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DEVELOPMENT OF A COMBINED QUANTITY AND QUALITY MODEL FOR OPTIMAL GROUNDWATER MANAGEMENT

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ABSTRACT

DEVELOPMENT OF A COMBINED QUANTITY AND QUALITY MODEL
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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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Keywords -- Groundwater Management/Optimization/Groundwater Quality/
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INTRODUCTION

A. Purpose and Objectives

Developing optimal regional quantitative water management strategies 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 optimizing 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 optimization problems having nonlinear constraints. However, depending on the problem, 'optimal' solutions resulting from problems incorporating nonlinear constraints may not be globally optimal. Such solutions 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 original nonlinear problem. Their adequacy depends on the degree to which the linear formulation appropriately represents the nonlinear system.

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 strategies while simultaneously considering groundwater quality constraints.

METHODS AND PROCEDURES

A. Modelling Methodology Overview and Functions

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

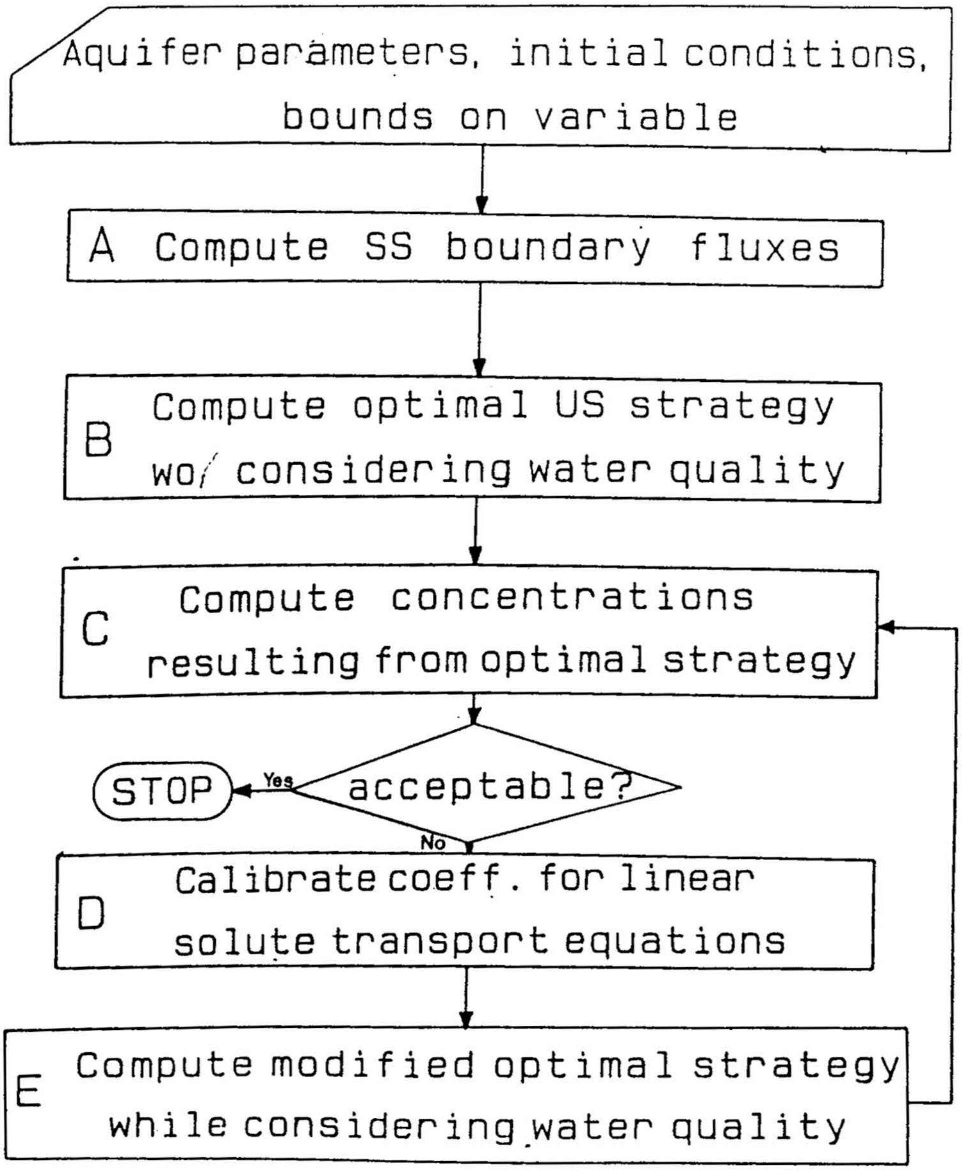

Figure 1. Flowchart of module functions in MODCON.

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 maintain initial heads (h_o)	2D steady flow
LGP. Pumping strategy (q^*_B) that best maintains initial subsystem heads (h_o) at future time T. Predicted heads (h^*_T).	2D unsteady flow $q^L \leqslant q^* \leqslant q^U$ $h^L \leqslant h^* \leqslant h^U$
Nonlinear MOC solute transport. Future concentrations (C^{MOC}_T) and heads (h^{MOC}_T) resulting from q^*. (used to Id. unacceptable C and verify h^*_T.)	2D advection-dispersion
LGP. Calibrated coefficients so linearly predicted concentrations (C^*_T)$\approx C^{MOC}_T$.	
LGP. Modified pumping strategy that best maintains h_o at time T with acceptable concentrations.	2D unsteady flow 2D advection-dispersion $q^L \leqslant q^* \leqslant q^U$ $h^L \leqslant h^* \leqslant h^U$ $C^*_T \leqslant C^U$

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]

$\{H*\} - \{D_+\} + \{D_-\} = \{H_o\}$ ..[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 concentrations are functions of initial concentrations, intermediary fluxes, advective and dispersive processes. The F coefficients and over- and under-achievement variables are determined by the model through optimization.

$$C_o + f\ (F_1,Q,C,V) + f\ (F_2,H,C,T,V) + f\ (F_3,H,C,P,V) - D_+ + D_- = C_{T,MOC} \qquad ..[6]$$

where

C_o,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.

$$\frac{2C_o}{C_o + C_{T,MOC}} \leq F_1 \leq \frac{2C_{T,MOC}}{C_o + C_{T,MOC}} \qquad ..[7]$$

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

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

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 gradients. F_2 represents the weight that is placed on initial concentrations 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 constraint 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 simultaneously 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.

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

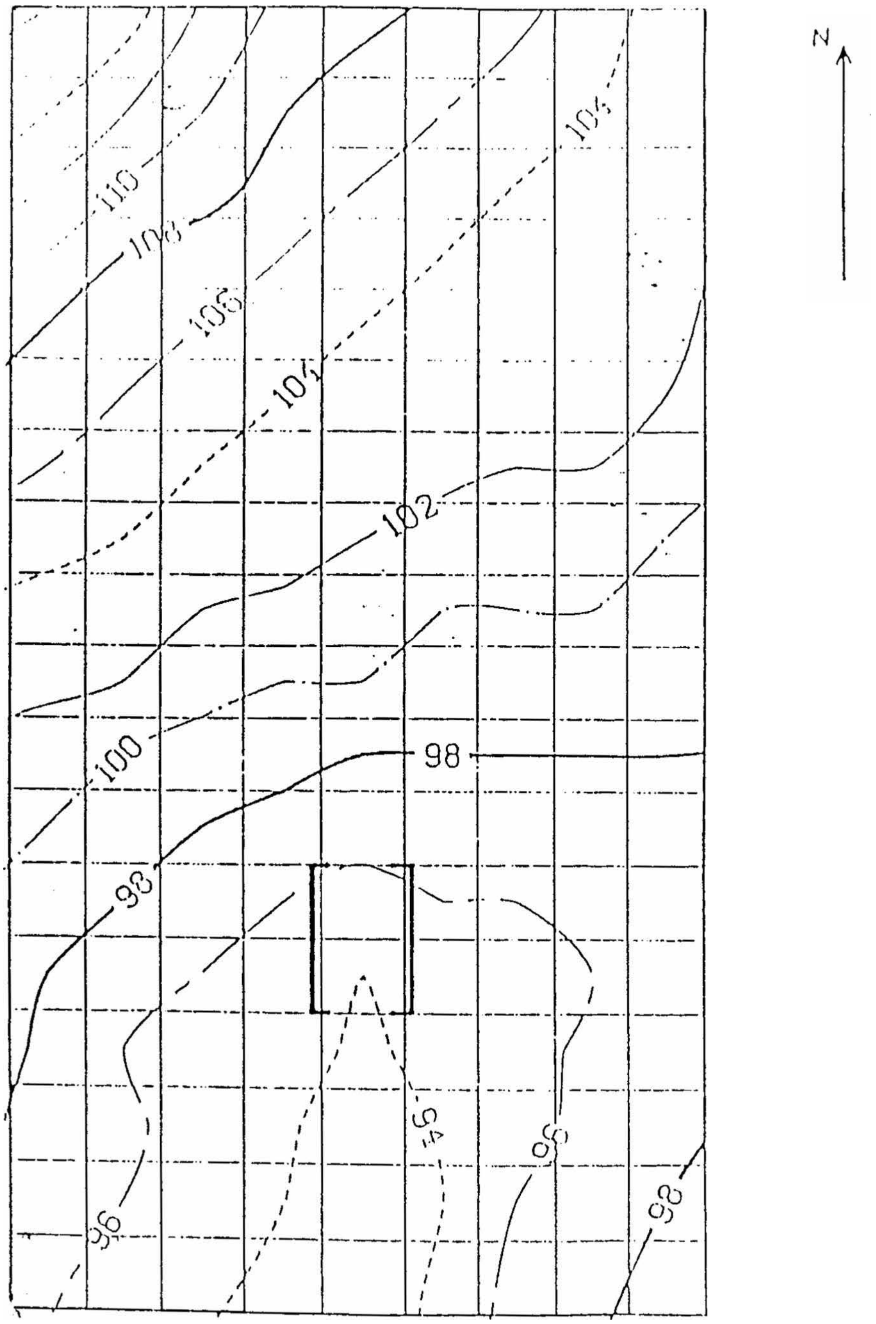

Figure 3. Assumed initial potentiometric surface, in ft above sea level. Critical cells are framed.

	J								
I	1	2	3	4	5	6	7	8	9
1	0	0	0	50	100	150	200	250	0
2	0	0	0	50	100	200	200	200	200
3	0	0	0	50	100	100	100	100	100
4	0	0	0	50	50	75	75	50	50
5	0	0	0	0	50	50	50	0	0
6	0	0	0	0	50	75	50	0	0
7	0	0	0	50	75	100	50	50	0
8	0	0	0	50	100	100	100	50	0
9	0	0	0	50	200	200	150	50	0
10	0	0	0	50	230	200	200	50	0
11	0	0	0	75	260	230	200	125	50
12	0	0	0	115	290	245	200	125	50
13	0	0	50	150	320	285	250	125	50
14	0	0	50	150	350	325	300	100	100
15	0	0	50	150	375	375	350	200	100
16	0	0	50	100	400	400	400	200	100
17	0	50	75	200	400	550	400	200	100
18	0	100	100	200	500	700	400	400	0

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

J

I	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	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

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

				J		
		3	4	5	6	7
	11	0	0	0	0	0
	12	0	0	0	0	0
I	13	0	0	797	0	0
	14	0	0	1112	0	0
	15	0	0	0	0	0
	16	0	0	0	0	0

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

				J		
		3	4	5	6	7
	11	0	0	0	-28	-23
	12	-145	0	0	0	0
I	13	-6	-111	648	0	0
	14	-6	-75	648	0	0
	15	-15	-211	0	-15	0
	16	36	0	-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.

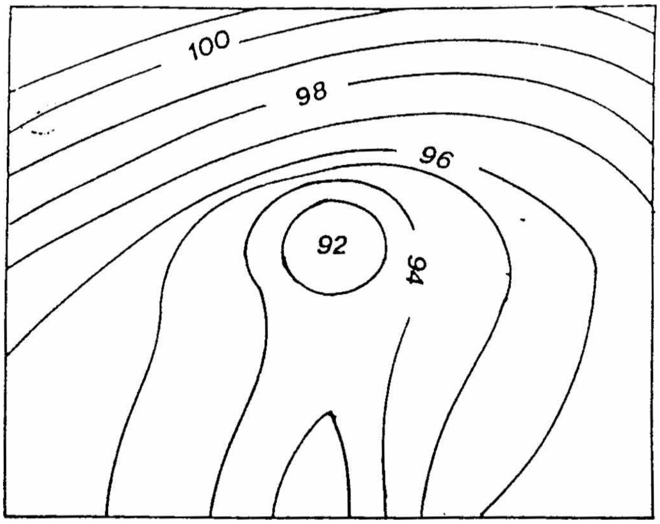

Figure 8. Heads that will result in a portion of the study area after 25 years of implementing the pumping strategy computed by module E, in ft above sea level.

				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.

	J								
I	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

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.