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Application of Multi-objective Optimization Techniques on Optimal Groundwater Remediation Design

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Abstract*—Aquifer parameters such as hydraulic conductivity, effective porosity and hydraulic head etc. play significant roles in groundwater remediation and management systems. They generally comprise multiple often conflicting objectives. This paper proposes a multi-objective groundwater remediation and management methodology based on pump-and-treat technology to determine optimal strategies for cleaning up the affected portion of a contaminated aquifer. Two objectives are considered namely (i) minimization of remediation cost and (ii) maximization of clean water extraction rate. Multi-objective optimization code NSGA II is employed along with MODFLOW and MT3DMS to obtain a remediation cost-extraction tradeoff. The Pareto front thus obtained consists of several optimal solutions to the problem. Sensitivity analyses on some important input parameters have been carried out to account for the effects of variability of these parameters on the model result.

Index Terms*—groundwater remediation, pump-and-treat, multi-objective optimization, Pareto front.

I. INTRODUCTION

Groundwater is one of the major natural resources that supply drinking water for human beings. Therefore, remediation of contaminated aquifers and development of appropriate management systems which include both groundwater quantity and quality management problems, are important from several aspects and deserve to draw great interests to researchers specializing in this field. The pump-and-treat method (P&T) is one of the most commonly used groundwater remediation methods. In this method a number of wells installed at several predefined locations of the affected aquifer and remove the contaminated water through extraction wells and treat it onsite, The treated water can either be injected back into the aquifer or it can be safely or it may be used agricultural purposes. P&T method has been extensively employed in the design of optimal groundwater remediation systems by many researchers by using Simulation-optimization technique. Major optimization approaches used for designing such systems include linear programming [1] non-linear programming [8], dynamic programming [4], genetic algorithms [11], multi-objective evolutionary algorithms [13]. Majority of these studies use a single objective for achieving a certain goal, such as, minimization of remediation cost, maximization of clean-up, minimization of risk to health etc. These works are mostly applied to the remediation of 2-dimensional aquifers affected with a single contaminant.

But real world groundwater remediation problems generally involve multiple conflicting objectives. Remediation designs dealing with multiple objectives and applied to 2-dimensional aquifers affected by multi-species contaminants are rarely found in the literature. In this work MODFLOW 2000 and MT3DMS 5.0 are coupled with NSGA-II for obtaining a set of optimal pump-and-treat groundwater remediation and management systems. The optimization problem under study has two conflicting objectives: (i) minimization of the total remediation cost and (ii) maximization of clean water extraction rate.

The variability of aquifer physical parameters, such as hydraulic conductivity, porosity etc. is ubiquitous. Owing to the inherent spatial variability of these parameters, design of an optimal groundwater system by any method encounters major difficulties. Sensitivity analyses are carried out to study the influence of variations in the values of some important aquifer parameters on the optimal remediation design.

II. MATERIALS AND METHOD

Groundwater flow is simulated by MODFLOW 2000 while contaminant transport is simulated by MT3DMS 5.0. NSGA II is used to solve the multi-objective optimization problem. A hypothetical 2-dimensional aquifer is used in the study. Sensibility analyses are carried out on three important aquifer properties. Explanations of the methodology are given in the following sections.

A. *Groundwater Flow Model*

MODFLOW 2000 (Harbaugh et al., 2000) is a computer program used to solve 2-dimensional flow of groundwater. It uses Finite Difference Method for solving the flow equation described by the partial differential equation (1) both for steady state and transient flow applications:

$$\frac{\partial}{\partial x}\left(K_{xx}\frac{\partial h}{\partial x}\right)+\frac{\partial}{\partial y}\left(K_{yy}\frac{\partial h}{\partial y}\right)-W=S_s\frac{\partial h}{\partial t} \qquad (1)$$

where K_{xx}, K_{yy} and K_{zz} are the values of hydraulic conductivities along the *x*, *y*, and *z* coordinate axes [LT^{-1}]; *h* is the hydraulic head [L]; S_s is the specific storage[L^{-1}]; *t* is the time [T]; W is the volumetric flux per unit volume and represents sources and/or sinks of water[T^{-1}].

B. *Contaminant Transport Model*

MT3DMS 5.0 (Zheng and Wang, 1999) is a modular three-dimensional multi-species contaminant transport model. It uses the hydraulic heads and sink/source terms generated by MODFLOW to simulate advection, dispersion, sink/source mixing, and chemical reaction in groundwater contaminant transport. The partial differential equation for

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describing three-dimensional contaminant transport in a aquifer system may be written as:

$$\frac{\partial C}{\partial t}=\frac{\partial}{\partial x_i}\left(D_{ij}\frac{\partial C}{\partial x_j}\right)-\frac{\partial}{\partial x_i}\left(v_i C\right)+\frac{q_s}{\theta}C_s+\sum_{k=1}^{N}R_k \qquad (2)$$

where D_{ij} is the hydrodynamic dispersion coefficient tensor [L^2T^{-1}]; x_i and x_j are the distances along the three-dimensional Cartesian coordinate axis directions [L]; C is the solute concentration in dissolved phase [ML^{-3}]; v_i is the average linear velocity [LT^{-1}]; θ is the porosity [dimensionless]; q_s is the volumetric flux of water per unit volume of aquifer representing sources (positive) and sinks (negative); C_s is the concentration of the source/sink flux[ML^{-3}]; t is the time [T]; $\sum_{k=1}^{N}R_k$ is the chemical reaction term [$ML^{-3}T^{-1}$]; and i and j are respective Cartesian coordinate axes.

C. *Multi-Objective Optimization*

Groundwater remediation problems generally have multiple conflicting objectives which require simultaneous optimization and are referred to as multi-objective optimization problems. Such a problem seeks a set of tradeoff solutions containing a large set of optimal solutions and provides a tradeoff curve known as Pareto front. The tradeoff curve provides the decision maker a variety of better-performing alternatives.

A multi-objective problem in its general form can be stated as:

min $f_m(x)$ *m= 1, 2, ……….M;*

subject to

$g_j(x)\geq 0$; *j=1, 2, …………J;*

$h_k(x)=0$; *k=1, 2, …………K;*

$x_i^{(L)}\le x\le x_i^{(U)}$; *i=1, 2, …………n;*

where M = the number of objectives to be optimized; J= the number of inequality constraints; K = the number of equality constraints; $x_i^{(L)}$ = lower bound of variable x_i ; $x_i^{(U)}$= upper bound of variable x_i; n = the number of decision variables; x_i = i^{th} decision variable.

Multi-objective optimization algorithms generally use the concept of Pareto domination. In these algorithms, two solutions are compared on the basis of whether one dominates the other solution or not (Deb, 2001). The concept of domination can be stated as one candidate solution dominates another only if it is at least equal in all the objectives and superior in at least one. The task of a multi-objective optimization algorithm is to determine a set of non-dominated solutions which constitute the Pareto front. A non-dominated solution is the one in which an improvement in one objective requires a degradation of another.

III. OPTIMIZATION MODEL FORMULATIONS

Groundwater is one of the major sources of drinking water. Every section of a society is directly or indirectly associated with groundwater. Remediation of contaminated groundwater involves input from several parties with multiple conflicting objectives. The application of multi-objective optimization for the design of an optimal remediation and management system is demonstrated in this work. The objective functions of the proposed optimization model are: (i) minimization of the total remediation cost and (ii) maximization of clean water extraction rate. Extraction rates and well locations are the decision variables of the optimization model. Constraints are imposed on hydraulic heads and contaminant concentrations at well locations. The model formulations are stated below:

$$\mathit{Min\ Cost}=G_{pump}+G_{carbon}+G_{capital}+G_{install}+G_{main} \qquad (3)$$

$$\min QC=\sum_{l=1}^{L}Q_l \qquad (4)$$

subject to

$$C_j\le C_{goal}\quad \forall j=1,2,.......N \qquad (5)$$

$$s_i\le s_{\max}\quad \forall i=1,2,........M \qquad (6)$$

$$M^*=\sum_{i=1}^{M}z_i \qquad (7)$$

where G_{pump} = pumping cost (\$), G_{carbon} = operational cost (\$) of the GAC treatment facility, and $G_{capital}$ = capital cost (\$) of GAC adsorbers; $G_{install}$ = installation cost of monitoring and/or pumping well (\$); G_{main} = maintenance cost of monitoring and/or pumping well (\$); C_j = contaminant concentration at the end of the remediation period at observation well j =1,2,….N (M/L^3); C_{goal} = water quality goal (M/L^3); s_i = drawdown at the end of remediation period at pumping well i (L). M = number of potential pumping wells installed;

Q_l = rate of extraction at well l (cum/day).

QC =total rate of extraction from L wells (cum/day).

$Cost$ = total remediation cost (\$).

z_i = installaition decision variable (binary). If z = 0, well is not installed and if z =1, well is installed.

t_{pd} = remediation time (days).

M^* = number of pumping wells installed.

L = number of wells from which uncontaminated water is extracted.

IV. FIELD SCALE APPLICATION

The coupled model is applied to a 2-dimensional hypothetical aquifer [Fig. 2]. The domain consists of a single layer, each of which is 15 m thick and is discretized into 570 finite difference blocks (each of size 50m × 50m). The hypothetical initial contaminant plume consisting of two chemical contaminant species and having a maximum concentration of 40 mg/l. The distribution coefficients for species 1 and species 2 are 0.245 cm^3/g and 0.0882 cm^3/g respectively. A steady flow toward the right boundary is manitained with a constant hydraulic head of 12 m and contaminant concentration of 0.0 mg/l on the left boundary, a constant hydraulic head of 0.0 m and contaminant concentration of 0.0 mg/l on the right boundary and no flow at the top and bottom boundaries. The aquifer is assumed to be homogeneous and confined. The contaminant plume is assumed to be developed in the middle layer. The concentration of each contaminant at these wells must not be greater than 0.5 mg/l at the end of the remediation period. Additional aquifer parameters are listed in Table 1.

Two existing wells (W19 and W20) downstream of the plume [Fig. 1] supply drinking water to the surrounding inhabitants. This study aims at developing several strategies via multi-objective optimization which are capable of achieving the clean-up level below the permissible contaminant concentration level by the end of a remediation period of five years and at the same time the supply of uncontaminated water through the existing two wells remains unaffected within the range from 900 m^3/day to 1700 m^3/day.

Table 1. Aquifer Parameters

Parameter	Value
Hydraulic Conductivity K (m/day) (layer 3)	18
Longitudinal Dispersivity α_L (m)	70
Transeverse Dispersivity α_T (m)	3
Porosity θ	0.2
Media bulk density ρ_b (g/cm^3)	2.12
Aquifer thickness b (m)	15

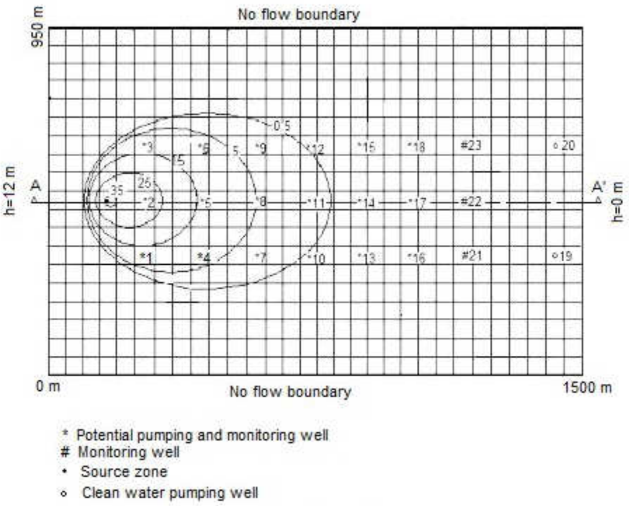

Fig. 1. Initial distribution of contaminant plume

Extraction rates of all pumping wells (W1 through W20) and locations of wells (W1 through W18) are the variables of the optimization problem. Two existing wells (W19 and W20) located at the unaffected portion of the aquifer are used to extract clean water. The locations of these two wells are on the downstream of the contaminant plume and remain unchanged. The lower and upper limits of extraction at each of these two wells are set to 450 and 850 m^3/day respectively. The NSGA II model provided a tradeoff between remediation cost and clean water extraction rate in the form a Pareto front as shown in Fig. 2. This feature of the Pareto front yielded a lot of insight into the model results because from the concept of non-domination, each of these points of the Pareto front represents an optimal alternative solution. Thus, out of these several alternative optimal solutions the decision maker or the analyst can conveniently choose the solution which is most appropriate to the prevailing conditions. This feature of multi-objective optimization algorithms is certainly an advantage over single-objective optimization routines because in order to obtain such a large number of solutions obtained from a single run by using a multi-objective optimization routine, a single-objective optimization algorithm would require impractically large computation time.

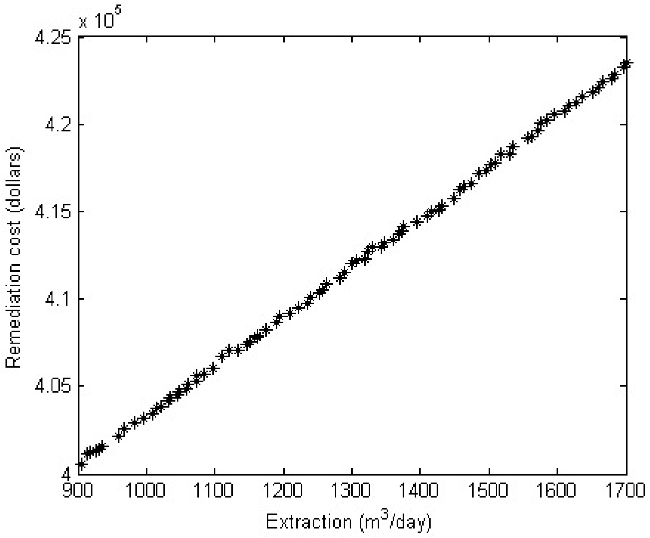

Fig. 2 Plot of Remediation cost vs. total clean water extraction for steady state condition

V. RESULTS AND DISCUSSIONS

The results of the investigations on a hypothetical contaminant plume show wide variations in remediation cost with changes in pumping strategies. The remediation cost decreases with decrease in extraction rates. Multi-objective optimization algorithms have an advantage over single-objective optimization algorithms because in order to obtain such a large number of solutions obtained from a single run by using a multi-objective optimization routine, a single-objective optimization algorithm would require impractically large computation time. Results also suggest that groundwater remediation problems are site specific and accuracy of the model result would be heavily dependent upon the quality of input data.

VI. CONCLUSION

In the optimal design of a contaminated groundwater remediation system which often involve multiple conflicting objectives, use of an efficient multi-objective optimization routine is highly benefitial because this technique simplifies the decision making processes by providing a number better-performing alternatives in a comparatively much lesser CPU time. Traditional optimization techniques would, on the other hand, require an impracticable amount of CPU time for obtaining these solutions. Extensive field exploration should carried out so that the values of the aquifer parameters

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represent the actual site as closely as possible. Slight deviation from the actual field condition would affect the model results. The developed model could be useful in achieving this goal along with other management objectives.

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