-PSO-BIO is shown in Figure 1. Optimal cost is attained by considering multi-objectives of optimal injection rate of oxygen, number of injection wells, and time of remediation. The objective function is given as (Minsker & Shoemaker 1998):

$$\text{Minimize cost } f = \sum_{i=1}^{N} a_i \sqrt{1 + Q_i^2} \tag{9}$$

where Q_i is the injection rate in m^3/day; a_i is the relative cost coefficient; N is the number of injection wells; and i is the node number. PSO parameters are initialized and the objective function is assessed. The equations are solved for contaminant concentration and oxygen with the constraints. If the termination criteria are encountered, the simulation results post-processed, otherwise the particles and swarm best values, velocities and positions of particles are restructured, and the objective function is recalculated.

The purpose of the present study is to get optimal injection rates for the wells for minimization of the total cost of remediation along with remediation time and number of

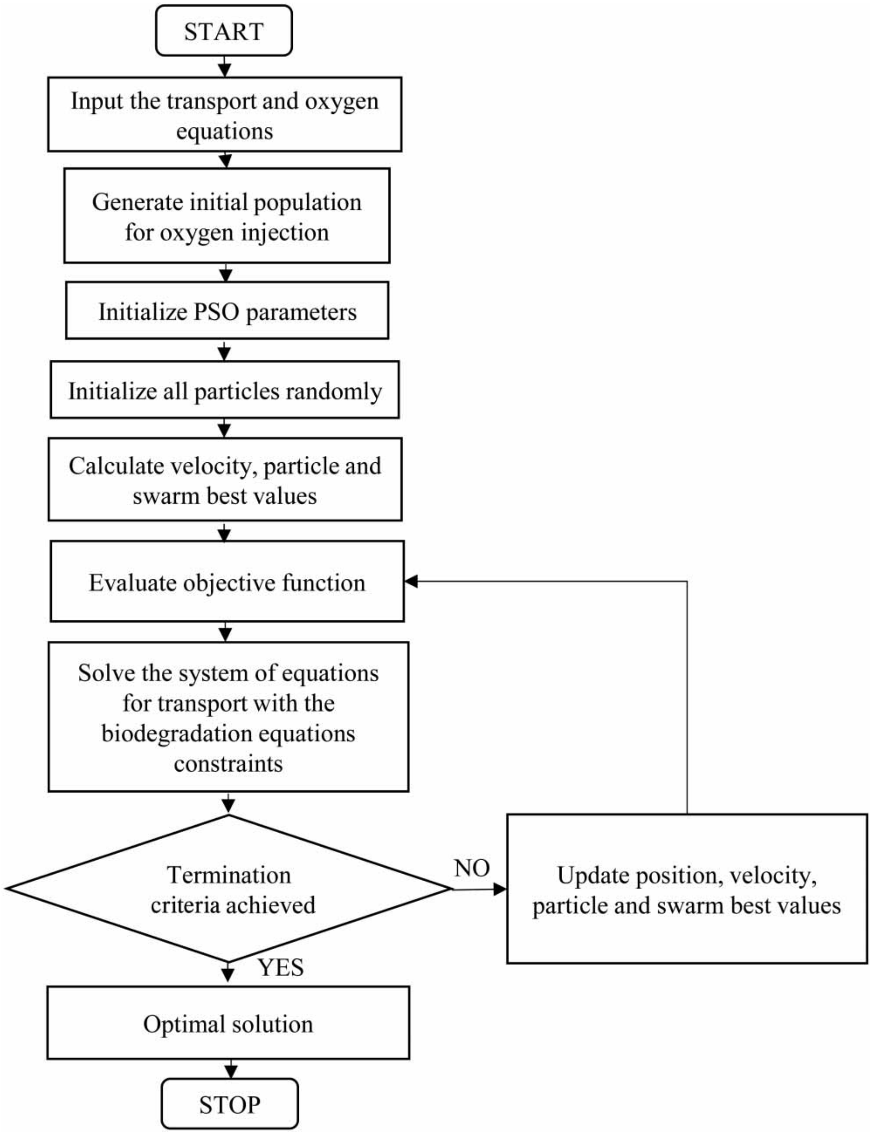

Figure 1 | Flow chart of PCM-BIO-PSO model.

wells. Concentration distribution is analyzed for different strategies for the entire remediation period.

Here, two scenarios of optimization are considered: cost minimization with number of wells and cost minimization with time of remediation.

Scenario A

$$\text{Minimize number of injection wells}\,(N) \tag{10a}$$

The aim of optimization for this scenario is to identify bioremediation designs that minimize cost of remediation and the number of injection wells by fulfilling the limitations on the specified contaminant concentration. The result causes the least number of wells for clean-up with the consideration of the plume position. Thus, the objective function contains the oxygen injection rate and number of wells to optimize.

Scenario B

$$\text{Minimize time of remediation}\,(t) \tag{10b}$$

The purpose of optimization for this scenario, is to identify bioremediation designs which reduce cost and time of remediation on the selected pollutant concentration. The solution gives the minimum time of remediation for different population sizes and thereby the remediation cost is reduced.

The objective function is given in Equation (9). For both cases, the set of constraints considered is:

$$c_m < c';\ h_n \le h_i \le h_m;\ 0 \le t < t_{\max} \text{ and } 0 \le Q_i < Q_m \tag{11}$$

where c_m and c' are the maximum and the specified limit of concentration, respectively, anywhere in the aquifer; h_n and h_m are the minimum and maximum head, respectively, anywhere in the aquifer; h_i is the groundwater head anywhere in the aquifer; and Q_m is the maximum injection/pumping rate.

The objective function comprises the injection rate of water containing oxygen, time of remediation, and the number of wells. Here, the cost of setting up of the injection well is considered as fixed and hence it is not considered in the objective function. Based on the above formulation, a multi-objective model PCM-BIO-PSO-MO is developed.

The oxygen content in injected water is fixed and hence cannot be considered as a decision variable. In this study, aerated oxygen containing 8 mg/L of oxygen concentration is considered (Hinchee *et al.* 1987; Minsker & Shoemaker 1998). Further, it is assumed by the model that the microorganisms are present in substantial amounts in the aquifer for bioremediation (Minsker & Shoemaker 1998). The rate of decay is assumed to be equal to the rate of biomass growth ensuring the indigenous nature of biomass.

MODELING PROCEDURE

A step-by-step procedure for the PCM-BIO-PSO-MO model is given below (Figure 1):

1. Input all physiological and hydrological parameters.
2. Discretize the aquifer into equidistant nodes in x and y directions. Consider a rectangular support domain for each node.
3. Apply PCM-BIO-PSO-MO model for three different cases:
   a. cost optimization with number of wells;
   b. cost optimization with time of remediation;
   c. cost optimization with number of wells and time of remediation.
4. The model is run to reach the contamination level to 5 ppb or less.

The developed PCM-BIO-PSO-MO has been applied to a hypothetical problem and verified as a single-objective model and found to be satisfactory (Mategaonkar & Eldho 2012c).

CASE STUDY

The application of the PCM-BIO-PSO model is investigated by considering a case study which is like a field problem (Figure 2). The primary components of the contamination are identified as TCE, originating from a nearby laundry. From the pumping and flow rate, the aquifer parameters are determined, and the location of contaminant plume is

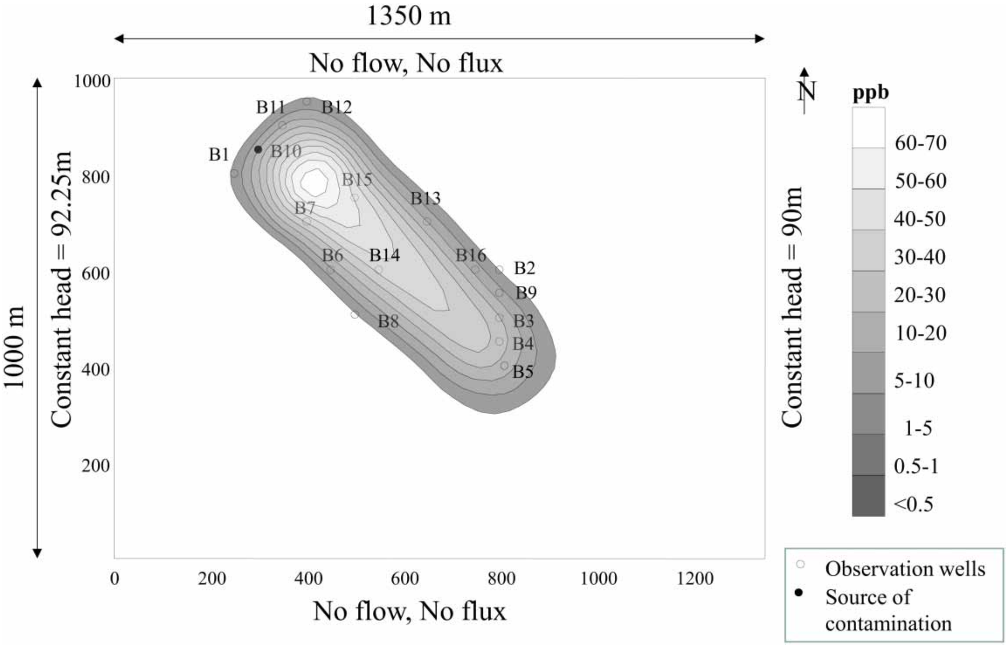

Figure 2 | Schematic representation of aquifer.

identified. The average groundwater velocity in the area is about 0.1 m/day. The aquifer is spread over approximately 1,350 m × 1,000 m with a thickness of 100 m (Figure 2). The maximum contamination concentration at the hotspot is about 70 μg/L. The adopted method should remediate the plume to a drinking water standard of 5 ppb (Hazen & Fliermans 1995). The hydrogeological and physical parameters for this case study are given in Table 1 (Minsker & Shoemaker 1998).

A specific quantity of oxygen is infused into the aquifer to start bioremediation. Decision variables do not influence the oxygen concentration in the injection of water. It is determined by the user quantified values. For the aquifer considered, 9 m and 4.5 m are the dispersivity values in longitudinal and transverse directions. The southern and northern boundaries are not flux boundaries. Constant head at the western boundary is 92.5 m and at the eastern boundary is 90.00 m.

Table 1 | Physical parameters for the case considered

Parameter	**Value**
Contaminant	Tri-chloro-ethylene (TCE)
Size	1,350 m × 1,000 m
Thickness of aquifer	100 m
Hydraulic conductivity	4.4×10^{-3} m/s
Porosity	0.25
Retardation factor	1
Longitudinal dispersivity	9 m
Transverse dispersivity	4.5 m
Substrate half-velocity coefficient K_c	49.6 mg/L
Oxygen half-velocity coefficient K_o	1 mg/L
Maximum gross specific growth rate $\mu_{\max}$	6.48/d
Ratio of oxygen to substrate	3
Maximum injection hydraulic head (h_m)	100 m
Minimum injection hydraulic head (h_n)	80 m
Water quality standard, $c_{\max}$	5 ppb

Application of the PCM-BIO-PSO-MO model

The case study, as mentioned above, is analyzed with the model. For the PCM-BIO-PSO model, 588 nodes are considered (Figure 3) with α_c value as 3 and $\Delta x = \Delta y = 50$ m. The value of Cs is taken as 150, $\Delta t = 1$ day and for every square support domain nine nodes are considered. The nodal assembly for the PCM-BIO-PSO-MO model and the position of injection wells are shown in Figure 3.

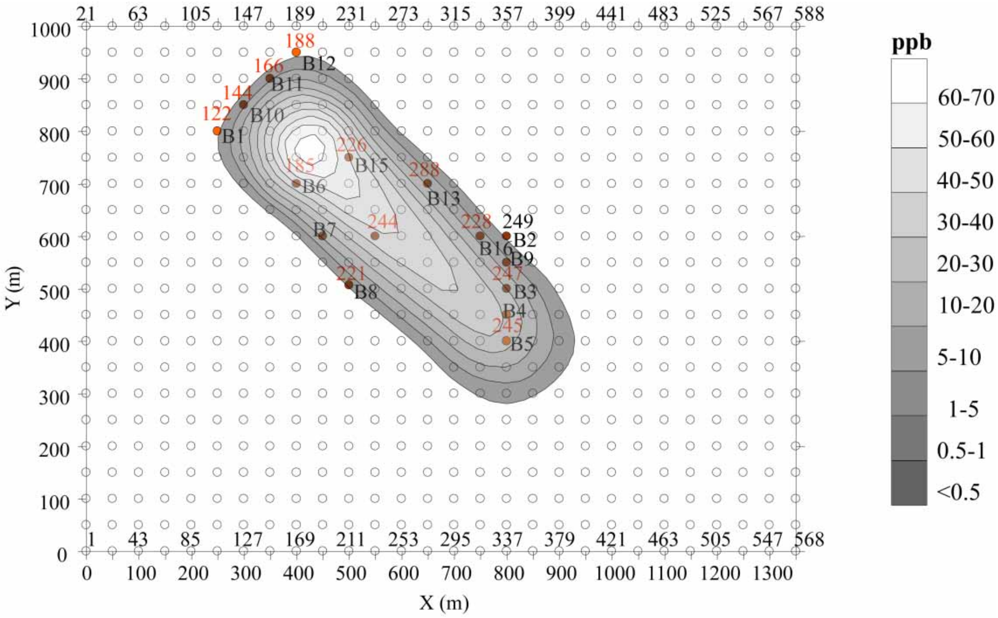

Figure 3 | Nodal arrangement for the aquifer (with location of injection wells).

The injection wells are provided at nodes 144, 183, 198, 227, and 239. The injection rates vary from 200 to 2,000 $\mathrm{m^3/d}$ for the simulation. Further parameters applied are $c_1 = c_2 = 0.5$ and $w = 1.2$. For the S/O model, the hydraulic heads of every node ought to be fewer than h_m and more than h_n (Table 1). h_m is selected to guarantee that the rise in the hydraulic head is equivalent to the most possible hydraulic head.

Original contaminant strength in the plume ranges from 0.5 to 70 μg/L with the peak concentration (>50 μg/L) at nodes 144, 183, 198, 227, and 239 (Figure 3). The primary biomass concentration at every node is assumed to be 0.005 mg/L. The plume is assumed to be enclosed in the oxygen concentration of 3 mg/L while at the center oxygen strength is assumed to be exhausted. The adopted method should remediate the plume to a drinking water standard of 5 ppb. The concentration levels in the 16 investigated observation wells are given in Table 2.

The PCM-BIO-PSO model is applied to remediate the groundwater by *in-situ* bioremediation. Three different cases are considered by applying the PCM-BIO-PSO with the cost and number of injection wells, cost and time of remediation, and cost and both number of wells and time of remediation. In all the cases, the three population sizes for PSO considered are 50, 75, and 100.

Table 2 | Concentration level at the observation wells

Observation well	Contamination level (μg/L)	Observation well	Contamination level (μg/L)
B1	6.3	B9	48.9
B2	5.9	B10	6
B3	44.1	B11	10.5
B4	12.8	B12	18.9
B5	0.9	B13	40.6
B6	66.7	B14	14.1
B7	22	B15	8.2
B8	0.7	B16	6.5

The purpose of the bioremediation is to decrease the contaminant plume up to 5 ppb; hydraulic heads at every node ought to be lower than h_m and higher than h_n. The assumed quantities of h_m and h_n are shown in Table 1. h_n is selected in such a manner that it does not rise above the top of the aquifer whereas h_m is selected to make sure that the rise in the hydraulic head is equivalent to the maximum possible injected hydraulic head (Minsker & Shoemaker 1998).

With the temporal interval of 1 day, the model is run for 100 days. The rate of aerated oxygen is taken as \$0.56 (INR 28 approx.) and the rate of injection/extraction is taken as \$14.41 (INR 720 approx.) per Q_i per month (Minsker & Shoemaker 1998).

Analysis 1

For the first case, three (at nodes 144, 183, and 198), four (at nodes 144, 183, 198, and 227), and five injection wells (at nodes 144, 183, 198, 227, and 239) are considered for remediation.

For this case, three population sizes of 50, 75, and 100 are considered. It is observed that the optimal solution for all the cases is achieved for a four wells' scenario. The cost variation with number of wells is shown in Table 3. The total cost ranges from Rs. 5.59×10^7 to Rs. 9.24×10^7 for a population size of 100 and 100 days.

Table 3 | Solution set for number of wells, time of remediation and population size

		Time of remediation		
Number of wells	**Population size**	**70 days** **Cost (Rs.)**	**100 days**	**200 days**
3	50	7.28×10^7	9.15×10^7	1.72×10^8
	75	6.82×10^7	8.63×10^7	1.70×10^8
	100	6.87×10^7	6.78×10^7	1.57×10^8
4	50	7.61×10^7	6.32×10^7	1.31×10^8
	75	7.42×10^7	6.25×10^7	1.28×10^8
	100	6.35×10^7	5.59×10^7	1.19×10^8
5	50	1.36×10^8	9.30×10^7	1.88×10^8
	75	1.35×10^8	9.26×10^7	1.86×10^8
	100	1.35×10^8	9.24×10^7	1.85×10^8

Analysis 2

For the second case, three different periods of remediation of 70, 100, and 200 days are considered. For this case, also three population sizes (50, 75, and 100) are considered. Cost variation with time for all the population sizes is shown in Figure 4. From Table 3 it is observed that the optimal solution is obtained for 100 days. The total cost for all scenarios range from Rs. 5.59×10^7 to Rs. 1.35×10^8 for all time periods.

Analysis 3

For the third case, both the number of wells and time of remediation were optimization functions along with cost. The results are shown in Table 4. It is observed that even if the number of injection wells is reduced, the cost is not reduced because of high injection rate, and cost is not reduced even if the time of remediation is reduced.

Sensitivity analysis

To figure out the model behavior along with various model parameters, a sensitivity study is conducted for time step, inter-nodal distance (Δx and Δy), and *Cs* value. An attempt is made to increase the accuracy to its maximum to achieve

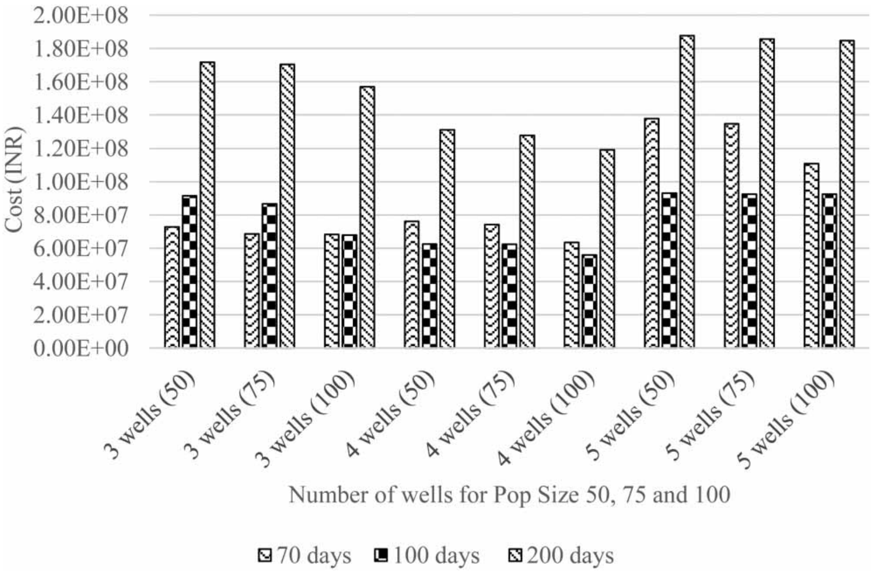

Figure 4 | Cost variation with time.

Table 4 | Solution set for injection rates, number of wells and time of remediation

		Time of remediation (days)			Time of remediation (days)		
		70	100	200	70	100	200
No. of wells	**Well locations (nodes)**	**Rate of injection (m^3/s)**			**Cost (Rs.)**		
3	144	1,582.44	750.98	624.91	6.87×10^7	6.78×10^7	1.57×10^8
	183	1,193.79	675.61	592.68			
	198	887.86	516.69	320.99			
4	144	1,218.45	979.75	804.14	6.35×10^7	5.59×10^7	1.19×10^8
	183	981.76	750.34	657.34			
	198	868.19	664.18	571.24			
	227	753.44	577.78	497.01			
5	144	1,107.89	902.56	753.12	1.35×10^8	9.24×10^7	1.85×10^7
	183	958.78	813.22	639.26			
	198	833.11	719.67	540.77			
	227	720.19	657.76	489.23			
	239	672.72	603.56	402.77			

the minimum concentration of 5 ppb (Minsker & Shoemaker 1998) following remediation for 100 days. For this study, divergence is calculated using the formula (Liu & Gu 2005):

$$\text{Divergence} = \left(\frac{1}{N}\right) \sum_{i=1}^{N} \left| (c_i^{obs} - c^{opt})/c^{opt} \right| \tag{12}$$

where N is the total number of nodes in the aquifer; c_i^{obs} is the contaminant concentration at the end of remediation period; c^{opt} is the optimum contaminant concentration to be achieved at the end of remediation period (5 ppb). The divergence is calculated and plotted with different parameters on semi-log plot by changing the parameters one by one keeping other parameters constant. The attempt is to reduce the divergence to its minimum to achieve the minimum concentration of 5 ppb (Minsker & Shoemaker 1998) after remediation for 100 days. The model is tested for the time steps (Δt) of 1 day, 2 days, 5 days, and 10 days for 100 days. It is found that the model results improve with a lesser time step. The results are shown in Figure 5. Second, the model is tested for inter-nodal distances, $\Delta x = \Delta y = 25m$, $\Delta x = \Delta y = 50m$, and $\Delta x = \Delta y = 100m$. It is observed that the divergence is reduced with the lesser Δx and Δy values. The results after two years of remediation are shown in Figure 6. Finally, the model is tested for different Cs values of 25, 50, 75, 100, and 150. The error reduces with the increasing value of Cs. It indicates that divergence reduces with the greater number of nodes in the support domain. The results after two years are shown in Figure 7. The results indicate that the model is sensitive for all the above-mentioned parameters. However, to achieve the

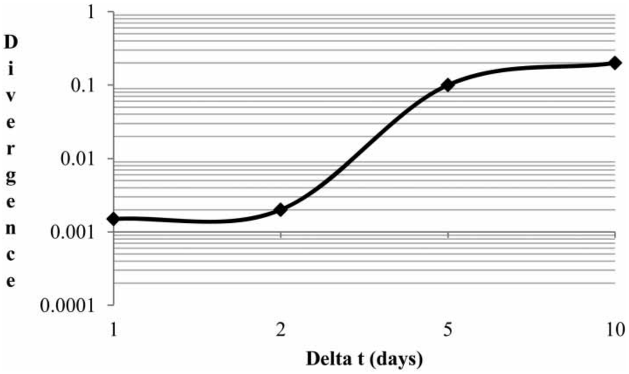

Figure 5 | Divergence for different time steps (Δt).

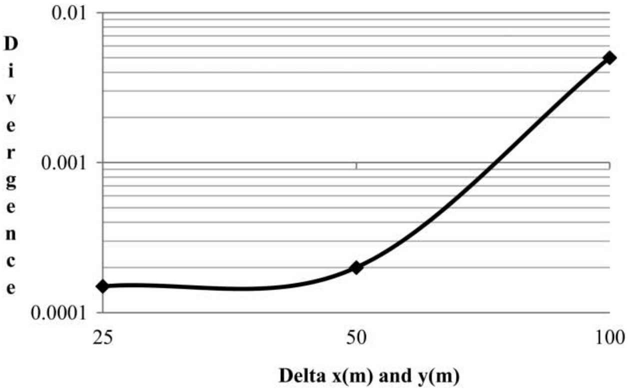

Figure 6 | Divergence for inter-nodal distances (Δx and Δy values).

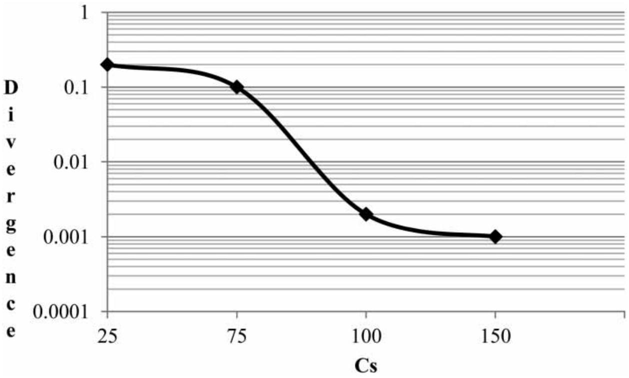

Figure 7 | Divergence for different *Cs* values.

optimum value of contaminant concentration to 5 ppb after bioremediation, the model gives satisfactory results for $\Delta t = 1$ day, $\Delta x = \Delta y = 50m$, and $Cs = 150$ for 100 days of remediation with optimal computational efforts.

CONCLUSIONS

The simulation-optimization models help to design optimal remediation of groundwater. In this study, a PCM-based meshfree model is developed for bioremediation simulation. Also, a PSO-based optimization model is developed for optimization. PCM is a very simple method to work with and apply. With the appropriate selection of shape parameters, the model provides efficient results. The PCM models are further coupled with PSO-based optimization techniques (PCM-BIO-PSO) for *in-situ* bioremediation of groundwater contamination to get an efficient and optimal solution to the bioremediation problem.

In this study, the PCM-BIO-PSO model is applied to a case study similar to a field problem for *in-situ* bioremediation with three scenarios, namely, cost and number of injection wells, cost and time of remediation, cost and number of wells and time of remediation together.

The total cost for three wells for 70 days, 100 days, and 200 days is Rs. 6.87×10^7, Rs. 6.78×10^7, and Rs. 1.57×10^8, respectively. The total cost for four wells for 70 days, 100 days, and 200 days is Rs. 6.35×10^7, Rs. 5.59×10^7, and Rs. 1.19×10^8 respectively. The total cost for five wells for 70 days, 100 days, and 200 days is Rs. 1.35×10^8, Rs. 9.24×10^7, and Rs. 1.85×10^8, respectively. In all the cases, it is observed that the PCM-BIO-PSO-MO model gives the optimal cost of Rs. 5.59×10^7 for four wells, 100 days, and 100 population size for four wells' scenario.

It is observed that as the number of injection wells increases the cost is increased, but at the same time, the remediation time is reduced. The injection rate increases for less time of remediation. Also, the problem solution is optimized with the increasing population size. The proposed methodology can be effectively used in the *in-situ* bioremediation of contaminated sites.

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