

OPTIMAL GRONDWATER MONITORING NETWORK DESIGN FOR POLLUTION PLUME ESTIMATION WITH ACTIVE SOURCES

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ABSTRACT

A new methodology has been developed to design optimal monitoring network to estimate the transient pollution plume resulting from active pollution sources in a contaminated aquifer. An optimization algorithm is linked with geostatistical kriging model as well as a numerical simulation model. Simulated annealing is used as the optimization tool. The physical process in the aquifer, i.e., the flow and contaminant transport processes are numerically simulated using numerical groundwater flow and transport simulation models. The spatial extrapolation of measured and simulated concentration is performed by using geostatistical estimation based on Kriging. The objective is to minimize the mass estimation error. The developed methodology is evaluated for an illustrative study area.

Keywords: Groundwater Monitoring Network Design, Groundwater Pollution Detection, Simulated Annealing, Kriging.

1 INTRODUCTION

Groundwater, under most conditions, is safer and more reliable for use than surface water. Groundwater may also be contaminated by some of the common activities which cause groundwater contamination like: illegal and unmonitored injection of pollutants in the aquifer, leakage from underground tanks and pipelines carrying sewage and other toxic contaminants, insufficient knowledge about the application of pesticides and fertilizers in agricultural fields, land disposal of wastes etc. The detection of groundwater contamination is difficult as it is not openly visible unlike surface water systems. A groundwater model can have two distinct components: (i) groundwater flow and (ii) groundwater contaminant transport components. The modeling of the groundwater systems include information about many hydrogeological parameters which have spatial and temporal variability and are highly complex in nature. These uncertainties in the groundwater may be intrinsic and informal. The first one is due to the variability of certain natural properties or processes and is irreducible such as recharge rate, hydraulic conductivity, porosity and dispersion coefficient etc. The second one is due to noisy or incomplete information.

For effective management of groundwater aquifer, monitoring is necessary for contaminant plume detection. The uncertainties involved in the prediction of plume movement and an economic constraint to limit the number of monitoring well

installations necessitates the design of an optimal monitoring network design. A methodology is developed for time varying optimal network design under uncertainty. A surrogate budgetary constraint is used to limit the number of monitoring wells to be installed in a particular management period.

Few examples of past attempts to develop methodologies for optimal design of a groundwater monitoring network are reported in: [1], [2], [3], [4], [5], [6] and [7].

Simulated Annealing (SA) is used as the optimization algorithm in our study. SA is used to solve the combinatorial optimization algorithm. The method of simulated annealing is a more flexible and generally applicable heuristic optimization technique and efficient in locating global optimal solutions. This method of optimization has been used successfully for large scale applications in groundwater [8]. This optimization algorithm is chosen for its efficiency in achieving a global optimal solution.

2 METHODOLOGY

The kriging linked SA model has three main components: (a) a groundwater flow and transport simulation, (b) a global mass estimation using Geostatistics, and (c) optimization using SA.

2.1 Groundwater flow and transport simulation

The equation describing the transient, two dimensional areal flow of groundwater through a

non – homogeneous, anisotropic, saturated aquifer can be written in Cartesian tensor notation [9] as:

$$\frac{\partial}{\partial x_i} \left(T_{ij} \frac{\partial h}{\partial x_j} \right) = S \frac{\partial h}{\partial t} + W; \quad i, j = 1, 2 \quad (1)$$

where

T_{ij} = transmissivity tensor (L^2T^{-1}) = $K_{ij}b$; K_{ij} = hydraulic conductivity tensor (LT^{-1}); b = saturated thickness of aquifer (L); h = hydraulic head (L); W = volume flux per unit area (LT^{-1}); x_i, x_j = Cartesian coordinates (L). In this study the flow model is simulated using MODFLOW (1996).

The partial differential equation describing the fate and transport of contaminants of species k in 3D, transient groundwater flow systems can be written as follows [10]:

$$\frac{\partial(\theta C^k)}{\partial t} = \frac{\partial}{\partial x_j} \left(\theta D_{ij} \frac{\partial C^k}{\partial x_j} \right) - \frac{\partial}{\partial x_i} (\theta v_i C^k) + q_s C_s^k + \Sigma R_n \quad (2)$$

Where

θ = porosity of the subsurface medium, dimensionless; C^k = dissolved concentration of species k , ML^{-3} ; t = time, T; $x_{i,j}$ = distance along the respective Cartesian coordinate axis, L; D_{ij} = hydrodynamic dispersion coefficient tensor, L^2T^{-1} ; v_i = seepage or linear pore water velocity, LT^{-1} ; it is related to the specific discharge or Darcy flux through the relationship, $v_i = q_i / \theta$; q_s = volumetric flow rate per unit volume of aquifer representing fluid sources (positive) and sinks (negative), T^{-1} ; C_s^k = concentration of the source or sink flux for species k , ML^{-3} ; ΣR_n = chemical reaction term, $ML^{-3}T^{-1}$. MT3D (1999) has been used as the contaminant transport simulation model for this study.

2.2 Geostatistics

Ordinary kriging (OK) is the most commonly used variant of the simple Kriging (SK) algorithm. Kriging (SK or OK) has been performed to provide a “best” linear unbiased estimate (BLUE) for unsampled values [11]. Different semivariogram models are used in the kriging which are selected by performing a sensitivity analysis using different sets of parameters. For this study spherical variogram model was selected and the package provided by [12] GSLIB (1998) was modified to estimate the plume concentration at all the unsampled locations within the study area.

2.3 Optimization Algorithm: Simulated Annealing

The optimization algorithm used for the design of the monitoring network is based on Simulated Annealing. Annealing is the cooling process of molten metals. At high temperature atoms with high energy move freely and when the temperature is reduced get ordered and finally form crystals having minimum possible energy. The SA parameters-temperature reduction factor, initial temperature, number of function evaluations for termination criteria are based on the sensitivity analysis as well as guidelines available in the literature [13] and [8].

3 OPTIMIZATION MODEL FORMULATION

The objective is to determine the optimal set of the monitoring locations for which the normalized mass estimation error is minimum, while constraining the total number of monitoring wells [14].

In the first step of the proposed methodology, before applying the monitoring network design model to the field, it is essential to have a calibrated flow and transport model for the study area. The simulation model is used to simulate the contaminant scenario of the site from initial time to some expected time t_n . It is assumed to represent the future conditions to be monitored using the given initial conditions, boundary conditions, flow and transport parameters, contaminant source characteristics, and potential monitoring locations. The simulated concentration value at the potential monitoring locations are assumed to be known, and these known values of the contaminant concentrations are used to construct the contaminant plume using spatial extrapolation.

In the second step, the concentration values at the potential monitoring wells and their coordinates are used to randomly generate the specified number of the groundwater monitoring well design plans, given as a maximum permissible number of wells in that particular analysis. In the third step the optimization process starts with the given sets of the initialized parameters. At a given iteration, the SA algorithm chooses a subset of monitoring locations from the set of potential locations. This subset is then used as an input to the kriging model which estimates the mass of the contaminant based on the set provided by the SA. All these different sets are evaluated for the objective function and the algorithm terminates when the final function value at the current temperature differs from the current optimal function value by less than error tolerance of

termination, and the optimal design set is evolved fulfilling the constraints.

4 MODEL APPLICATION

The size of the illustrative study area is 2800m x 2700m. The study area for illustrative application of the proposed monitoring network models are discretized into identical grids of 100m x 100m, as shown in Fig. 1.

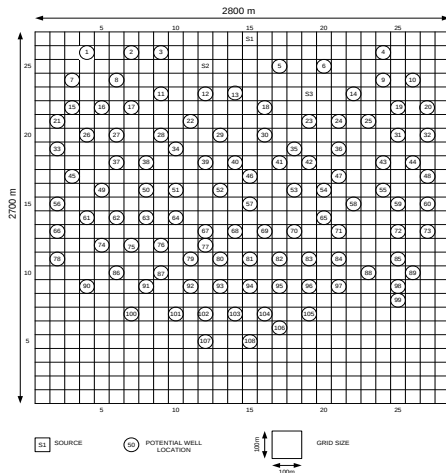


Fig. 1 Illustration of study area showing its physical parameters and potential monitoring well locations

The study area is assumed to have three continuous sources each with an injection mass flux of value 27.4 g/s. The injection rate of the contaminant sources are assumed to be 45m³/day, which is approximately half liter per second. One hundred eight potential observation wells are distributed in the area, for possibly collecting the concentration data in all management periods.

Sensitivity analysis has been performed on Simulated Annealing model and Kriging model to find out the best sets of parameters utilized for the linked optimal model [14] (Singh, 2008).

4.1 Performance Evaluation

The performance of the proposed methodology is evaluated for the illustrative study area for a specified contamination and management Scenario.

4.1.1 Scenario 1

The study area as shown in Fig. 1 is considered as the aquifer which is unconfined, homogeneous and isotropic in nature. All the flow and transport parameters remain constant over time. The recharge rate, pumping rate, and boundary conditions change with time. Contaminant sources are continuous, and mass flux rate is constant over time for all the

sources. Three contaminant sources S1, S2, S3 and 108 potential monitoring well locations are considered. The monitoring network is designed for a management period of one year duration. Each 1 year management period is divided into two time intervals. Total mass estimate based on concentration values simulated at the end of the one year management period at the specified 108 potential monitoring locations constitute an input to the kriging linked SA model. The objective function which minimizes the mass estimation error is utilized for solution of the model.

Table 1 gives the mass estimation error in percentage with the optimal number of wells as 35, 45, and 55, respectively. The error decreases with the increase in maximum permissible number of wells. This is expected, and it can be seen that the contaminant mass estimation error is not varying much from 45 to 55 wells.

Table 1 Number of wells and their corresponding mass estimation error in percentage in Scenario 1

No. of wells	Mass Estimation Error in %
35	0.2322
45	0.0021
55	0.0018

Figs. 2, 3 and 4 show the optimal locations of the 35, 45 and 55 wells respectively. The well locations chosen as solution of the design model are spatially spread over the study area. The performance in terms of the mass estimation errors as shown in Table 1 can be judged as satisfactory. However, the order of the mass estimation errors decreases with 35 to 45 and 55 optimal monitoring locations.

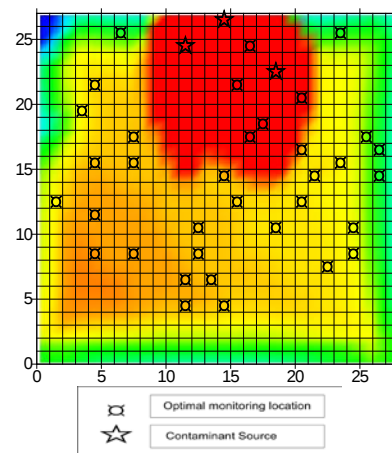


Fig. 2 Optimal location of monitoring wells for design set of 35 wells in Scenario 1

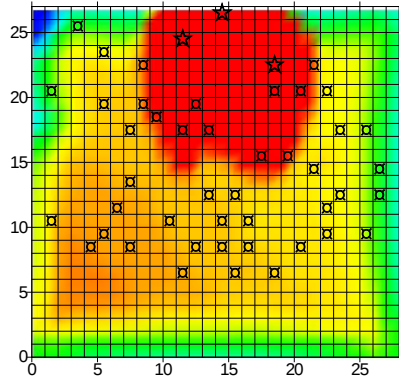


Fig. 3 Optimal location of monitoring wells for design set of 45 wells in Scenario 1

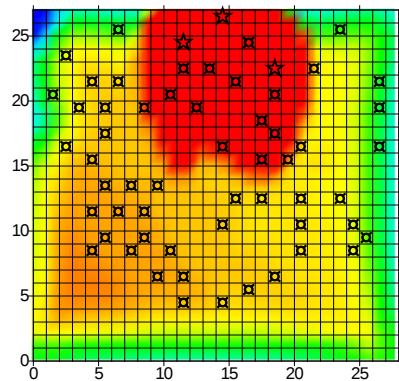


Fig. 4 Optimal location of monitoring wells for design set of 55 wells in Scenario 1

4.1.2 Scenario 2

All the conditions are same as in Scenario 1 except with the modifications in the contaminant source strength is considered uncertain. The mean contaminant source strengths are specified as 52608.0 mg/l. Uncertainties in terms of percentage are incorporated on the source concentration. Uncertainties in the source strength are incorporated by specifying a range of values for the source strengths. The range of upper bound and lower bound are shown in Table 2. These lower bound and upper bounds are utilized to generate different realizations of the source concentration using a uniform distribution. Ten realizations are generated from the uniform distribution for each of the sources. The simulation of the concentration plumes is performed for all 10 sets realizations. The mean concentration values at all the 108 potential monitoring locations obtained for these 10 realizations are utilized for spatial estimations of the concentration over the entire study area by kriging. This total contaminant mass estimate based on a number of realizations of the contaminant plume is used as input to the kriging linked SA model.

Monitoring design model is solved to obtain the optimal monitoring network design.

Table 2 Range of contaminant source strengths for Scenario 2

Uncertainty Level	Lower Bound in mg/l	Upper Bound in mg/l
10 %	47347.2	57868.8
20 %	42086.4	63129.6
30 %	36825.6	68390.4

For each of the uncertainty levels the optimal design set is obtained for 35 wells, 45 wells and 55 maximum number of permissible wells. Fig. 5 shows that for each set of wells, the mass estimation error increases with increase in the uncertainty level. The error values are compared with the values obtained for Scenario 1 without uncertainty. Fig. 6 also shows that the mass estimation error decreases as the number of monitoring wells increases. These values are also given in Table 3.

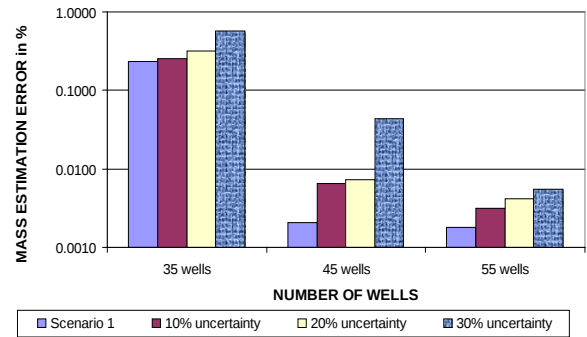


Fig. 5 Comparison of contaminant mass estimation error for Scenario 1 and 2

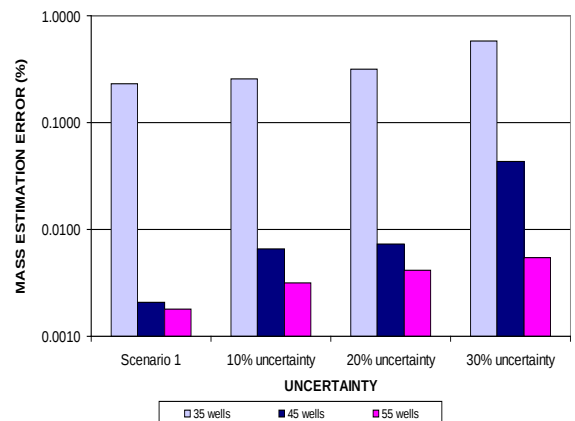


Fig. 6 Comparison of mass estimation errors with different levels of uncertainty

Table 3 Mass Estimation Error in percentage for Scenario 2

No. of Wells	Uncertainty			
	Scenario 1	10 %	20 %	30 %
35	0.2322	0.2541	0.3139	0.5772
45	0.0021	0.0065	0.0073	0.0431
55	0.0018	0.0031	0.0042	0.0054

For the optimal design set of 35 wells the level of error is very high as shown in the Table 3. Some of the locations are common to all these designs. It can be noted from Table 3, that the mass estimation errors decrease with the increase in total number of monitoring wells, and it increases with the increase in the level of uncertainty in estimating the contaminant sources and therefore, the total mass of the contaminant. The optimal monitoring design locations for the different maximum permissible number of monitoring wells are shown in Figs. 7. (a), (b); Figs. 8. (a), (b); and Figs. 9. (a), (b). These Figures show the variations in the designed networks for different permissible number of monitoring wells.

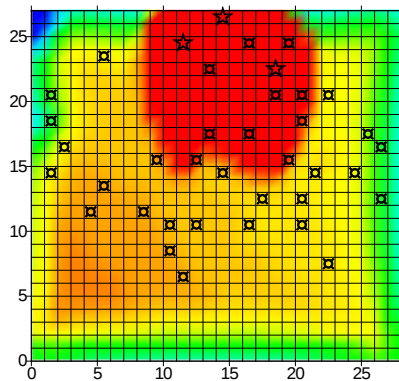


Fig. 7 (a) 10% uncertainty

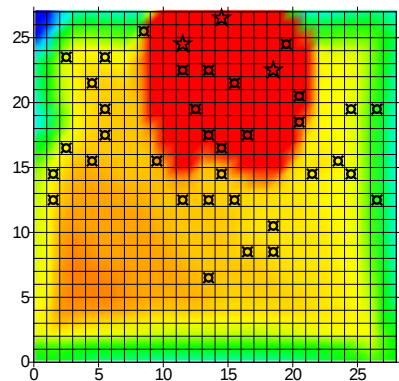


Fig. 7 (b) 30% uncertainty

Fig. 8 Optimal monitoring locations for 35 monitoring wells with different uncertainties levels in Scenario 2

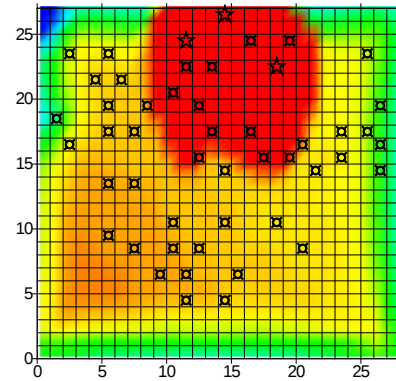


Fig. 8 (a) 10% uncertainty

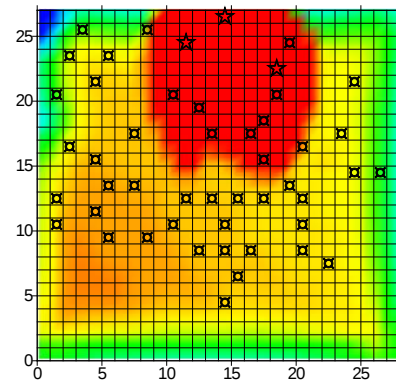


Fig. 8 (b) 30% uncertainty

Fig. 9 Optimal design locations for 45 monitoring wells with different uncertainties in Scenario 2.

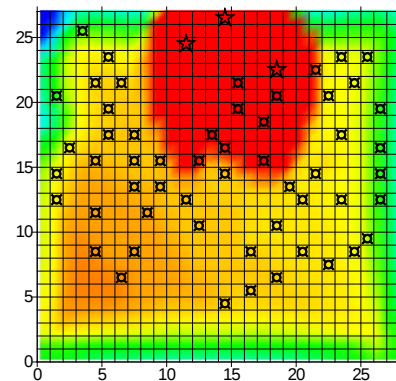


Fig. 9 (a) 10% uncertainty

5. CONCLUSIONS

Proposed groundwater monitoring network design models are solved for an illustrative study area with different scenarios. The solution results are primarily useful for evaluation of the performance of the proposed models. These results appear to be consistent with intuitive solutions and therefore acceptable.

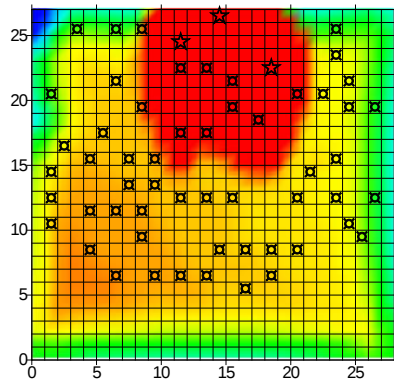


Fig. 9 (b) 30% uncertainty

Fig. 9 Optimal design locations of 55 monitoring wells with different uncertainties in Scenario 2

However, much more rigorous performance evaluations may be necessary to establish the applicability of the proposed methodologies. These performance evaluation results appear encouraging. The utility and feasibility of using a kriging model for spatial estimation of variables with an optimization algorithm i.e. Simulated Annealing is demonstrated. These solution results show the potential applicability of this approach for optimal design of groundwater contamination monitoring networks, including dynamic network design.

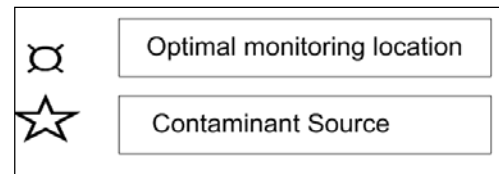
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CONVENTION FOLLOWED FOR FIGURES



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