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Meshfree PCM and PSO Model for *in-situ* Bioremediation of Groundwater

Mategaonkar Meenal[1], Kamat Sahajanand[2], Meenal Mategaonkar[3]
[1, 2]*Assistant Professor, Department of Civil Engineering, NMIMS's MPSTME, Mumbai 400056, India*

Abstract: Analysis of groundwater stream, transport and remediation is an intricate procedure. This procedure can be comprehended with the help of Simulation based Optimization models. Simulation-Optimization (S/O) demonstrate consolidating meshfree Point Collocation Method (PCM) with Particle Swarm Optimization (PSO) optimization is an effective model for optimizing in situ bioremediation system design. This S/O demonstrate utilizes meshfree PCM model to simulate the subsurface power through pressure and bioremediation and PSO to scan for an optimal design. This methodology thinks about every single feasible parameter in one objective function. The investigation proposes a one-stage management approach with the thought of pumping/treatment, well establishment, and facility capital expenses alongside limiting the expense of a time-varying pumping strategy exploitation utilizing the optimal system. Applying the optimal time-varying pumping strategy in the one phase reduces pumping cost. The anticipated PCM-BIO-PSO-MO (PBPM) show are regularly viably utilized for the in-situ bioremediation design of contaminated sites.
Keywords: Groundwater pollution; In situ bioremediation; Simulation-optimization model; Meshfree Point Collocation Method; Particle Swarm Optimization

I. INTRODUCTION

In situ bioremediation for contaminated groundwater clean-up can be considered as a manageable remediation technology as a result of its cost proficiency and capacity to accomplish total decimation of natural contaminants. Bioremediation demonstrating comprises of solutions for biodegradation conditions and fixing the time of remediation. It additionally includes following the oxygen injection and extraction wells. High cost of designing and working groundwater remediation frameworks has propelled scientists to look at for and develop optimization strategies for discovering structures with the best execution (Akbarnejad-Nesheli et al., 2016)

A simulation/optimization (S/O) the management model, that incorporates a groundwater flow and transport simulation model installed in an optimization program, will encourage specialists to plan an in situ bioremediation framework that best fulfills the management objectives and management (Shieh and Peralta, 2005). Since the remediation of groundwater contamination could be a non-linear and complicated method, it is expected to build up a one phase multi-objective function for differed parameters like pumping rate, injection/extraction well areas and time of remediation along the edge of the expense of remediation.

Different numerical models are utilized for the simulation of groundwater pollutant transport and remediation issues. Numerical models are required for building up an efficient usable design and upkeep of in-situ bioremediation arrangement. S/O model will give the economical injection approach, proper places of wells for remediation and duration of remediation. The capacity of S/O models for bioremediation is approved by numerous analysts (Minsker and Shoemaker (1998), Yoon and Shoemaker (2001), Prasad and Mathur (2008), Mategaokar and Eldho (2012c), and so forth.)

Meshfree (MFree) methods got acknowledgment in various engineering issues attributable to their meshfree character. Pre-processing time of simulation is condensed because of the removal of grid. Working in higher dimensions does not expand the complexity and computational expense of the technique in view of the simplicity in computing the distances in any degree of spatial dimensions, (Liu, 2003, Liu and Gu, 2005; Liu, 2006). Mugunthan et al. (2005) showed that function approximation methods could be a more efficient alternative to heuristic and derivative□based strategies for automatic calibration of computationally costly bioremediation models. MFree strategies are developed coupled flow and transport model successfully to groundwater flow and transport problems by many investigators (Li, et al., 2003, Praveenkumar and Dodagaudar, 2008, 2010). Mategaonkar and Eldho (2012a, b) developed coupled flow and transport model for groundwater and applied it to different theoretical and field contextual analyses. Mategaonkar and Eldho (2012c, 2018) also witnessed that the PCM-BIO-PSO display is a successful model for in situ bioremediation of groundwater pollution. Parno et al. (2012) applied surrogate PSO to improve the effectiveness of PSO for simulation based problems. Mategaonkar and Eldho (2014) likewise developed a multi-objective model for pump and treat method for the remediation of total dissolved solids (TDS). Kazemzadeh-Parsi (2015,a,b) built up a coupled simulation– optimization solution approach, in view of the finite element method (FEM) and a modified firefly calculation (MFA), for contaminated groundwater remediation design.

In this study an S/O model PCM-BIO-PSO-MO (PBPM) based on the coupled Meshfree Point Collocation Method (MFree-PCM) and Particle Swarm Optimization (PSO) is proposed for *in situ* bioremediation.

A. Governing Equations And Boundary Conditions

The following scheme of equations (Freeze and Cherry, 1979; Borden and Bedient, 1986; Mategaonkar and Eldho, 2012c) can be used in the simulation.

$$\frac{1}{S_y}\nabla\left(K\nabla h\right)-\partial_t h \pm Q - q - = 0 \qquad (1)$$

According to Darcy's law,

$$v_x = -K_x\left(\partial_x h\right); v_y = -K_y\left(\partial_y h\right) \qquad (2)$$

$$\partial_c t - \frac{1}{R_c}\left(\nabla(D\nabla c - vc) - M_t \frac{\mu_{\max}}{R_c}\left(\frac{c}{K_c + c}\right)\left(\frac{O}{K_o + O}\right)\right) \qquad (3)$$

$$\partial_c t - \frac{1}{R_c}\left(\nabla(D\nabla O - vO) - M_t \frac{\mu_{\max}}{R_c}\left(\frac{c}{K_c + c}\right)\left(\frac{O}{K_o + O}\right)\right) \qquad (4)$$

The symbols used in the above equations are given in Table 1.

Table 1: Symbols of the parameters

Symbol	Parameter	Symbol	Parameter
K_x	Hydraulic conductivities in the x direction	K_y	Hydraulic conductivities in the y direction
h	Piezometric head	S_y	Specific yield
v_x	Velocity in x direction	v_y	Velocity in y direction
Q_w	Flow rate from the well	q	Volume rate of steady uniform recharge per unit area per unit thickness of the aquifer
n_e	Porosity	c	Contaminant concentration
M_t	Total microbial concentration	$\mu_{\max}$	Maximum contaminant utilization rate per unit mass of microorganisms
K_c	Contaminant half saturation constant	K_o	Oxygen half saturation constant
M_t	Concentration of microbes	O	Oxygen concentration
Δt	Time interval	F	Ratio of oxygen to contaminant consumed
R_c	Retardation coefficient	D_{xx}	Dispersion coefficient x direction
D_{yy}	Dispersion coefficient y direction		

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Actual velocity is obtained as $V_x = v_x / n_e$ and $V_y = v_y / n_e$. For the above stated 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 normally used boundary conditions are: $h(x,y,t) = h_1(x,y,t)$; $c(x,y,t) = g_1$; $T\frac{\partial h}{\partial n} = q_1(x,y,t)$ and $\partial/\partial x(D_{xx}\partial O/\partial x)n_x + \partial/\partial x(D_{yy}\partial O/\partial y)n_y = g_2$ for $x, y \in \Gamma$; 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.

B. Meshfree model preparation for 2D 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 and Gu, 2005; Mategaonkar and Eldho, 2012c)

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

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

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

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 and Gu, 2005). First and second derivatives of the shape function with respect to x and y are calculated as given in Mategaonkar and Eldho (2012a, b). Forward finite difference scheme is adopted for time discretization. Therefore, from Equations (1) - (4) we get (Mategaonkar and Eldho, 2012c),

$$\left([K_1] - \frac{\Delta t}{R_c}\left((D_{xx})[K_3] + (D_{yy})[K_5]\right)\right)\{c_i\}^{(t+\Delta t)} = \left(\begin{array}{l}\left([K_1] - \frac{\Delta t}{R_c}\left((V_x)[K_2] + (V_y)[K_4]\right)\right)\{c_i\}^t - \\ \frac{\Delta t}{R_c}\left(M_t \mu_{max}\left(\frac{[K_1]c_i^t}{K_c + [K_1]c_i^t}\right)\left(\frac{[K_1]O_i^t}{K_o + [K_1]O_i^t}\right)\right)\end{array}\right) \tag{6a}$$

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

… (6b)

Where,

$[K_1]$ - global matrix of shape function

$[K_2]$ - global matrix of first derivative of shape functions with respect to x

$[K_3]$ - global matrix of second derivative of shape functions with respect to x

$[K_4]$ - global matrix of first derivative of shape functions with respect to y

$[K_5]$ - global matrix of second derivative of shape functions with respect to y

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.

Two dimensional MFree model for groundwater transport is developed based on above formulation. The developed transport and bioremediation equations were verified using attainable analytical and numerical solutions (Mategaonkar and Eldho, 2012a, b, c). Further an efficient model with PCM-BIO model for bioremediation simulation is developed. To simulate the passage of pollutant and oxygen in the subsurface in aerobic bioremediation, Eq. (6a) and (6b) are solved simultaneously.

C. PSO Based Optimization Model

Particle swarm optimization (PSO) is a stochastic optimization populace based strategy developed by Dr. Eberhart and Dr. Kennedy in 1995. It simulates the social behavior of bird flocking or fish schooling. In PSO, each solution is a "bird" in the hunt space called as a "particle". All particles have fitness values which are evaluated by the fitness function to be delicate, and have velocities which direct the drifting of the particles. The particles fly through the problem planetary by following the recent optimum particles. The 'particles' are the numerical speculations, involving three fundamental components: location, velocity and fitness. Location signifies the obscure variable of the Location, velocity characterizes the rate of change of location and the fitness is a degree to solve the objective function optimally. The PSO concept includes acceleration of individual particle toward its pbest and lbest spots. Acceleration is biased by a arbitrary term that splits random numbers being induced for acceleration to pbest and lbest positions (Parsopoulos et al., 2001).

$$m^i{}_{k+1} = m^i{}_k + n^i{}_{k+1} \quad (7a)$$

with velocity calculated as:

$$n^i{}_{k+1} = wn^i{}_k + c_1 r_1 (p^i{}_k - x^i{}_k) + c_2 r_2 (p^g{}_k - m^i{}_k) \quad (7b)$$

Where, $m^i{}_{k+1}$ is the updated position; $m^i{}_k$ is the particle position; $n^i{}_{k+1}$ is the updated velocity; $n^i{}_k$ is the particle velocity; $p^i{}_k$ is the best "remembered" individual particle position; $p^g{}_k$ 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.

D. Simulation Optimization (S/O) model

For getting the optimal result of *in-situ* bioremediation of subsurface water, simulation model PCM-BIO is coupled with the PSO optimization model and PCM-BIO-PSO-SO (PBPS) is developed. Optimal cost consists of fixed costs and variable costs. Fixed costs involve injection/extraction well installation costs, injection facility cost and treatment facility cost however pumping cost is the variable cost. The objective function is given as (Minsker and Shoemaker, 1998, Sheih and Peralta, 2005):

Minimize
$$Z = \left(\sum_{i=1}^{N} C^{IP}(i) IP(i)\right) + \sum_{t=1}^{T}\left\{\frac{1}{(i+i_r)^{ty_p}} \sum_{i=1}^{N} A\sqrt{1+Q_i^{2}}\right\} + \left\{D\left(\sum_{i=1}^{Ni} P(i,t)\right) + E\left(\sum_{i=1}^{Ne} P(i,t)\right)\right\}_{t=1}^{T} \quad (8)$$

Where, $C^{IP}(i)$ is the cost of installation of injection or extraction well at location *i* ($ per well); *IP (i)* is zero one integer for injection or extraction well existence at location; i is the node number; A is the relative cost coefficient; Q_i is the injection rate in

m^3/day; i_r is the discount rate; t is the stress period ; y_p is the duration of stress period; $P(i,t)$) is the injection or extraction rate at location i ; $D\left(\sum_{i=1}^{Ni} P(i,t)\right)$ is oxygen and nutrient injection facility capital cost, a function of total injection rate ($); $E\left(\sum_{i=1}^{Ne} P(i,t))\right)$ is the treatment facility capital cost, a function of total extraction rate ($);T is total number of stress periods; Ni is total number of injection wells; Ne is total number of extraction wells and $N = Ni + Ne$.
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 is 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.

In the present study, an attempt is made to get optimal solution for *in situ* bioremediation of contaminated groundwater with respect to cost, number of injection wells and duration of remediation in one stage using one objective function. Concentration and oxygen distribution is analyzed for the entire remediation period.
The set of constraints considered are

$$c_m < c' ; h_{\min} \le h_i \le h_{\max}; 0 \le t < t_{\max} \text{and } 0 \le Q_i < Q_m \tag{9}$$

where, c_m and c' are the maximum and the stated limit of concentration, respectively anyplace in the aquifer; $h_{\min}$ and $h_{\max}$ are the least and maximum head, respectively anyplace 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 covers the cost of setting up of injection well, injection or extraction rate at location the duration of stress period, oxygen and nutrient injection facility capital cost and the number of wells. Based on the above formulation, the PCM-BIO-PSO-MO (PBPM) model is developed. Parameters c_1 and c_2 are not critical for PSO's convergence. However, 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 0.6-1.2. 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 and population size is taken as 100 in this study.

E. Model Development

PBPM model is developed for the optimal design of *in situ* bioremediation of polluted groundwater. It includes two simulation models i.e. coupled flow and transport model and biodegradation model using meshfree PCM along with optimization model using PSO. For the system design some assumptions are made. In this study, aerated oxygen containing 8 ppm of concentration of oxygen is considered (Hinchee et al. 1987; Minsker and Shoemaker, 1998). Further, it is assumed that the microorganisms are present in the substantial amount in the aquifer for bioremediation. Also, the biomass growth rate is assumed to be equal to the rate of decay ensuring the aboriginal nature of biomass.
The flow chart for the PBPS model is shown in Fig. 1. Primarily, all physiological and hydrological parameters are given as input. An aquifer is discretized into equidistant nodes in x and y directions. A rectangular support domain for each node is considered.

An initial population is generated for transport and oxygen equations. PSO parameters like c_1, c_2 and w are initialized. Randomly all particle positions are also initialized. The values of position velocity, local best and global best are calculated for all particles. Objective function is calculated taking into consideration all the above parameters. The system of equations for transport and oxygen is solved using PBPS with all the constraints. If the objective is achieved (reaching minimum cost) then it is stopped else the particles' positions and velocities of particles are updated and the objective function is evaluated again. Procedure is repeated till the end of the remediation time. Optimal pumping rates and costs are noted. PBPS model is applied to get an optimal solution in one stage in an attempt to reach the contamination level to 5ppb or less. The developed PBPS model is applied to a hypothetical problem and substantiated with the results of S/O model based on BIOPLUME II and Parallel Recombinative Simulated Annealing (PRSA).

F. Case Study

The application of PBPM model is investigated by considering a case study which is similar to a field problem (Fig.2). The aquifer is spread over approximately 690 m x 510m with a thickness of 15 m. From pumping and flow rate, the aquifer parameters are determined and the location of contaminant plume is identified. The average groundwater velocity in the area is about 0.1 m/day. The maximum contamination concentration is about 20 ppm. The adopted design should optimize the system to remediate the plume to drinking water standard of 5ppb (Hazen and Fliermann, 1995). The physical and hydrogeological parameters for this case study are given in Table 2 (Shieh and Peralta, 2005). The Northern and Southern boundaries are no flux boundaries. Western boundary is with constant head 35.5 m and at the Eastern boundary is 27.7 m. Hydraulic conductivity is $6x10^{-5}$ m/s and gradient is 0.004. Groundwater flow is from West to East. The dispersivity values are 10m and 2m respectively in longitudinal and transverse direction.

G. Application of PBPM Model

The case study, as mentioned above, is analyzed with the model. In the PBPS model, 391 nodes are considered (Fig. 2). $\Delta x = \Delta y = 30m$ and $\Delta t = 1$. The value of Cs is taken as 90 with the α_c value as 3 and for every square support domain 9 nodes are considered. The nodal assembly for the PBPS model, position of injection, extraction and monitoring wells are shown in Fig. 2.

The injection wells are provided at nodes 111,127, 128, 129, 145 and 162. The rates of injection are varying from 0–1.26 Lps for the simulation. For S/O model, $h_{\min}$ is preferred in such a way that it does not drop below the top of the aquifer while $h_{\max}$ is selected so as to guarantee that the rise in the hydraulic head is equivalent to most potential drawdown. Original contaminant strength in the plume ranges from 1-20 ppm. The initial oxygen concentration is five ppm except within the contaminant plume space, where the oxygen concentrations have been consumed by aerobic biodegradation. The vertical exchange of oxygen with the unsaturated zone is assumed to be inconsequential. The injected oxygen concentration is 8 ppm. The adopted method should remediate the plume to drinking water standard of 5ppb. The concentration levels in the investigated nine observation wells are shown in Fig. 2. In this study, hydraulic heads at every node ought to be lower than hydraulic heads at every node ought to be lower than $h_{\max}$ and higher than $h_{\min}$ (Refer Table 1).

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II. RESULTS AND DISCUSSION

With the temporal interval of one day, the model is run for three years with the management period of one year. The cost coefficients are given in the Table 2. (Shieh and Peralta, 2005). The injection coefficient is based on the oxygen, nutrient and pumping operation costs. The extraction cost coefficients consider the cost of treating and pumping contaminated groundwater. Treatment includes air stripping and granular activated carbon. Injection and capital costs are based on their capacities.

In all the cases, it is observed that PBPM gives optimal cost of 1.92E+05$ for four wells with three injection wells at nodes 111,127,129 and one extraction well at node 230. The optimal solution is shown in Fig. 3.This cost is compared with other evolutionary algorithms like Simulation Annealing (SA), Genetic algorithm (GA) and Parallel Recombinative Simulated Annealing (PRSA) models and it is found that it is in line with these models and lies in between GA and PRSA. The comparison is given in Table 4.

A. Time varying pumping strategy

For better groundwater management, it is essential to minimize injection, extraction, treatment and facility cost which are eventually the functions of flow rates. As per the finding of Shoemaker and Minsker (1998) time varying strategy works better than steady pumping for effective *in situ* bioremediation. Similar findings were seen in Shieh and Peralta (2005). In this study, the model is developed for one stage management through time varying approach with the management periods of one year. It is found that PBPS is having good comparison with PRSA. The combined results are shown in Fig. 4 and the contamination plume after three years is shown in Fig. 5.

In single objective PSO, cost optimization is done by considering injection/extraction rates where fixed costs are not considered (Mategaonkar et al., 2012 c). However there are some more parameters like number of wells, time of remediation, initial fixed costs are to be considered for optimal solution for *in-situ bioremediation*. Mategaonkar et al. (2018) also developed a single objective model where number of wells and time of remediation are considered as different scenarios along with cost optimization for *in situ* bioremediation. In this paper, all the costs and objectives are included in one equation making it multi-objective which performs better than the single objective approach.

III. CONCLUSION

S/O model helps in providing solution for optimal remediation of groundwater. In this study, a meshfree simulation model dependent on PCM is proposed for in situ bioremediation. Likewise a PSO optimization model is developed for optimization. PCM is an modest method to work with and apply. With the suitable selection of shape parameters, the model delivers competent outcomes. The PCM models are further coupled with multi-objective PSO founded optimization methods and PBPM model is developed for in-situ bioremediation of groundwater contamination to get proficient and optimal solution for the complex remediation problem. In this study, the PBPM model is applied to a hypothetical case study for in-situ bioremediation with some static costs and variable costs. The proposed model is compared and other algorithms like SA, GA and PRSA and it is seen that it is competitive with these robust methods and can be meritoriously utilized in the in-situ bioremediation of contaminated sites.

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A. List of Tables

B. List of Figures

Table 2: Physical parameters for the case considered

Parameter	Value
Contaminant	Tri-chloro-ethylene (TCE)
Size	690m x 510m
Thickness of aquifer	15m
Hydraulic conductivity	6 x 10^{-5} m/s
Porosity	0.3
Retardation factor	1
Longitudinal dispersivity	10m
Transverse dispersivity	2m
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)	33.5m
Minimum injection hydraulic head(h_n)	27.7 m
Water quality standard, $c_{\max}$	5 ppb

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Table 3: Cost Function Coefficients (Shieh and Peralta, 2005)

Coefficient	Value
i_r (Discount rate)	0.05
C^{IP} (Installation cost)	12,000 $
C^P for injection cost (Oxygen, Nutrient and pumping operation)	4755 $ (LPS-Year)
C^P for extraction cost (Treatment and pumping operation)	15,850 $ (LPS-Year)
D (Injection facility cost for 1.26 -8.83 LPS)	20,000-44,000 $
E (Treatment facility capital cost for 1.26-8.83 LPS)	30,000-70,000 $

Table 4: Optimal Systems from SA, GA, PRSA and PBPM

Optimization algorithm	Well installation cost ($)	Injection cost ($)	Extraction cost ($)	Injection facility capital cost ($)	Treatment facility capital cost ($)	Total Cost ($)
SA	60000	36200	43100	28000	30000	1.97E+05
GA	48000	38100	52400	28000	30000	1.97E+05
PRSA	48000	37600	44900	28000	30000	1.89E+05
PBPM	48000	37700	48704	28000	30000	1.92E+05

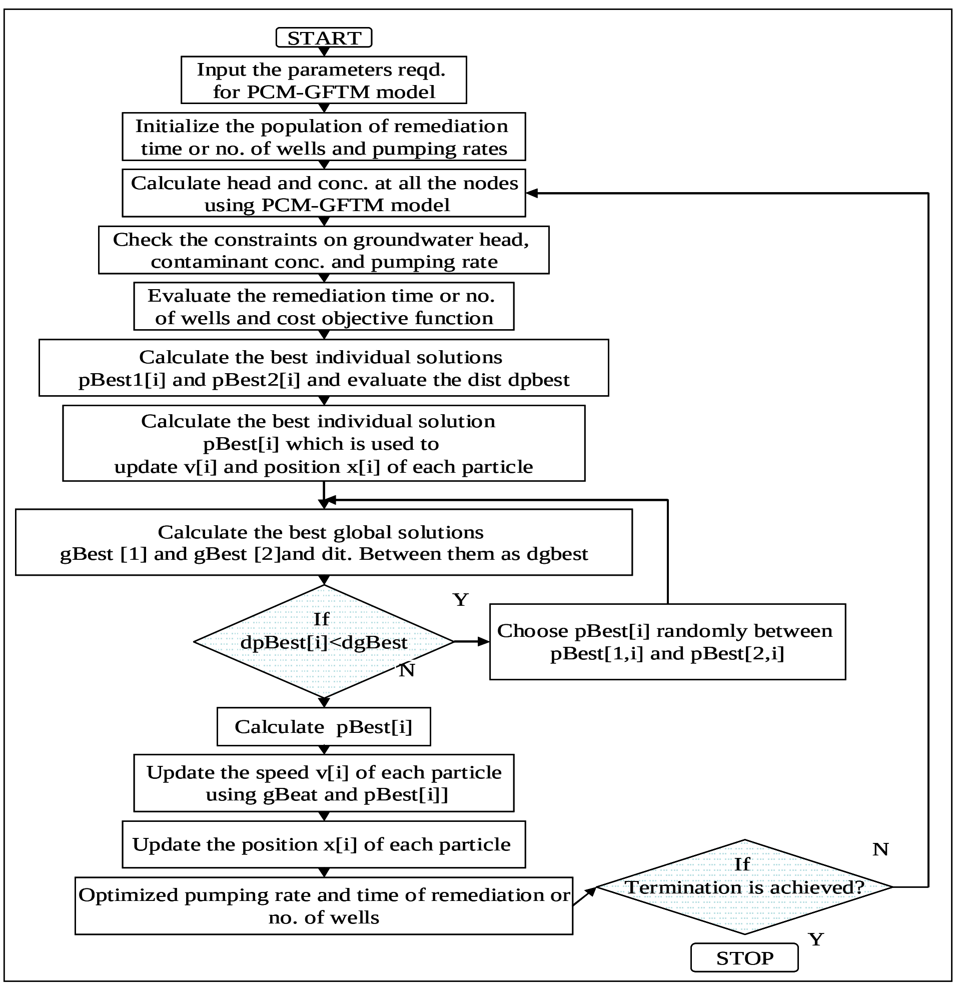


Fig.1. Flow chart of PCM-BIO-PSO-MO (PBPM) model

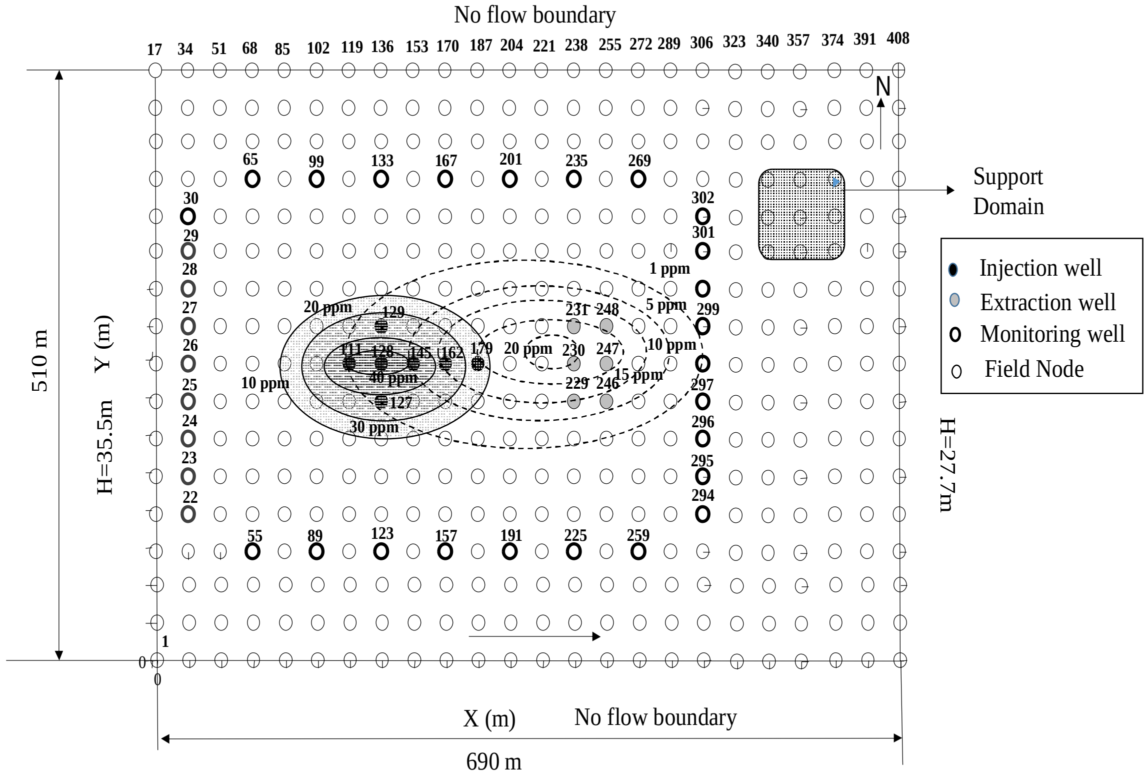


Fig.2. Schematic representation of aquifer

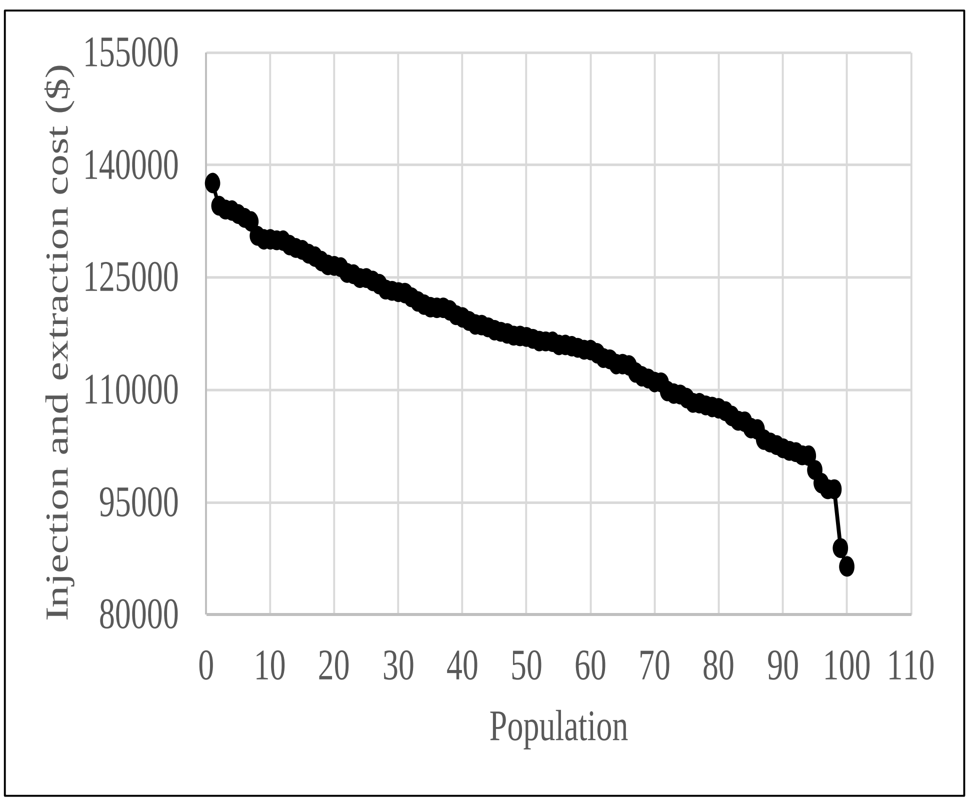


Fig. 3: Optimal cost for injection and extraction ($)

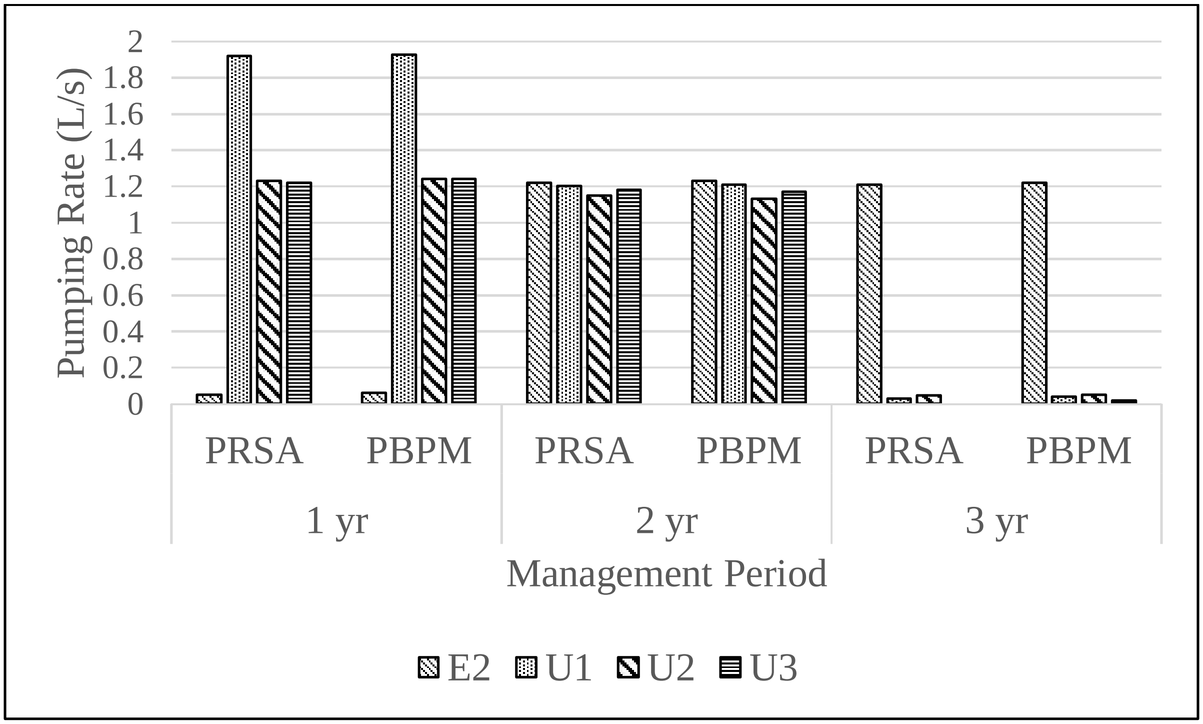


Fig.4. Time varying Pumping Strategy

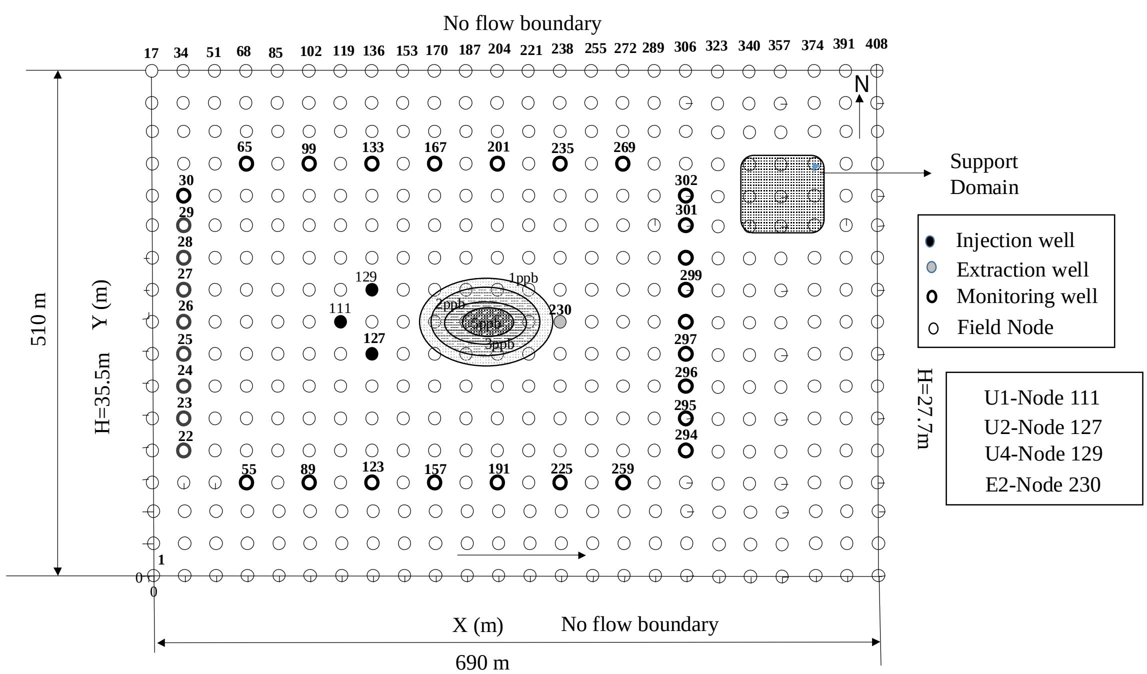
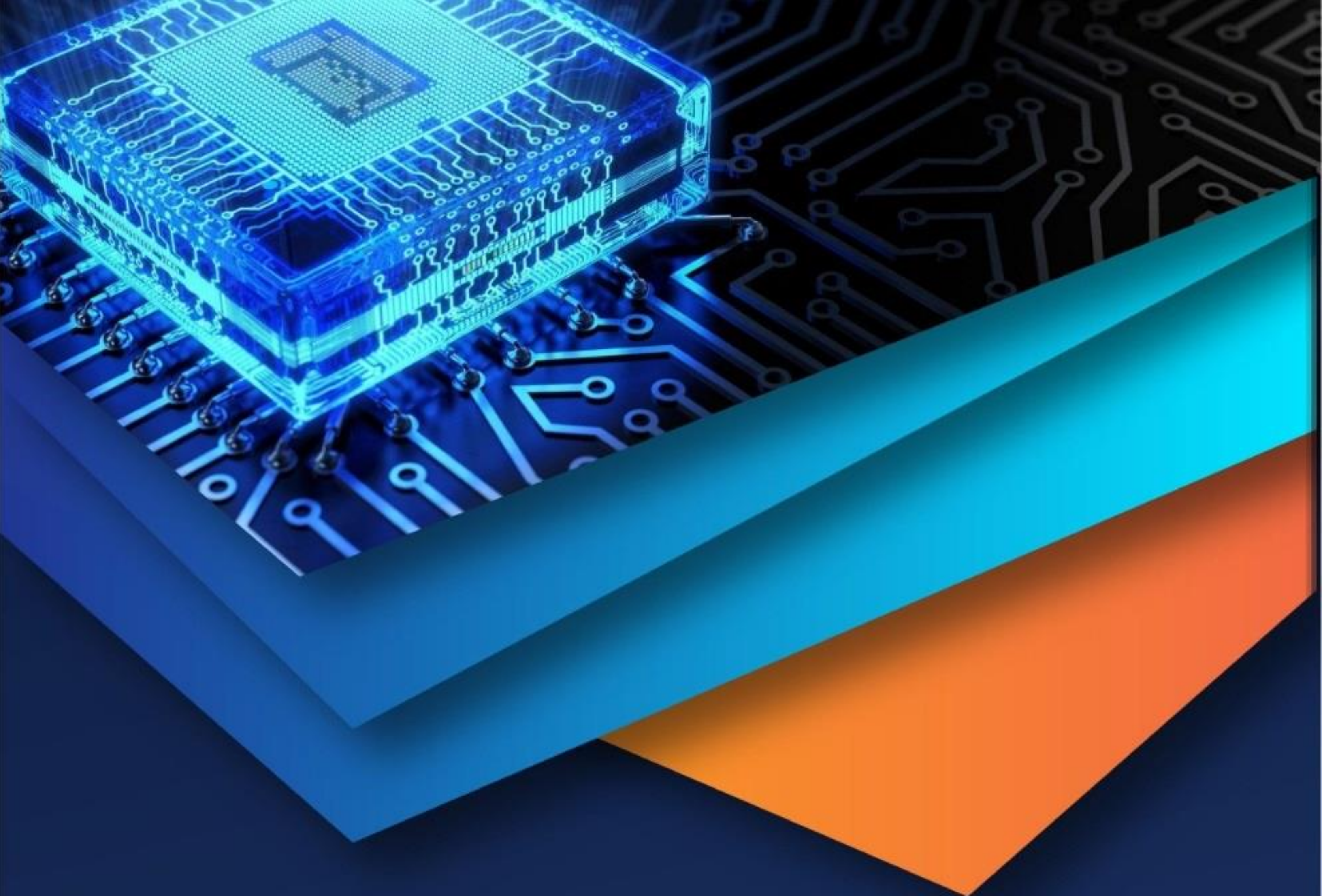


Fig.5. Contaminant plume after *in situ* bioremediation (after 3 years)



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