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Aquifer Decontamination Studies Using a Meshfree Point Collocation Method (PCM)

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Abstract

Groundwater contamination is a major problem in many parts of the world. Generally, the complex problem of groundwater and its contamination can be studied by solving the governing equations of flow and transport by using numerical methods such as Finite Difference Method (FDM), Finite Element Method (FEM) or Boundary Element Method (BEM). While using FDM or FEM, a grid or mesh has to be formed over the domain and their connectivity has to be checked carefully. Meshfree (MFree) method is an alternative numerical approach to solve the complex groundwater problems by simple and accurate manner. MFree method uses a set of nodes scattered within the problem domain and on the boundaries of the domain. In this method, the governing equations and equations for boundary conditions are directly discretized at the field nodes using simple collocation techniques to obtain a set of discretized system equations. In this paper, a MFree point collocation method (PCM) with radial basis function (RBF) is used for the coupled groundwater flow, contaminant transport simulation and decontamination in porous media. The concentration distribution in the system from the simulation results is considered as initial condition for the decontamination strategies for aquifer system. The simulation is carried out to study the effects of decontamination strategies like flushing and pumping effects with a Total Dissolved Solids (TDS) contaminated hypothetical aquifer. It is found that the flushing along with pumping is an effective remediation strategy. The study shows that MFree PCM is a simple method to simulate coupled groundwater flow and contaminant transport and for remediation studies. It saves the time for pre-processing such as meshing or remeshing.

Keywords: Aquifer, Groundwater Flow, Contamination Transport, Meshfree Point Collocation Method, Decontamination.

1. Introduction

Groundwater contamination is a major problem in many parts of the world and it has become a very a serious issue as the contaminated water puts everyone at risk for potential health problems. The level of contamination and vast variations of the contamination make it nearly impossible to determine the exact potential for health threats. Once an aquifer is contaminated, it is nearly impossible to decontaminate to a satisfactory level. Moreover aquifer decontamination process is very time consuming and costly affair. Due to the non-linear nature of the groundwater pollutant transport problem, numerical methods are a must to solve the flow and transport problem. The main idea in most of the numerical simulation is to transform a complex practical problem into a simple discrete form of mathematical description, recreate and solve the problem on a computer numerically, and represent the phenomena virtually according to the requirements of the modeler. It is often possible to get a numerical or approximate solution as long as proper numerical method is used. Many researchers and engineers tried to solve the complex problem of groundwater flow and transport by grid based methods such as Finite Difference Method (FDM) or Finite Element Method (FEM). While using FDM or FEM, a grid or mesh has to be formed over the domain and their connectivity has to be checked carefully.

Since last decade, meshfree methods have gained popularity in many engineering applications due to their mesh-free character and easy extension to higher dimensions (Liu, 2003). In most of the MFree methods, a set of nodes scattered within the problem domain as well as on the boundaries of the domain to represent the problem domain and its boundaries is used, regardless of the connectivity information between them. Since there is no grid, the time one would spend on meshing and remeshing (pre-processing) can be saved. This can lead to substantial cost and time savings when solving large scale field problems. In the last two decades of development in the MFree techniques, number of MFree methods have been formulated by mathematicians and researchers. Kansa (1990) used Multi –Quadrics (MQ) as the spatial approximation scheme for parabolic, hyperbolic and the elliptic Poisson's equation and showed that MQ is an extremely accurate approximation scheme for interpolation and partial derivative estimates for a variety of two-dimensional functions over both gridded and scattered data. Later on, this idea was extended to various types of problems by Franke and Shaback (1997), Hon and Mao (1998), Hon et al.(1999), Hon and Shaback (2001), Wu and Hon(2003), Khattak and Siraj (2008) and Mategaonkar and Eldho (2011a,b and 2012a,b). The choice of radial basis functions is a flexible feature of meshfree methods. Many researchers like Li et al.(2003), Liu(2006), Praveen Kumar and Dodagoudar (2008), Mategaonkar and Eldho (2011a,b and 2012a,b) investigated and found that MFree methods are simple and very effective in solving complex groundwater problems. In this study, the meshfree models are developed for groundwater flow and transport problems using point collocation method (PCM). Further, the developed models are applied for the decontamination study of a confined aquifer problem.

2. Governing Equations and Boundary Conditions

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

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

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.

Following initial conditions are used for transient flow analysis

$$h(x,y,0)=h_0(x,y) \qquad x,y\in\Omega \qquad (2)$$

Generally, the boundary conditions can be of two types, the prescribed head or flux. It can be written as,

$$h(x,y,t)=h_1(x,y,t) \qquad x,y\in\partial\Omega_1$$

$$T\frac{\partial h}{\partial n}=q_1(x,y,t) \qquad x,y\in\partial\Omega_2 \qquad (3)$$

where, h_0 and h_1 are the known head values and q_1 is the known flux value. Here, $\partial\Omega$ 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).

According to Darcy's law,

$$v_x = -K_x \frac{\partial h}{\partial x}\,;\; v_y = -K_y \frac{\partial h}{\partial y} \tag{4}$$

where 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. Actual velocity is obtained as $V_x = v_x / n_e$ and $V_y = v_y / n_e$, where, n_e is the porosity.

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

$$R\frac{\partial c}{\partial t} = \frac{\partial}{\partial x}\left(D_{xx}\frac{\partial c}{\partial x}\right) + \frac{\partial}{\partial y}\left(D_{yy}\frac{\partial c}{\partial y}\right) - \frac{\partial}{\partial x}(V_x c) - \frac{\partial}{\partial y}(V_y c) - \frac{c'W}{n_e b} - R\lambda c \tag{5}$$

where, D_{xx}, D_{yy} are the components of dispersion coefficient tensor [L^2T^{-1}]; c is the dissolved concentration [ML^{-3}]; λ is the reaction rate constant [T^{-1}]; W is the elemental recharge rate with solute concentration c'; n_e is the local porosity; t is the time; b is the aquifer thickness under the element and R is the retardation factor.

The initial conditions used are:

$$c(x, y, 0) = f \qquad x, y \in \Omega \tag{6a}$$

The boundary conditions used are:

$$c(x, y, t) = g_1 \qquad x, y \in \Gamma_1 \tag{6b}$$

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

where, f and g_1 are the known concentrations and g_2 is the known concentration gradient

3. PCM- flow and transport model (PCM-GFTM) Formulation

For the simulation of groundwater flow, it is required to solve Eq. (1). The formulation for groundwater flow equation, PCM-flow (Mategaonkar and Eldho, 2011a,b), is used to obtain the head distribution in the domain considered. The PCM-flow model is coupled to the PCM-transport model to get PCM-GFTM (Mategaonkar and Eldho, 2012a, b) model to simulate the groundwater flow and transport in an aquifer.

For the PCM based models, the first step is to define the trial solution $\widehat{h}(x, y, t)$ and $\hat{c}(x, y, t)$ as,

$$\widehat{h}(x, y, t) = \sum_{i=1}^{n} h_i(t) R_i(x, y) \tag{7}$$

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

where, 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; Kansa, 1990). The shape function is given as:

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

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 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 shape function ($R_i(x,y)$), the first derivatives ($(\partial R_i(x,y)/\partial x),(\partial R_i(x,y)/\partial y)$) and second derivatives ($(\partial^2 R_i(x,y)/\partial x^2)$ and $(\partial^2 R_i(x,y)/\partial y^2)$) are to be calculated for each support domain (Mategaonkar and Eldho,2011,2012) and then they are incorporated in the global matrix for the whole problem domain, with consideration of Kronecker delta property. The final form of the PCM-flow model with source or sink terms is:

$$\left([K_1]-\left(\frac{T\Delta t}{S}\right)([K_2]+[K_3])\{h_i\}^{(t+\Delta t)}\right)=[K_1]\{h_i\}^{(t)}\pm\left(\left(\frac{\Delta t}{S}\right)[K_1]\{Q_w\}\right) \tag{10}$$

The final form of PCM-transport model is:

$$\begin{aligned}&\{[K_1]-\Delta t((D_{xx})[K_3]+(D_{yy})[K_5])\}\{c_i\}^{(t+\Delta t)}\\&=\{[K_1]-\Delta t((v_x)[K_2]+(v_y)[K_4])\}\{c_i\}^{(t)}+\Delta t[K_1]\{c_2\}\end{aligned} \tag{11}$$

Where, $[K_1]$ is the global matrix of shape function; $[K_2]$ is the global matrix of first derivative of shape functions with respect to x; $[K_3]$ is the global matrix of second derivative of shape functions with respect to x; $[K_4]$ is the global matrix of first derivative of shape functions with respect to y; $[K_5]$ is the global matrix of second derivative of shape functions with respect to y and $\{Q_w\}$ is the global matrix of the entire source and sink terms and $\{c_2\}$ is the known value of the contamination from ponds or recharge wells. The respective value of contamination is considered for all the nodes that lie in the support domain where that pond or recharge well lies.

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. After the unknown head values are found, the velocities at nodes are found by using Darcy's law and further the system of equation is solved by Gauss Jordan method.

4. PCM-GFTM Model Development

The PCM flow models for confined and unconfined aquifers and solute transport models are coupled together so that flow and transport model (PCM-GFTM) is developed (Mategaonkar and Eldho, 2012a, b). The steady state and transient state head distribution are calculated from the flow models. Then using the Darcy's law, velocities at all the nodes are calculated. This velocity is used for the transport model and then simulation of concentration distribution is carried out. The detailed steps of the model are given below.

The values of transmissivity, porosity, storativity, dispersivity and details of the area are taken from the source data. For the numerical accuracy, the grid spacing and time step is chosen to ensure that the Peclet number is less than 2 and Courant number is less than 1(MacQuarrie et al., 1990). The equidistant nodes are added in the aquifer domain and on the boundary. For every node in the domain, one support domain is to be constructed. For every support domain, the values of shape function $R_i(x,y)$, its first and second derivative with respect to x and y are calculated and then they are incorporated in the global matrices for the whole problem domain. The nodes lying on the boundary should be assigned the values as per the Dirichlet or Neumann boundary conditions. For transport model, the initial concentration at all the nodes is considered to be zero.

As per the Eq. (1), the head values at all the nodes at the next time step are calculated. The velocities at nodes are calculated using the Eq. (4). Using these velocities, the concentration at all the nodes in the aquifer are calculated using Eq. (5) after application of boundary conditions. The procedure is repeated until the prescribed total simulation time is reached. For successive time steps, the head and concentration values from the previous time steps are used as initial conditions. The PCM based flow model and transport model are verified with the available analytical solutions (Mategaonkar and Eldho, 2012a,b).

5. Case Study

Once the aquifer is contaminated, it is very difficult to clean or decontaminate to satisfactory levels. To decontaminate an aquifer, the commonly used techniques include: self cleaning (only natural process), flushing the aquifer by recharging with pure water and pumping out the contaminated water of the aquifer. In this study, the decontamination strategies of: flushing; and pumping and flushing together are considered for aquifer decontamination. To study the effectiveness of PCM model to analyze the decontamination strategies, here a hypothetical case study in 2D is considered. Fig. 1 shows the confined aquifer considered. There is a pond on the West side, recharging the aquifer at a rate of 0.009 m/d. Also, there are 2 recharge wells located (Fig. 1) recharging at a rate of 0.009 m/d. Both pond and well is contaminated by TDS with 1000ppm

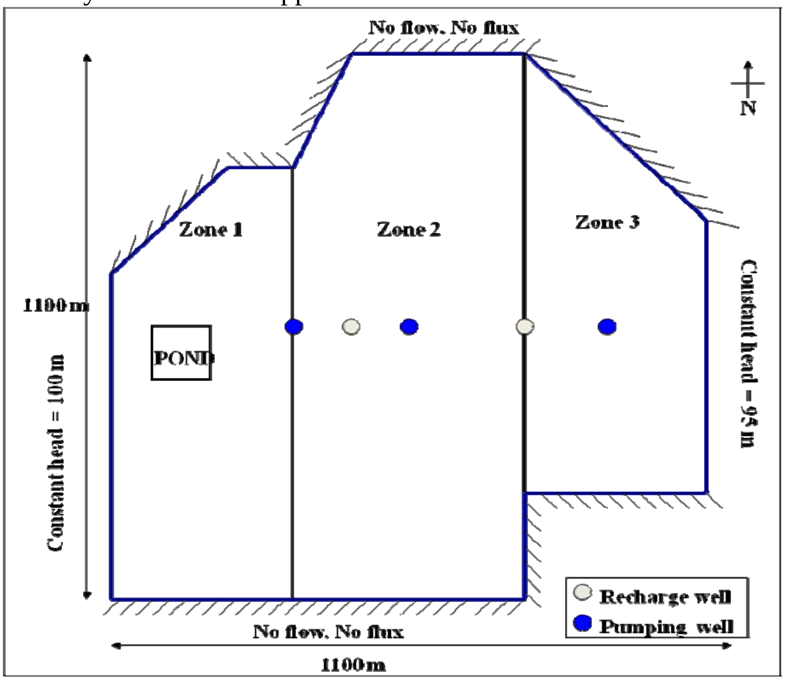

Fig. 1: Schematic representation of aquifer (for decontamination study)

The input data for the problem considered is given in Table 1. The boundary conditions for the problem considered are: constant head on the Western side as 100 m; constant head on Eastern side as 95m. Specific storage is 0.004 and the average depth of ground surface to datum is 40m.

Table 1: Parameters for the aquifer problem considered

Properties	**Zone 1**	**Zone 2**	**Zone 3**
Transmissivity T_x (m^2/d)	500	450	300
Transmissivity T_y (m^2/d)	400	300	250
Porosity	0.3	0.3	0.3
Longitudinal dispersivity (m)	220	220	220
Transverse dispersivity (m)	20	20	20

The Northern and Southern boundaries are considered as no flow boundaries. The aquifer is contaminated by TDS due to recharge from pond. Initially the problem is simulated by PCM-GFTM model. The number of nodes is taken as 110 with 9 nodes in the support domain (see Fig.2). The value of *Cs* is considered as 300 and the time step of 1 day is considered. The maximum concentration of TDS near to pond is 995.87 ppm. During the simulation process, the system was affected by various sources like seepage from the polluted pond, concentration entering from the recharge wells and the abstraction wells pumping at a rate of 500 m^3/d (Fig. 1). Using the PCM model, the flow and transport in the aquifer is simulated for 5 yrs. The concentration distribution in the system is identified from the simulation results as shown in Fig.3

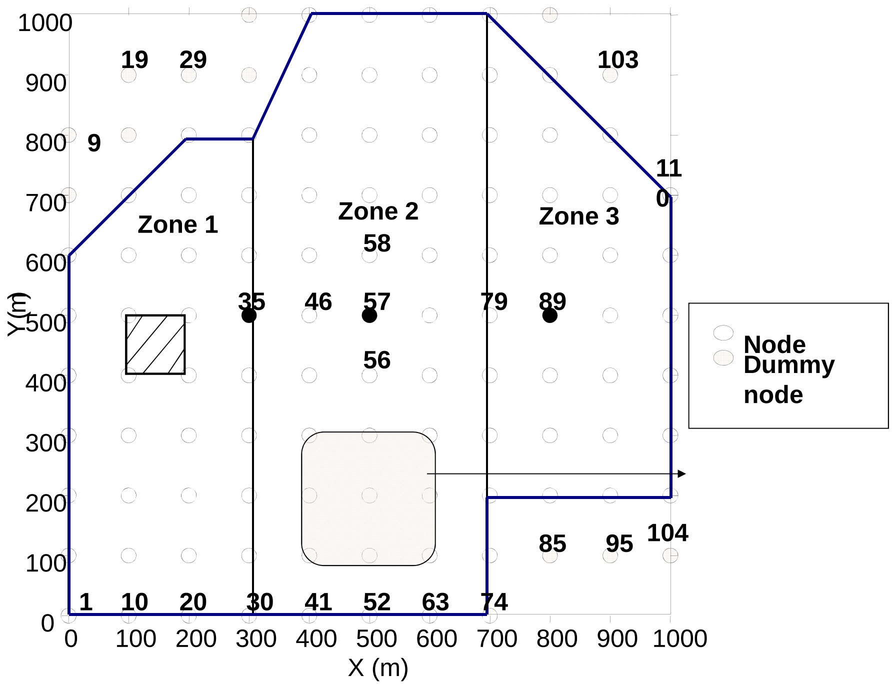

Fig. 2: Nodal arrangement in aquifer (for decontamination study)

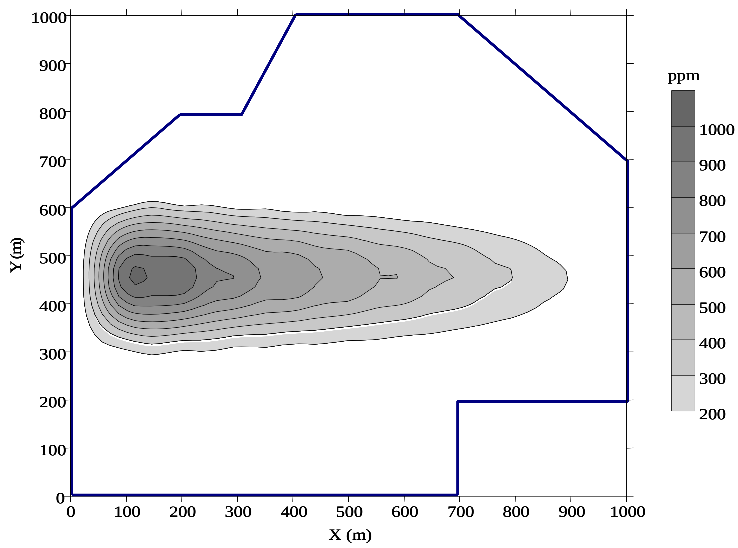

Fig. 3: Initial concentration in the aquifer (after 5 yrs of pollution)

6. Strategies for Ddecontamination of Aaquifer

The concentration distribution at the end of 5 years is considered as initial conditions for the remediation of the aquifer system and it is assumed that contamination is stopped and remediation process is undertaken. In this study, for cleanup of the contaminated aquifer, two decontamination alternatives have been considered. These include: (1) decontamination by flushing and (2) decontamination by combination of flushing and pumping. In an aquifer contaminated by pollutants, if the source of the pollutants is removed, alternatively entry of the pollutants to the aquifer is stopped, then the pollutants move away and the decontamination process takes place in the aquifer with the natural flow process. It is assumed that from the beginning to a specified period, the contamination process is going on. At a particular time, the contamination source is removed and the resulting concentration movement is analyzed using the PCM model.

6.1 Aquifer decontamination by flushing

The alternative considered here is to clean up the contaminated aquifer by flushing through the recharge pond and wells with pure water at the same rate of seepage (0.009m/d) for the flow field. The condition at the end of 5 years of pollution (Fig. 3) is considered for cleaning. During the decontamination process of 3 years, the pumping wells are not in operation. The progress of the aquifer decontamination by flushing for 3 years is shown in Fig 4.

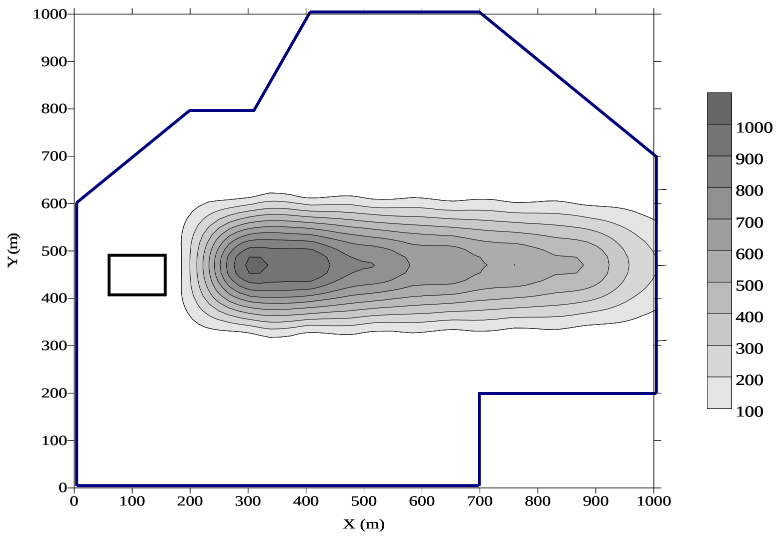

Fig. 4: Concentration distribution after flushing

Based on the results obtained in this remediation alternative, it is observed that the area of 700 ppm plume in the aquifer is reduced from 0.28 Km^2 to 0.11 Km^2 within 3 years. The area of the plume is reduced in this alternative, as the plume moves towards the right side of the aquifer due to flushing. The cleaning process can be enhanced if the flushing rate is increased. The cleanup time in this alternative mainly depends on the rate of recharge from the pond.

6.2 Aquifer decontamination by flushing and pumping

The second decontamination strategy considered is combination of flushing and pumping. Here the aquifer was flushed by recharging with clean water from the pond with a rate of 0.009 m/d. With reference to the plume location, here the three pumping wells are considered (nodes 35, 57 and 89) extracting contaminated water at the rate of 700, 500 and 300 m^3/d (Fig. 2). Here it is assumed that the recharging wells are not in operation. The concentration contours after flushing and pumping for 3 years is shown in the Fig. 5. Based on the results obtained here, it is observed that the area of 700 ppm plume in the aquifer is reduced from 0.28 Km^2 to 0.088 Km^2 within 3 years. It could be possible that if the rate of recharge/pumping is increased, the cleanup time will be reduced.

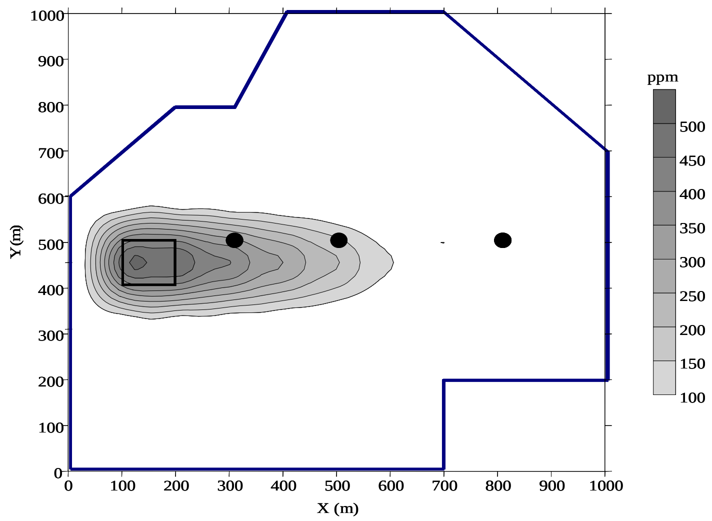

Fig. 5: Concentration distribution after pumping and flushing

6.3 Discussion

For the considered confined aquifer, two decontamination alternatives are considered to clean up the aquifer. The aquifer was polluted due to seepage from a polluted pond and a polluted recharge wells. The system is simulated for a period of 5 years to find out the concentration distribution in the aquifer system. After 5 years, the 700 ppm plume occupied in an area of 0.28 Km^2. By considering 3 years of decontamination by flushing, the area of 700 ppm plume is 0.11 Km^2 in flushing. In the second method (pumping and flushing), the maximum extent of plume in the system is nearly 0.088 Km^2 area. The concentration at nodes 35, 57 and 89 after 3 years for all the strategies is plotted and shown in Fig. 6.

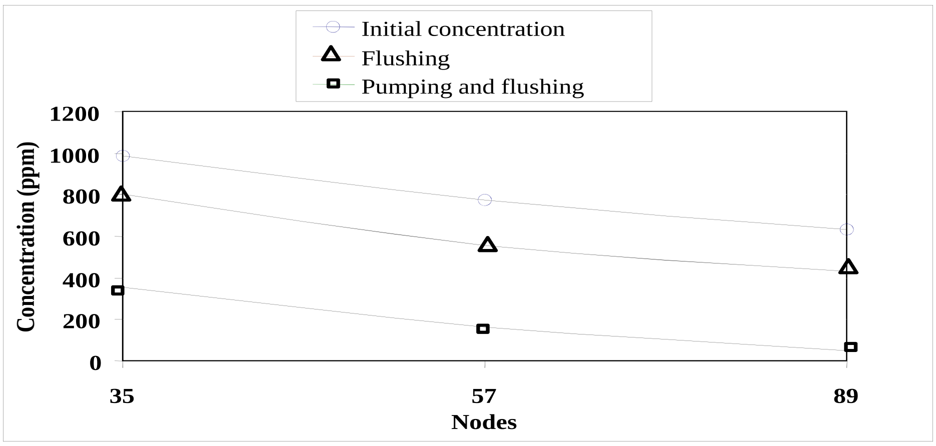

Fig. 6: Concentration distribution for all decontamination strategies after 3 years at some nodes

Further considering 6 years of decontamination, the area of plume is reduced to 0.09 Km^2 in flushing and the plume is reduced to 0.031 Km^2 in the case of pumping and flushing. For the problem considered, Table 2 and Table 3 show the contaminant spread area after 3 years and 6 years of simulation. Based on the performance of the two decontamination methods, it is possible to identify the best strategy to reduce the concentration level in the system.

Table 2: Effectiveness of decontamination strategies (after 3 years)

Strategy	**Initial spread area of 700 ppm plume (Km^2)**	**Spread area of 700 ppm after 3 yrs. of remediation (Km^2)**
Flushing	0.28	0.11
Flushing and pumping	0.28	0.088

Table 3: Effectiveness of decontamination strategies (after 6 years)

Strategy	**Initial spread area of 700 ppm plume (Km^2)**	**Spread area of 700 ppm after 6 yrs. of remediation (Km^2)**
Flushing	0.28	0.09
Flushing and pumping	0.28	0.031

Based on the performance of the two decontamination methods, it is possible to identify the necessary strategy to reduce the concentration level in the aquifer system depending on the problem condition. Using the pump and flushing option, after 3 years of decontamination period, the effect of the plume on the system is insignificant. In other words, the system has become nearly free from contamination. The results have shown that the best strategy that can be considered in the present case is the combination of flushing and pumping alternative.

7. Concluding Remarks

In this study, the coupled flow and transport models using Meshfree Point Collocation Method are used for the investigation of decontamination strategies of a contaminated confined aquifer. Two decontamination strategies investigated include: flushing; and pumping and flushing together. The decontamination strategies are investigated for a hypothetical problem. The effectiveness of the self cleaning depends upon natural groundwater flow velocities and recharge from the pond. If favorable hydraulic gradients are produced contaminated plume may move away from the pond to the desired region. Decontamination by pumping depends upon rate of pumping, location of pumping wells and contamination properties. The contamination spread can be controlled with the effectiveness of these parameters. For better decontamination, the pumping wells will have to be located at the location of maximum concentration which can be predicted using the PCM-GFTM model.

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