Calibration and Reliability in Groundwater Modelling (Proceedings of the ModelCARE 99 Conference held at Zürich, Switzerland, September 1999). IAHS Publ. no. 265, 2000.

An optimal decision for contaminant plume capture design in a groundwater system under parameter and boundary uncertainty

BERNARD B. HSIEH

US Army Engineer R&D Center, Waterways Experiment Station, 3909 Halls Ferry Road, Vicksburg, Mississippi 39180-6199, USA

e-mail: hsieh@hl.wes.army.mil

Abstract An integrated modelling technique, which includes numerical simulation, optimization, and uncertainty analysis, was developed for investigating an optimal decision of contaminant plume capture design in groundwater. A generalized linkage between a numerical model, such as FEMWATER (a three-dimensional finite element code) from the GMS (Department of Defence Groundwater Modelling System), and an optimization solver based on the unit-response matrix method, was first constructed. The next step was to insert the parameter and boundary uncertainties into the hydraulic gradient control schemes. The developed sensitivity coefficients were then combined with the response coefficient calculation and considered as additional design constraints in the optimization process. A real case study to examine the optimal capture zone design for the uncertainties of hydraulic conductivity, infiltration rate, and constant head boundary was demonstrated.

INTRODUCTION

Numerical simulation in groundwater has been commonly used as a decision-making tool for predicting flow and contamination transport and designing pump-and-treat systems. However, the available numerical tools are usually insufficient to design aquifer restoration needs and to meet specified management goals because of the tremendous number of trials that have to be repeatedly simulated. The combined simulation–optimization technique definitely provides quick decisions of well locations and pumping rates. However, previous investigations (Gorelick *et al.*, 1984; Atwood & Gorelick, 1985; Colarullo *et al.*, 1984), have all assumed that aquifer parameters are known with complete certainty, which never exists in any field study. To save project resources and to obtain a high probability of achieving project goals, an optimal design should include the integration of simulation, optimization, and uncertainty components.

Methods for the design of capture and containment systems can be developed using linear simulation management models if the hydrodynamic dispersion is ignored. Since there are always insufficient data on the physical parameters associated with pollutant movement through aquifers, another major objective is to decrease the sensitivity of the system to unforeseen changes in errors of the physical parameters. Valocchi & Eheart (1987) described a technique to incorporate parameter uncertainty into coupled linear optimization groundwater simulation models.

In this paper, an extension using a three-dimensional (3-D) numerical model and developing a generalized linkage between the numerical model and optimization schemes via hydraulic gradient control are reported. A real case study using investigations of the uncertainties of hydraulic conductivity in pumping the well layer, infiltration rate, and constant head boundary that affect the optimal design strategies was addressed.

SYSTEM DEVELOPMENT

The system consists of three components: the numerical simulation module, the optimization module, and the uncertainty module.

Groundwater simulation module

The linkage developed between numerical simulation and optimization was a generalized procedure, which can fit both simulation tools in GMS. FEMWATER is a three-dimensional finite element model of density-dependent flow and transport through saturated and unsaturated porous media.

The procedures for constructing a simulation model include the development of a hydrogeological conceptual model, the development of the computational mesh, the determination of boundary and initial conditions, the estimation of model parameters and performing the model run, the conducting of model calibration/verification, and the demonstration of pre-processing and post-processing.

Optimization linkage module

The optimization module includes the steps of formulating the management problem, generating the response matrix, inputting the objective functions and constraints, solving the optimization problem, and post-processing of optimal results. This module uses the hydraulic gradient control method (Atwood & Gorelick, 1985; Gorelick *et al.*, 1993) which is based on a unit-response matrix, to perform the linkage between the FEMWATER model and an optimization solver. The main idea for using hydraulic gradient control is to select wells and pumping or recharge rates so that the contaminant plume does not migrate during cleanup. As long as the plume is stationary, contaminated water can be removed, treated, and disposed or discharged. In the absence of hydraulic controls, the plume will migrate and disperse within the existing and future groundwater flow fields.

Minimizing well rates could mean extracting the most water, or, injecting the least water. Objectives based on well rates may include all or select managed wells. Once the management problem is converted into a mathematical formulation via response theory, it can be written in a format suitable for input into a linear or nonlinear programming solver. The original code, the revised simplex method, was adopted from numerical recipes (Press *et al.*, 1988) and was extensively modified to conduct the construction of this module.

Uncertainty module

We assume that a best estimate of the aquifer parameter, such as hydraulic conductivity, has been described in the traditional model as the management scheme to determine an optimal pumping strategy. However, in some specific regions or layers, the hydraulic conductivity values are uncertain. We used the hydraulic gradient control concept to incorporate the sensitivity criterion into the management model by constraining the maximum possible value of the sensitivity coefficients. The sensitivity coefficients are used to measure the impact of a small change in this parameter upon contaminant plume containment.

OPTIMIZATION OF PUMPING TO CONTROL TCE PLUME MIGRATION ON ONE RESTORATION SITE

The developed system with three modules was applied to a restoration site to develop an optimal pumping strategy for determining the contaminant plume.

Problem identification

This remediation site is approximately 12.1 ha (30 acres) in size and contains several locations where past spills, disposal practices, and operations have contaminated soil and groundwater. This site and its surrounding vicinity is hydrologically characterized as a valley-fill aquifer system. The main aquifer appears to be unconfined and is observed to have a water table approximately 30 m below the ground surface at the site.

In response to TCE (trichloroethylene) contamination found in on-site wells, the study site installed a ground treatment facility and is continuing detailed studies of subsurface contamination at the site and its surroundings. Currently, groundwater extraction comes from five pumping wells with four of the five being deep-well pumps, with a daily pumping rate of about 3780 m^3 day^{-1} (one million gallons). The treatment system is based on physical separation through air stripping to isolate TCE, with the treated water then being discharged into the river.

Development of the numerical flow model

The numerical model used in this study was based on a hydrogeological conceptual model. The extent of the esker deposit and geometry of the basement surface are of critical importance to the hydrogeological model. The map module of GMS was used to create a new surface two-dimensional (2-D) mesh (Fig. 1(a)). The basement and sediment geometry with nine different materials classified are shown with the 3-D finite element mesh overlay in Fig. 1(b). Under the hydrogeological condition modelled, the mesh is vertically divided into nine materials and 21 layers. The 3-D mesh consists of 11 000 nodes and 20 139 elements.

The western and northwestern model boundaries are represented by the river and are defined by constant fixed head elevations of 116 m. The eastern boundary is a constant head of 165 m. The southern and northeastern boundaries are defined as no-flow boundaries. The recharge and water-well boundary conditions were also assigned to the model. A value of 1.32×10^{-3} m day^{-1} was used as a precipitation influx. Well-pumping boundary conditions were assigned to five locations. A numerical procedure

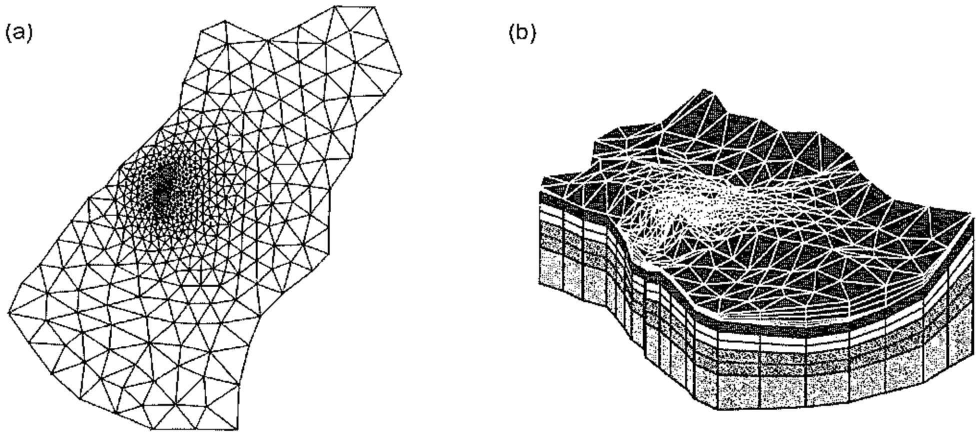

Fig. 1 (a) 2-D and (b) 3-D computational meshes.

was developed to estimate initial conditions with an iteration process because the field measurements were not sufficiently dense enough.

Hydraulic conductivity was assumed to be homogeneous within each model layer. Unsaturated zone curves were required for moisture content, relative conductivity, and water capacity as a function of pressure head. The highest hydraulic conductivity is in the esker layer (86.4 m day^{-1} for horizontal and 50.0 m day^{-1} for vertical).

OPTIMAL SOLUTIONS FOR PUMPING AND MIGRATION CONTROL OF TCE PLUME AT SITE

Design of optimal pumping strategies

Since there presently is no planning for new wells and no injection activities for any pumping wells, hydraulic gradient control is based on the pumping strategies for the five existing wells. Using the information from the past two years of pumping history, the average demand for each well and the total demand can be estimated.

The plume is located upgradient of the existing well system. Due to the hydrogeological conditions and management strategies at the site, the hydraulic gradient control for preventing the plume migration was designed by assigning 15 control pairs on the down-gradient side of the well system. Each pair occupies two computational nodes: one is inward and other is outward. The objective is to minimize pumping rates. Five constraints were associated with the capacity, demand, usage and individual pumping rates and migration control. The constraints are as follows:

- Restrict the total volume pumped to allow a low-cost, low-capacity treatment system.
- Restrict the total volume pumped to meet cooling-system demands.
- Restrict the least usage of pumping well 3.
- Restrict individual pumping rates to allow the use of small, inexpensive pumps.
- Restrict heads outside the contaminated zone to values greater than or equal to the heads inside (no spreading).

Optimal solutions and post-optimization verification for the site

To determine the response matrix, this study only requires six numerical simulation runs which significantly reduces the computer memory and time required to obtain the optimal solution. The optimal pumping solutions for the five wells are illustrated in Table 1. The total pumpage for satisfying the objective function and constraints is 7484 m^3 day^{-1}. This amount is about 86% of the full-operating capacity of the entire treatment system. This preliminary result could indicate that current usage must be increased to meet all specified constraints.

Table 1 Optimal pumping rate (m^3 day^{-1}) compared with full capacity and average usage for each treatment well.

Well	Average usage	Full capacity	Optimal scheme
1	1171	2286	2014
2	501	1986	1827
3	1566	1566	1050
4	131	1219	1422
5	1261	1589	1171
Total	4530	8646	7484

It is necessary to verify the optimal solutions by checking the optimized values with respect to the desired constraints. Three different variables were used to present this process: velocity field, hydraulic head, and gradient at control pairs. Using the optimal pumping solutions as the pumping rate input and then re-running the numerical model does this. The flow field and total head around the pumping and the hydraulic control area show the resulting depression cone formed around the wells. Contaminated water will be trapped by these wells and will not be discharged to the river. The clear water in the up-gradient could bypass the contaminated area and discharge into the river. These results show that each control pair under the optimal pumping schemes satisfies the hydraulic gradient control strategy.

INCORPORATING THE UNCERTAINTY OF HYDRAULIC CONDUCTIVITY AND CONSTANT HEAD BOUNDARY INTO OPTIMAL DESIGN

The sensitivity coefficient is defined as the total gradient change when the parameter or boundary value has some uncertainty associated with it. Actually, this total change is based on the regional hydraulic gradient change plus the total drawdown change due to the pumping activities.

Three experiments were investigated, 10% (8.6 m day^{-1}) increase of hydraulic conductivity in the esker layer, 0.01×10^{-3} m^3 day^{-1} of infiltration rate, and 1 m of constant head boundary over the northeastern side of the model increases. These changes are considered as the uncertainty due to the measurement or estimate error. For each experiment, six computer runs are made—one for the background run due to parameter or boundary change, and five for estimating the response coefficient matrix due to parameter or boundary change. Fifteen estimated sensitivity coefficients for each control pair were used as the sensitivity constraints for solving the optimization problem.

Table 2 Optimal pumping solutions (m^3 day^{-1}) the uncertainty-constraints of hydraulic conductivity, infiltration rate, and constant head boundary.

Parameter	S_{avg}	S_{max}	$Q1$	$Q2$	$Q3$	$Q4$	$Q5$	Total
No uncertainty	N/A	N/A	2014	1827	1050	1422	1171	7484
Hydraulic conductivity	6.2×10^{-3}	6.0×10^{-3}	2095	1913	1089	1282	1218	7698
		3.0×10^{-3}	2228	2264	1151	1565	1293	8296
		1.0×10^{-3}	unfeasible solution					
Infiltration rate	2.5×10^{-3}	2.5×10^{-3}	2030	1841	1062	1437	1184	7554
		2.0×10^{-3}	2047	1855	1073	1451	1197	7623
		1.0×10^{-3}	2112	1912	1120	1510	1248	7902
Constant head boundary	5.5×10^{-2}	5.0×10^{-2}	2132	1973	1120	1539	1241	8013
		2.5×10^{-2}	2242	2165	1174	1673	1283	8637
		1.0×10^{-2}	unfeasible solution					

The S_{max} for the tests of each experiment needs to be estimated. Usually, the average response coefficient (S_{avg}) and the average drawdown can be used as the initially estimated S_{max}. Table 2 summarizes the optimal pumping with given S_{max} for each experiment. Due to the scale difference among these parameter or boundary changes, the optimal pumping scheme changes are difficult to compare. However, for each individual parameter or boundary value, these results are very useful for determining what is allowable error in order to obtain reliable optimal pumping values. For those more sensitive control pairs, it might indicate a need for more field measurement to support the reliable study. That some S_{max} obtain unfeasible optimal solutions is due to the limitation of the capacity constraint in the system.

CONCLUSIONS

A very effective and computationally efficient scheme was developed and then applied at a restoration site to determine the optimal pumping alternatives for groundwater remediation. An optimization procedure using GMS and FEMWATER was developed that could be used to contain the contaminant plume while minimizing pumping rates. The sensitivity constraint is used to examine the uncertainty of parameter or boundary values.

Considering the capacity, demand, individual pumping limit, usage priority, and migration control of contamination, the results indicate that the optimal total pumping (7484 m^3 day^{-1}) was less than the full operating capacity (8646 m^3 day^{-1}) at this demonstration site. However, the optimal results with the uncertainty constraint indicate that if the maximum sensitivity of hydraulic conductivity is less than 1.5×10^{-3}, or the maximum sensitivity of constant boundary head is less than 1.0×10^{-2}, total optimal pumping might need more than the water with full-operating capacity.

Acknowledgements This work was funded by the US Army Environmental Center. Permission to publish this information was granted by the Chief of Engineers.

REFERENCES

Atwood, D. & Gorelick, S. (1985) Hydraulic gradient control for groundwater contaminant removal. *J. Hydraul.* **76**, 85–106.

Colarullo, S. J., Heidari, M. & Maddock III, T. (1984) Identification of an optimal groundwater management strategy in a contaminated aquifer. *Wat. Resour. Bull.* 20(5), 747–760.

Gorelick, S., Freeze, A., Donohue, D. & Keely, J. (1993) *Groundwater Contamination: Optimal Capture and Containment.* Lewis Publishers, Boca Raton, Florida, USA.

Gorelick, S. M., Voss, I., Gill, P. E., Murry, W., Saunders, M. A. & Wright, M. H. (1984) Aquifer reclamation design: the use of contaminant transport simulation combined with nonlinear programming. *Wat. Resour. Res.* 20(4), 415–427.

Press, W., Flannery, B., Teukolsky, S. & Vetterling, W. (1988) *Numerical Recipes.* Cambridge University Press, Cambridge, UK.

Valocchi, A. J. & Eheart, J. W. (1987) Incorporating parameter uncertainty into groundwater quality management models. In: *Systems Analysis in Water Quality Management* (ed. by M. B. Beck), 251–257. Pergamon Press, London, UK.