DEVELOPMENT OF A COMBINED QUANTITY AND QUALITY MODEL

FOR

OPTIMAL GROUNDWATER MANAGEMENT

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Research Project Technical Completion Report

Project G-1212-04

ABSTRACT

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Presented is a procedure for incorporating solute transport as linear constraints within computer models for optimizing regional groundwater extraction strategies. The MODCON modelling procedure uses linear goal programming, embedded linearized equations for flow and solute transport and a MOC simulation model. Assumed is 2D flow and solute transport and a dispersed conservative contaminant. The MODCON procedure develops steady groundwater extraction strategies that will satisfy future groundwater quality constraints while simultaneously causing future piezometric heads to be as close to current heads as possible. The procedure is applied to a 160 square mile area in southeastern Arkansas.

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INTRODUCTION

A. Purpose and Objectives

Developing optimal regional quantitative water management strate-
gies has been accomplished with increasing frequency in recent years.
Consideration of groundwater quality constraints is not common in
such models, however. This results from the fact that when optimiz-
ing groundwater extraction (rather than injection), mass flux of
contaminant extraction is the product of unknown concentrations and
unknown extraction rates. In other words, constraint equations
describing extraction are nonlinear.

There are many commercially available codes that can solve opti-
mization problems having nonlinear constraints. However, depending
on the problem, 'optimal' solutions resulting from problems incorpo-
rating nonlinear constraints may not be globally optimal. Such solu-
tions may be merely locally optimal in the decision space. It is
possible to perform enough repetitive nonlinear optimizations, using
different initial feasible solutions, to become somewhat sure that
one has attained a true global optimal strategy. Depending on the
number of variable, it may be impractical or uneconomical to do so.

Some researchers advocate linearizing nonlinear equations to
derive globally optimal solutions. This tack has its own weakness.
Such solutions are merely optimal for a linear surrogate of the orig-
inal nonlinear problem. Their adequacy depends on the degree to
which the linear formulation appropriately represents the nonlinear
system.

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The purpose of this report is to describe a MODCON (MODel for MODifying CONtaminant CONcentrations) approach for developing globally optimal groundwater management strategies that include consideration of groundwater quality. MODCON relies on the repetitive use of linear optimization/simulation goal-programming models and an externally developed nonlinear solute transport model.

B. Related Research and Activities

Several techniques have been used to represent solute transport in optimization models (Gorelick, 1983). Each method has limitations. Gorelick (1984) represented solute transport as nonlinear constraints. However, when nonlinear water quality constraints are used, it is difficult to assure global optimality. A second category of models use gradient control and velocity influence coefficients (Colarullo et al., 1984; Gorelick and Lefkoff, 1985). Such models may be overly restrictive if some contaminant movement (in addition to dispersion) is acceptable, or impractical for regional use if the area of contamination is large. A third method utilizes influence coefficients describing the effect of a change in potentiometric head on steady state contamination (Datta and Peralta, 1986). This approach is also overly restrictive, since it takes a very long time for steady state concentrations to develop, and impractical, if groundwater quality constraints must be considered for many locations. Other approaches also have been utilized (Louie et al., 1984). No previously reported techniques seem well suited for the task of developing volumetrically optimal regional extraction strate-

gies while simultaneously considering groundwater quality constraints.

METHODS AND PROCEDURES

A. <u>Modelling Methodology Overview and Functions</u>

We assume: 1) an unconfined isotropic heterogeneous aquifer in which the change in water levels with time will cause insignificant change in transmissivity, 2) two-dimensional groundwater flow, 3) two-dimensional solute transport and insignificant vertical density gradients, and 4) conservative dispersed contaminant. Although anisotropic hydraulic conductivity can be readily considered, isotropic conductivity is assumed here.

The purpose of the proposed model is to develop a regional groundwater extraction strategy that will, as much as possible, maintain an existing potentiometric surface, while assuring that future groundwater contaminant concentrations are acceptable. It is assumed that the developed annual pumping strategy will be unchanging with time during the planning period. In order to achieve these goals, the iterative optimization and simulation process described below is used (Figure 1 contains a flowchart).

The complete modelling procedure (MODCON) consists of four optimization/simulation modules (A,B,D,E) and an externally developed solute transport model (module C). Optimization is accomplished using GAMS/MINOS (Kendrick and Meeraus, 1985; Murtagh and Saunders, 1983). Components A, B and E incorporate the two-dimensional linearized Boussinesq equation to model groundwater flow. Modules D and E

Figure 1. Flowchart of module functions in MODCON.

incorporate linearized solute transport equations. In this paper, module C is the method of characteristics (MOC) model of Konikow and Bredehoeft (1978). The functions of each part of MODCON are discussed below. Their most important characteristics are summarized in Figure 2.

Model A uses steady-state simulation and weighted linear goal-programming (LGP) optimization to determine acceptable boundary flux rates for the subsystem. This function is important when it is impractical to model an entire aquifer system. It aids developing a pumping strategy for only a portion of the aquifer in such a way as to prevent disruption of flow outside that subsystem. To do this, one assumes that aquifer stimuli outside the system during the management period will maintain the regional flow patterns that exist at the beginning of the era (t=0), as long as pumping within the subsystem does not induce more groundwater flow into the subsystem than occurred initially. The recharge fluxes computed for boundary cells by submodel A are used as upper limits on recharge in subsequent optimization models.

Submodel B uses unsteady simulation and weighted LGP optimization to compute a pumping strategy that will cause future potentiometric heads to be as close to current heads as possible. It does not consider solute transport.

In module C, a nonlinear solute transport model provides multi-time-step nonlinear simulation. It computes the future concentrations that will result from implementation of the pumping strategy

Module Type. Output   Constraints

Linear goal-programming (LGP).
Boundary fluxes ($q^{ss,CH}$) that best   2D steady flow
maintain initial heads (h_o)

LGP. Pumping strategy (q_a^*) that   2D unsteady flow
best maintains initial subsystem $q^L \leqslant q^* \leqslant q^u$
heads (h_o) at future time T. $h^L \leqslant h^* \leqslant h^u$
Predicted heads (h_T^*).

Nonlinear MOC solute transport.
Future concentrations (C_T^{MOC}) and   2D advection-dispersion
heads (h_T^{MOC}) resulting from q^*. (used
to Id. unacceptable C and verify h_T^*.)

LGP. Calibrated coefficients so linearly
predicted concentrations (C_T^*)$\approx C_T^{MOC}$.

                                        2D unsteady flow
LGP. Modified pumping strategy that   2D advection-dispersion
best maintains h_o at time T with $q^L \leqslant q^* \leqslant q^u$.
acceptable concentrations. $h^L \leqslant h^* \leqslant h^u$
                                             $C_T^* \leqslant C^u$

Figure 2. Significant characteristics of MODCON modules.

developed by model B. Assuming future concentrations will be unacceptable in some locations, the pumping strategy will need to be modified. To accomplish strategy modification, solute transport must be appropriately included in a model similar to model B.

The next step is to create an adequate linear representation of solute transport. Submodel D uses LGP to calibrate two-dimensional linear solute transport equations so that they can replicate concentrations predicted by the nonlinear model. By including only a single time-step, model D avoids using unknown concentrations (final concentrations are assumed known from module C) in its solute transport equations and is able to be linear. (Transmissivities are computed for both beginning and final heads.)

Module E includes the objective function and unsteady volumetric simulation of model B, as well as the calibrated linear solute transport equations of model D. It develops a modified pumping strategy that considers groundwater quality constraints. Its objective function is the same as that for module B.

Because of the bold assumptions made in the linearized solute transport constraints, one should verify the concentrations predicted by model E. The MOC model is used for this purpose. Figure 1 shows that iteration through models D, E and the nonlinear model is continued until concentrations predicted by model E are acceptable and close to those predicted by nonlinear model.

B. Model Development

For an n cell subsystem, the objective function for models A, B,

D and E is (Yazdanian and Peralta, 1986):

minimize $y = (W) \{ D_+ \} + (W) \{ D_- \}$ ..[1]

where

(W) = a 1 x n vector of weighting factors, (dimensionless)

$\{ D_+ \}$ and $\{ D_- \}$ are m x 1 column vectors of over- and under-
achievement variables, respectively, units of
L for modules A, B, & E, units of ppm for
module D.

Optimal solutions for submodels A and B are constrained subject to
the following, simply described for either steady-state flow (A) or
a single time step of unsteady flow (B). (For t time steps, array
dimensions of magnitude n become n x t.)

$\{L_q\} \leq \{Q_*\} = \{B\} - [A] \{H_*\} \leq \{U_q\}$ ..[2]

$\{L_h\} \leq \{H_*\} \leq \{U_h\}$ ..[3]

$\{H_*\} - \{D_+\} + \{D_-\} = \{H_0\}$ ..[4]

$\{D_+\}, \{D_-\} \geq 0.0$ ..[5]

where

$\{L_q\}$ and $\{U_q\}$ = n x 1 column vectors of lower and upper bounds,
respectively, on pumping (or recharge), L^3

$\{Q_*\}$ = n x 1 column vector of optimal net annual steady pumping or
recharge) rates, where discharge is positive valued, L^3

{B} = n x 1 vector describing initial heads, effective porosities,

     cell sizes and time step sizes, L^3

[A] = n x n symmetric banded matrix of aquifer properties, L^2

{H*} = n x 1 column vector of optimal final or intermediate

     heads, depending on the number of time steps, L

{L_h} and {U_h} = n x 1 column vectors of lower and upper bounds

          on head, L

{H_o} = initial heads, L

Note that the objective function considers all cells, not merely
internal cells. Thus, in this example, boundary cells are treated as
variable head/restrained flux boundary conditions (equation [2]),
rather than as classical constant head (Dirichlet) or constant flux
(Neumann). The use of weights of large magnitude for boundary cells
effectively forces heads to approximate desired values.

The constraints for module D reflect its function of calibrating
coefficients contained in linearized solute transport equations. It
uses objective function [1] subject to conditions mentioned below,
including constraint [6] for each cell. Note that over- and under-
achievement variables have dimensions of concentration in equation
[6], as they do in equation [1] when it is applied to model D. Based
on simulation using the MOC model, future heads and concentrations
are known. Equation [6] reflects the fact that these future concen-
trations are functions of initial concentrations, intermediary
fluxes, advective and dispersive processes. The F coefficients and

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over- and under-achievement variables are determined by the model

through optimization.

$C_0 + f\ (F_1,Q,C,V) + f\ (F_2,H,C,T,V) + f\ (F_3,H,C,P,V)$

$$- D_+ + D_- = C_{T,MOC} \qquad\qquad ..[6]$$

where

C_0,C = initial and intermediate concentrations

$C_{T,MOC}$ = final concentrations predicted by MOC model in module C

F_1,F_2,F_3 = linear coefficients for processes of accretion,

             advection and dispersion

V = volume

T = transmissivity and other problem specific parameters

P = dispersivity and other parameters

subject to bounds on F values to aid realistic representation of

transport.

$$\dfrac{2C_0}{C_0 + C_{T,MOC}} \le F_1 \le \dfrac{2C_{T,MOC}}{C_0 + C_{T,MOC}} \qquad\qquad ..[7]$$

$$0.0 \le F_2 \le 1.0 \qquad\qquad ..[8]$$

$$0.0 \le F_3 \le 1.0 \qquad\qquad ..[9]$$

The bounds on F_1 assure that the concentration of that being pumped

from a cell is between initial and final concentrations of the cell.

The finite-difference function describing concentration change due to

advection considers both initial and final concentrations and gra-
dients. F_2 represents the weight that is placed on initial concen-
trations and gradients (if F_2 equals 1) versus the weight placed on
final concentrations and gradients (if F_2 equals 2). F_3 performs the
same function for dispersive mass flux that F_2 performs for advective
flux. Module D also contains bounds [5]. As a result, it determines
the coefficient values that cause best replication of concentrations
predicted by nonlinear simulation.

Module E uses objective function [1], calibrated F coefficients
and constraint equations [2-5] and [10], which is a vectorized con-
straint form of [6].

$$\{f_\#(F,C,Q,V,H,T,P)\} - \{D_+\} + \{D_-\} \leq \{U_c\} \qquad ..[10]$$

This final model computes a pumping strategy that will cause future
heads to be as close as possible to initial heads, while simulta-
neously assuring that future groundwater contaminant concentrations
are acceptable.

PRINCIPAL FINDINGS AND SIGNIFICANCE

Flow assumptions are as mentioned previously. The study area
aquifer is unconfined, consisting of unconsolidated sands and gravels
with a hydraulic conductivity of 250 ft/day and a specific yield of
0.25. A longitudinal (and transverse) dispersivity of 1320 ft is
assumed in the MOC model for a dispersed contaminant and large cell
size. Diffusion is assumed to be insignificant.

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Figure 3 shows a grid of 1 mi^2 cells taken from the Bayou Bartholomew basin in Arkansas. The displayed potentiometric surface is one that would evolve from implementation of one of the optimal sustained yield pumping strategies developed by Peralta et al. (1985). Cells in which future (25 year) concentration are to be modified are framed in this and subsequent figures. Current (assumed initial) concentrations of NaCl are shown in Figure 4 (Fitzpatrick, 1985).

Module A provides boundary fluxes needed to prevent disruption of the regional flow regime. Module B computes optimal steady pumping values needed to most closely maintain heads of Figure 3 after 25 years. The MOC model predicts the 25-year concentrations that will result from implementing the strategy computed by model B (Figure 5). Note that predicted concentrations in cells (13,5) and (14,5) are 300 and 330, respectively.

Assume that future development plans make it desirable that 25-year concentrations in cells (13,5) and (14,5) be no greater than 250 and 275 ppm, respectively. Module D calibrates the F coefficients to permit linear expression of the mass density changes predicted by MOC model. Module E uses those results to compute a revised optimal pumping strategy (Figure 6 shows the strategy for a selected portion of the system).

Figure 7 shows the differences in annual pumping between the strategies developed by Module B (which does not consider water quality) and Module E (which does consider future water quality). Figure 8 shows the potentiometric surface that will result in the
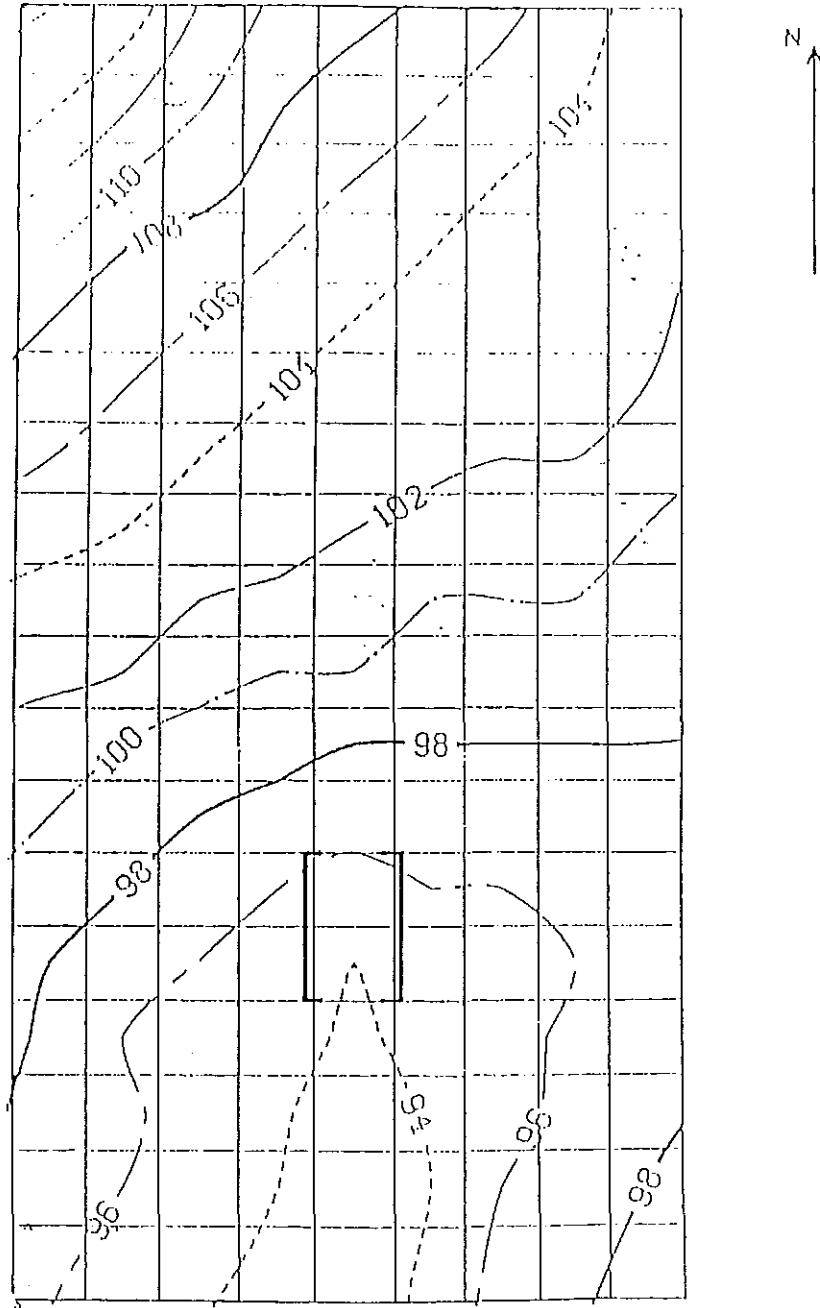
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Figure 3. Assumed initial potentiometric surface, in ft above sea level. Critical cells are framed.

Figure 4. Assumed initial NaCl concentrations in groundwater, in ppm.

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	1	2	3	4	5	6	7	8	9
1	0	0	5	26	100	153	200	242	0
2	0	0	6	27	103	178	191	1·98	197
3	0	0	4	47	92	106	107	104	102
4	0	0	4	41	56	74	75	51	47
5	0	0	0	7	47	53	49	4	3
6	0	0	0	6	50	72	49	5	0
7	0	0	3	45	75	94	56	44	3
8	0	0	4	50	102	107	97	50	3
9	0	0	4	57	181	189	147	54	2
10	0	0	5	62	210	203	188	60	6
11	0	0	7	84	239	229	197	120	51
12	0	0	14	120	269	247	202	126	52
13	0	4	51	152	[300]	286	245	125	57
14	0	5	54	157	[330]	325	292	116	97
15	0	4	51	153	365	373	341	198	107
16	0	6	52	125	377	408	377	209	109
17	4	47	80	198	398	518	398	227	107
18	0	97	105	212	565	428	419	387	0

I

Figure 5. Twenty-five year concentrations, in ppm, predicted by MOC model to result from implementing pumping strategy computed by module B.

J

I	3	4	5	6	7
11	Ø	Ø	Ø	Ø	Ø
12	Ø	Ø	Ø	Ø	Ø
13	Ø	Ø	797	Ø	Ø
14	Ø	Ø	1112	Ø	Ø
15	Ø	Ø	Ø	Ø	Ø
16	Ø	Ø	Ø	Ø	Ø

Figure 6. Annual groundwater extraction strategy computed by Module E for a selected portion of the study area, in ac-ft/yr.

J

I	3	4	5	6	7
11	Ø	Ø	Ø	-28	-23
12	-145	Ø	Ø	Ø	Ø
13	-6	-111	648	Ø	Ø
14	-6	-75	648	Ø	Ø
15	-15	-211	Ø	-15	Ø
16	36	Ø	-73	-341	-66

Figure 7. Difference between annual groundwater extraction strategies computed by Modules E and B, (E − B), for a portion of the study area, in ac-ft/yr.

vicinity of the critical cells after 25 years of implementing the Module E strategy. Figure 9 shows the differences in potentiometric surface elevations that will result depending on whether one implements the strategy from Module E or the strategy from Module B.

Consequences of implementing the strategy from Module E are tested using MOC model. Figure 10 shows that MOC-predicted future concentrations resulting from pumping strategies implementation achieves acceptable future concentrations.

CONCLUSIONS

A linear finite-difference equation is presented to approximate two-dimensional solute transport by advection and dispersion. The equation is calibrated and used within an optimization/simulation procedure (MODCON). MODCON develops optimal pumping strategies that will as much as possible maintain present potentiometric surface elevations, while satisfying future water quality constraints. The procedure seems promising, but judgement and experience in optimization/simulation procedures are important for successful application.
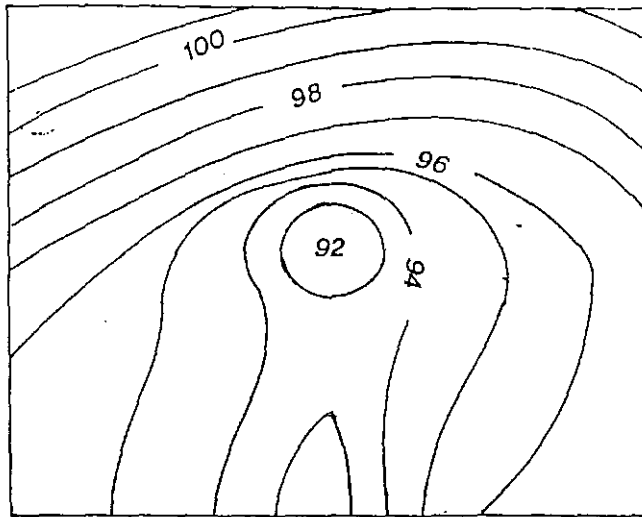
Figure 8. Heads that will result in a portion of the study
area after 25 years of implementing the pumping
strategy computed by module E, in ft above sea level.

J

	3	4	5	6	7
11	0.2	-0.1	-0.3	-0.1	-0.0
12	0.3	-0.3	-0.9	-0.6	-0.2
I 13	-0.0	-0.6	-2.5	-1.0	-0.3
14	0.0	-0.5	-2.2	-0.8	0.0
15	0.5	0.0	-0.3	0.1	0.7
16	0.3	0.5	1.0	0.8	0.9

Figure 9. Difference between twenty-five year heads resulting
from implementing strategies computed by modules E
and B, (E-B), for a portion of the study area, in ft.

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					J				
	1	2	3	4	5	6	7	8	9
1	0	0	5	26	100	153	200	242	0
2	0	0	6	27	103	178	191	198	197
3	0	0	4	47	92	106	107	104	102
4	0	0	4	41	56	74	75	51	47
5	0	0	0	7	47	53	49	4	3
6	0	0	0	6	50	72	49	5	0
7	0	0	4	45	75	94	55	44	3
8	0	0	4	50	102	107	97	50	3
9	0	0	4	57	181	189	147	54	2
10	0	0	5	63	209	204	187	60	7
11	0	0	8	87	235	229	197	121	51
12	0	1	18	125	256	249	203	127	52
13	0	5	53	158	[233]	284	246	127	57
14	0	5	57	167	[265]	322	290	118	97
15	0	3	54	156	355	370	342	200	104
16	0	5	52	116	389	409	383	206	107
17	4	47	81	199	405	518	399	222	105
18	0	97	105	212	568	517	424	390	0

I

Figure 10. Twenty-five year concentrations, in ppm, predicted by MOC model to result from implementing optimal pumping strategy computed by model D.

LITERATURE CITED

Colarullo, S. J., M. Heidari and T. Maddock. 1984. Identification of an optimal groundwater management strategy in a contaminated aquifer. Water Resources Bulletin. v. 20, no. 5, pp. 747-760.

Datta, B. and R. C. Peralta. 1986. Optimal modification of regional potentiometric surface design for groundwater contaminant containment. Transactions of the ASAE. v. 29, no. 6.

Fitzpatrick, D.J. 1985. Occurrence of saltwater in the alluvial aquifer in the Boeuf Tensas basin, Arkansas. USGS Water Resources Investigations Report 85-4029. Little Rock, Arkansas.

Gorelick, S.M. 1983. A review of distributed parameter groundwater management modeling methods. Water Resources Research. v. 19, no. 2, pp. 305-319.

Gorelick, S.M., C.I. Voss, P.E. Gill, W. Murray, M.A. Saunders and M.H. Wright. 1984. Aquifer reclamation design: The use of contaminant transport simulation combined with non linear programming. Water Resources Research. v. 20, no. 4, pp. 415-427.

Gorelick, S. M., and L. J. Lefkoff. 1985. Design and cost analysis of rapid aquifer restoration systems using flow simulation and quadratic programming. Groundwater. v. 24, no. 6, pp. 777-790.

Kendrick, D. and A. Meeraus. 1985. GAMS An introduction. The World Bank. Washington, D. C.

Konikow, L.F. and J.D. Bredehoeft. 1978. Computer model of two-dimensional solute transport and dispersion in groundwater. Techniques of water resources investigations of the United States Geological Survey. Book 7. Chapter C2. 91 pp.

Louie, W.F., W. Yeh and N.S. Hsu. 1984. Multiobjective water resources management planning. Journal of Water Resources Planning and Management. ASCE. v. 110, no. 1, pp. 39-56.

Murtagh, B. A. and M. A. Saunders. 1983. MINOS 5.0 user's guide. Technical Report SOL 83-20, Stanford University, California.

Peralta, R. C., B. Datta, J. Solaimanian, P. J. Killian and A. Yazdanian. 1985. Optimal sustained yield groundwater withdrawal strategies for the Boeuf Tensas basin in Arkansas. Miscellaneous Publication No. 29. Water Resources Research Center, Fayetteville, AR 72701.

Yazdanian, A. and R. C. Peralta. 1986. Sustained yield groundwater planning by goal programming. Groundwater. v. 24, no. 2, pp. 157-165.