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PC Software for Optimizing Groundwater Contaminant Plume Capture and Containment

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I. INTRODUCTION

Simulation/optimization (S/O) models can be used to speed the process of computing desirable groundwater pumping strategies for plume management. They make the process of computing optimal strategies fairly straightforward and can help minimize the labor and cost of groundwater contaminant cleanup.

Differences between S/O models and the simulation (S) models currently used by over 98% of practitioners are discussed in Section II [1], followed by an overview of the two most common forms of groundwater management S/O models, their strengths and limitations, in Section III. In Section IV, currently available PC-based S/O models are discussed, and the ways in which they would be applied to representative situations are illustrated. Included is US/WELLS^D, an easy-to-use deterministic model that requires minimal data but will address aquifer and stream-aquifer systems where the analytical solutions of Theis [2] and Glover and Balmer [3] are appropriate. Also included is US/REMAX^B, appropriate for heterogeneous, multilayer systems. To ease use, that code accepts data in format readable by MODFLOW [4], the most widely used flow simulation model in the United States today.

These two S/O models are selected because they are the only ones we are aware of that (1) are available for use on PCs, (2) include with them the optimization algorithms necessary for solution, and (3) use superposition. As explained later, these characteristics make them especially useful for plume management by consultants and water resource managers.

II. COMPARISON BETWEEN COMMONLY USED SIMULATION MODELS AND SIMULATION/OPTIMIZATION MODELS

A simulation/optimization (S/O) model contains both simulation equations and an operations research optimization algorithm. The simulation equations permit the model to appropriately represent aquifer response to hydraulic stimuli and boundary conditions. The optimization algorithm permits the specified management objective to serve as the function driving the search for an optimal strategy. The model computes a pumping strategy that minimizes (or maximizes) the value of the objective function.

Table 1 shows generic inputs and outputs of the generally used simulation (S) model and those of an S/O model. The normal S models compute aquifer responses to assumed (input) boundary conditions and pumping values. Using such models to develop acceptable pumping strategies can be tedious and involve much trial and error. For example, simulated system response to an assumed pumping strategy might cause unacceptable consequences. In that case, the user must assume another pumping strategy, reuse the model to calculate aquifer response, and recheck for acceptability of results. This process of assuming, predicting, and checking might have to be repeated many times. The number of repetitions increases with the number of pumping locations and control locations (places where acceptability of system response must be evaluated and ensured).

When using an S model, as the number of possible pumping sites increases the likelihood that the user has assumed an "optimal" strategy decreases. Also, as the number of restrictions on acceptable system response to pumping increases, the ability of the user to assume an optimal strategy also decreases. Assuming a truly optimal strategy becomes impractical or nearly impossible as problem complexity increases. There are too many different possible combinations of pumping values. Furthermore, even if the computation process is automated in a computer program, the act of checking and ensuring strategy acceptability becomes increasingly painful as the number of control locations becomes large. In essence, it becomes impossible to compute mathematically optimal strategies for complicated groundwater management problems using S models.

Alternatively, S/O models directly calculate the best pumping strategies for the specified management objectives and ensure that the resulting heads and flows lie within prespecified limits or bounds (Table 1). The upper and lower bounds reflect the range of values that the user considers acceptable for cell pumping rates and resulting heads. The model automatically considers the bounds while calculating optimal pumping strategies. The user might choose to use lower bounds on pumping at currently operating public supply wells. He/she might choose to limit pumping at the upper end of the range, depending on hardware availability or legal restrictions. The user might impose lower bounds on head, at a specific distance below current water levels or above the base of the aquifer. Upper bounds might be the ground surface or a specified distance below the ground surface.

Assume, for example, a situation in which a planning agency is attempting to determine the least amount of groundwater pumping needed to capture a contaminant plume and the locations where it should be pumped, i.e., the spatial distribution of the withdrawals and injections. If a pumping strategy is not implemented to achieve capture, the contaminant will reach public supply wells, resulting in litigation and undesirable costs.

Table 1 Comparison Between Simulation and Simulation/Optimization Models

Model type	Input values	Computed values
Simulation (S)	Some boundary flows Some boundary heads Pumping	Some boundary flows Heads at "variable" head cells
Simulation/optimization (S/O)	Some boundary flows Some boundary heads Bounds on pumping, heads, flows	Optimal boundary flows Optimal heads at "variable" head cells Optimal pumping

An S/O model can be used to directly calculate an optimal pumping strategy for the goal of minimizing the pumping needed to capture the plume without causing unacceptable consequences. For example, assume that no injection mounds should reach the ground surface and that no drawdowns should exceed 2 m. In addition, assume that potentiometric surface gradients near the plume should be toward the plume source.

The S/O model will directly calculate the minimum total pumping rate needed and will identify how much should be pumped from each pumping location. The potentiometric surface heads and gradients that will result from the optimal pumping will lie within the bounds specified initially (Table 1). In other words, future heads will not reach the ground surface, future heads will not be more than 2 m below current heads, and final gradients will be toward the contaminant source. Thus, the very first optimal pumping strategy computed by an S/O model will satisfy all specified management goals.

III. COMMON S/O MODELING APPROACHES AND LIMITATIONS

Most S/O models employ either an embedding or a response matrix approach for representing system (head) response to pumping [5]. Embedding models contain finite-difference or finite-element equations embedded directly as constraints. In a finite-difference embedding model, head and pumping values (or other flows) must be computed for each time step at each cell. This is a very useful approach for those situations in which (1) pumping should be a decision variable at most cells, (2) head must be constrained in a high proportion of cells, and (3) either a steady-state strategy should be developed or there need be very few time steps. It is not as desirable if there are relatively few pumping cells and control points or if many time steps are needed. Thus, embedding models have been mainly used for steady-state regional planning and for small hypothetical problems.

Response matrix S/O models use linear systems theory and superposition with influence coefficients (e.g., [6]–[14] and many others). The matrix containing the influence coefficients and superposition (summation equations) is termed the response matrix. Response matrix (RM) models use a two-step process. First, normal simulation (analytical or numerical) is used to calculate system response to assumed unit stimuli. Then optimization is performed by an S/O model that includes summation equations (discretized forms of the convolution integral).

Response matrix models are ideal for transient management situations. They require constraint equations for only those specific cells and time steps at which head or flow (other than pumping) must be restricted during the optimization. To predict system response to the optimal strategy at locations and times other than those constrained in the S/O model, an external simulation model is used after the optimization.

Regardless of the simulation approach used, S/O models share some of the limitations of standard simulation models. Poor physical system representation or inadequate data will cause error. One cannot properly optimize management of system processes that one cannot correctly simulate. Useful simulation/optimization modeling presupposes that aquifer parameters are appropriate and that actual boundary conditions are represented adequately within the model.

Both embedding and RM S/O models generally assume system linearity during at least some part of their processing operation. Confined aquifers are linear, unless they become unconfined. Unconfined aquifers are nonlinear, but frequently the change in transmissivity is insignificant, and they can be treated as if they were linear. Most commonly, system nonlinearity is addressed by cycling. Cycling involves (1) assuming aquifer parameters (and computing influence coefficients for RM models), (2) calculating an optimal strategy, (3) recalculating system parameters, (4) comparing assumed and newly calculated parameter values, and (5) either stopping or returning to step 2 and repeating the process (if the assumed parameter values are still inappropriate for the problem or if the optimal strategy is still changing with cycling). Frequently, three cycles are sufficient for this convergence process. Thus, although both types of models are completely applicable for confined aquifers, some adjustments must be made to accurately apply them to unconfined aquifers.

Within S/O models, plume capture is generally achieved by controlling hydraulic gradients and thus controlling advective transport. Generally, nonlinear transport equations are not included. This approach permits the modeler to retain use of the characteristics of linear systems (superposition, etc.). All of the RM model applications presented below achieve capture via gradient control.

Concerning data input, S/O models require all of the data needed by simulation models, plus information on lower and upper bounds on decision variables (pumping rate, location) and state variables (head, gradient, etc.). Although the same sort of information should be required when using an S model, the forced codification of these data as S/O model input is helpful. It causes the modeler to specify strategy acceptability criteria earlier than he/she might otherwise.

Concerning model results, an S/O model might tell a user that the posed problem is infeasible. This means that the user has posed a problem for which all the constraints cannot be satisfied simultaneously. For example, the user might have instructed the model to cause the head near an injection cell to reach at least 100 m above mean sea level and simultaneously told it that the upper bound on injection in 50 m^3/day. If that injection rate is inadequate to cause the required change in head, the model will declare the problem to be infeasible. The model will be unable to determine even one pumping rate that can satisfy both conditions.

Of course, if there is more than one potential injection well, the same problem might be feasible. In that case, the model can compute an optimal pumping strategy (probably the user would have requested a strategy that minimizes the total pumping needed to achieve that head).

Fortunately, S/O model users rapidly get beyond the stage wherein they try to develop impossible pumping strategies (force the model to achieve goals that are impossible or mutually exclusive when considering both the laws of nature and the goals of humans). Experience brings the S/O modeler great ability to address common management problems.

IV. PC-BASED S/O MODELS AND SAMPLE APPLICATIONS

A. US/WELLS^D for Systems Addressable Using Analytical Solutions

1. Model Background

US/WELLS^D (Utah State extraction/injection well system for optimal groundwater management) is a deterministic version of an RM model. It uses influence coefficients based on analytical equations for potentiometric surface response to pumping and river depletion resulting from pumping. It is appropriate for systems where those analytical approaches are appropriate—presumably relatively homogeneous systems. (Of course, in the management and consulting arena, such approaches are commonly applied to heterogeneous systems, with acceptable error.)

Characteristics of US/WELLS^D are summarized in Table 2. The overview below is derived from the user's manual [15].

The objective function of the optimization module in US/WELLS is generally applicable and easily used for a variety of situations. The user can select either a linear or a quadratic form. The linear objective function is to minimize

$$\sum_{x=1}^{2} [W_{E,x} \sum_{j=1}^{J} E_{j,x} + W_{I,x} \sum_{k=1}^{K} I_{k,x}] \tag{1}$$

Table 2 Characteristics of US/WELLS[D] and US/REMAX[B]

	US/WELLS[D]	US/REMAX[B]
Systems addressed	One Layer, homogeneous Stream/aquifer Stream stage not affected by pumping	Multilayer heterogeneous Stream/aquifer Stream stage affected by pumping
Management period	One or two stress periods of equal or unequal duration Steady state or transient Can rep. transient evolutionary era with terminal steady-state conditions.	One or multiple stress periods of equal duration Steady state or transient
Influence coefficients	Deterministic Based on analytical expressions by Theis and Glover and Balmer	Deterministic Based on finite-difference simulation (MODFLOW+STR)
Objective function	Min or max pumping or combination Time-varying weight for extraction and injection	Min or max pumping or combination Diff. weight for each pumping location
Bounds and constraints	$g^L \le g \le g^U$ $h^L \le h \le h^U$ $G^L_{1,2} \le G_{1,2} \le G^U_{1,2}$ $\frac{\Sigma\,(\text{Ext})}{\Sigma\,(\text{Inj})} \le 1.X$ $= 1.0$ $\ge 1.X$ $d^L \le d \le d^U$	$g^L \le g \le g^U$ $h^L \le h \le h^U$ $\Delta h^L_{1,2} \le \Delta h_{1,2} \le \Delta h^U_{1,2}$ $G^L_{1,2} \le G_{1,2} \le G^U_{1,2}$ $V^L_{1,2} \le V_{1,2} \le V^U_{1,2}$ $\frac{\Sigma\,(\text{Ext})}{\Sigma\,(\text{Inj})} \le 1.0$ $= 1.0$ ≥ 1.0 $\Sigma(\text{Ext})^L \le \Sigma(\text{Ext}) \le \Sigma(\text{Ext})^U$

Notes: Superscripts L and U refer to lower and upper bounds; g = extraction or injection, [L^3/T]; h = head.; Δh, $G_{1,2}$, $V_{1,2}$ = head-difference, gradient, and velocity, respectively, between any two locations, [L], dimensionless, or [L/T]; Σ (Ext), Σ (Inj) = total extraction or injection, [L^3/T]; d = stream depletion, [L^3/T].

where $W_{E,x}$ and $W_{I,x}$ are the cost coefficient or weight assigned to extraction (E) or injection (I) rates in the x_{th} time period, [\$/($L^3 \cdot T$)] or dimensionless; $E_{j,x}$ and $J_{k,x}$ are extraction (E) or injection (I) rate at well j (or k) in the x_{th} time period, [L^3/T]; and J and K are number of extraction (J) or injection (K) wells.

Potential constraints are the following.

1. Hydraulic gradient between any gradient control pair of wells at any time period must be within user-specified bounds. This can ensure that water is moving only in the desired direction. The maximum value can differ for each gradient control pair and time period. This constraint is useful, for example, when US/WELLS[D] is used for groundwater contaminant plume immobilization or for any situation where hydraulic gradient control is desired.
2. Extraction or injection rate at any well must be within user-specified bounds (lower and upper limits). If the user cannot decide if a certain well should be used for extraction or injection, he can locate one of each at the same location. The model will then determine either an extraction or an injection rate, or neither, for that location.

3. Hydraulic head at any injection, extraction, or observation well must be within user-specified lower and upper bounds. For example, a lower bound may be used to maintain adequate saturated thickness. An upper bound may be used to prevent surface flooding or to eliminate the need for pressurized injection. These lower and upper bounds can differ for different locations. The bounds are the same for both time periods.
4. Total import or export of water can be controlled to be within a user-specified range. The user can also completely prevent import or export of water or both. If no import or export of water is allowed, the total optimal extraction must equal the total optimal injection.
5. Depletion from the river must be within user-specified bounds (lower and upper limits). This is applicable only if a river exists in the considered system.
6. Constraint 3 is modified such that the probability that the actual change in head at any point in the groundwater system is not less than the change calculated by the model or is not greater than the change calculated by the model and is at least equal to the reliability level specified by the user. (This ability is found only in an alpha-test chance-constrained version of the model, US/WELLS^S, which considers the stochastic nature of hydraulic conductivity. The utilized chance constraint is more accurate than previously reported formulations.)

Optionally, US/WELLS^D can use a quadratic objective function to minimize

$$\sum_{x=1}^{2} [WW_{E,x} \sum_{j=1}^{J} E_{j,x} H_{j,x} + W_{E,x} \sum_{j=1}^{J} E_{j,x} + W_{I,x} \sum_{k=1}^{K} I_{k,x}] \tag{2}$$

where $H_{j,x}$ is the dynamic lift, the difference between ground surface elevation and optimal potentiometric head resulting at extraction well j at the end of the x_{th} time period, [L]; and $WW_{E,x}$ is the weight assigned to the power used for extraction in the x_{th} time period, [\$/L·T)].

The weighting factors can be used to emphasize different criteria and different time periods. For example, assume a problem of minimizing the total extraction using the linear objective function. If the second time period is chosen to be much longer than the first time period and the weights assigned to extraction and injection in the second time period are larger than those used for the first time period, then the solution will tend to minimize steady-state extraction/injection rates, and less attention will be given to the short-term transient rates. Through the weighting factors, US/WELLS^D can also be used for maximizing pumping rates for water supply problems.

2. Application and Results

Here we illustrate the use of US/WELLS^D to determine the optimal time-varying sequence of extraction and injection of water in prespecified locations needed for first immobilizing and then extracting a groundwater contaminant plume. In this example, the user specifies *potential* locations of extraction and injection wells around the contaminant plume (Figure 1). US/WELLS^D then determines optimal extraction and injection rates for different time periods.

To illustrate model flexibility, four potential extraction wells and five potential injection wells are considered for placement outside the contaminant plume during the first period. In the second time period, three extraction wells are considered for placement inside the plume (to extract contaminated water) and five potential downgradient injection wells are considered. During both periods, the resulting hydraulic gradients (between 10 pairs of head observation locations) must be toward the center of the plume. Alternatively, the user could choose to minimize the pumping needed to capture the plume using only internal extraction wells in one or both periods.

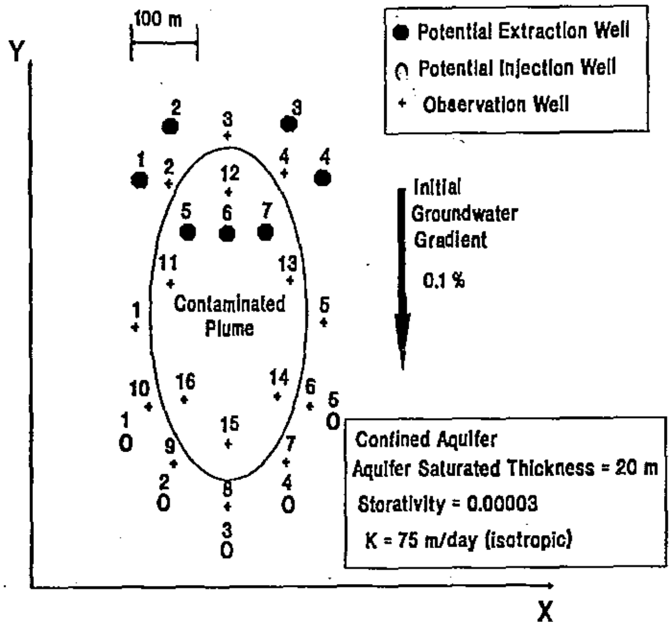

Figure 1 Hypothetical study area for Example A, addressable with US/WELLS^D.

Here, the quadratic objective function is used and employs greater weights for the second time period than the first period. This supports the fact that the second period is much longer than the first. In addition, neither export nor import of water is allowed—total injection must equal total extraction in each period. All the above considerations are incorporated within the model via the input data [15]. The user also specifies lower and upper bounds on head and pumping rates.

Figure 2 shows US/WELLS^D output, in meters and m^3/day. This contains, in addition to the input bounds (L. Bound and U. Bound), the optimal values of the decision variables (pumping), state variables (head and gradient), and marginal values.

The marginal is defined as the value by which the objective function will change if a tightly bounded variable changes one unit. If a variable's optimal value is not equal to either its lower or upper bound, its marginal will be zero. That is, the marginal will be nonzero only if the optimal value of the variable equals one of its bounds. In this case, the marginal shows the improvement of the value of the objective function resulting from relaxing this bound by one unit. Marginals are valid only as long as no other variable also changes in value. Thus they might be valid for only a small range of change in the bound.

To illustrate, the output file (Figure 2) shows that the marginal of the optimal injection rate in the first time period at injection well 3 is −45.3. The objective function value was 334,668.1. If the upper bound on injection in the first time period is relaxed by one unit at the mentioned well (that is, the new upper bound is 901 instead of 900), one would expect the value of the objective function to change by about −45.3 to 334,622.8. If this change is actually made and the model is rerun, the resulting change in objective function value is −45.4.

Marginals are useful in determining how to refine an optimal strategy. They help one to decide which bounds or constraints should be looked at more closely and perhaps relaxed. They also indicate the trade-off between that bound and objective achievement. They show how much one is giving up in terms of objective attainment to satisfy that restriction.

MODEL STATUS : OPTIMAL SOLUTION FOUND
VALUE OF OBJECTIVE FUNCTION 334668.1

OPTIMAL EXTRACTION RATES

FIRST TIME PERIOD

Well No	L.Bound	Optimal	U.Bound	Marginal
1	0.00	745.42	900.00	0.000
2	0.00	447.60	900.00	0.000
3	0.00	448.71	900.00	0.000
4	0.00	747.86	900.00	0.000
5	0.00	0.00	0.00	0.000
6	0.00	0.00	0.00	0.000
7	0.00	0.00	0.00	0.000

SECOND TIME PERIOD

Well No	L.Bound	Optimal	U.Bound	Marginal
1	0.00	0.00	0.00	81.955
2	0.00	0.00	0.00	81.627
3	0.00	0.00	0.00	81.605
4	0.00	0.00	0.00	81.913
5	0.00	426.53	900.00	0.000
6	0.00	883.77	900.00	0.000
7	0.00	428.90	900.00	0.000

OPTIMAL INJECTION RATES

FIRST TIME PERIOD

Well No	L.Bound	Optimal	U.Bound	Marginal	
1	0.00	211.66	900.00	0.000	
2	0.00	328.89	900.00	0.000	
3	0.00	900.00	900.00	-45.342	<=== *explained in text*
4	0.00	900.00	900.00	0.000	
5	0.00	49.04	900.00	0.000	

SECOND TIME PERIOD

Well No	L.Bound	Optimal	U.Bound	Marginal
1	0.00	0.00	900.00	132.584
2	0.00	293.53	900.00	0.000
3	0.00	900.00	900.00	-4.3E+2
4	0.00	545.67	900.00	0.000
5	0.00	0.00	900.00	132.583

OPTIMAL HEADS AT OBSERVATION WELLS

FIRST TIME PERIOD

Well No	L.Bound	Optimal	U.Bound	Marginal
1	30.00	35.69	40.00	0.000
2	30.00	35.54	40.00	0.000
3	30.00	35.60	40.00	0.000
4	30.00	35.55	40.00	0.000
5	30.00	35.70	40.00	0.000
6	30.00	35.79	40.00	0.000
7	30.00	35.92	40.00	0.000
8	30.00	35.88	40.00	0.000
9	30.00	35.84	40.00	0.000
10	30.00	35.77	40.00	0.000
11	30.00	35.65	40.00	0.000
12	30.00	35.60	40.00	0.000
13	30.00	35.65	40.00	0.000
14	30.00	35.79	40.00	0.000
15	30.00	35.88	40.00	0.000
16	30.00	35.77	40.00	0.000

Figure 2 US/WELLS[D] output file for Example A.

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SECOND TIME PERIOD

Well No	L.Bound	Optimal	U.Bound	Marginal
1	30.00	35.62	40.00	0.000
2	30.00	35.62	40.00	0.000
3	30.00	35.68	40.00	0.000
4	30.00	35.62	40.00	0.000
5	30.00	35.63	40.00	0.000
6	30.00	35.66	40.00	0.000
7	30.00	35.75	40.00	0.000
8	30.00	35.74	40.00	0.000
9	30.00	35.71	40.00	0.000
10	30.00	35.64	40.00	0.000
11	30.00	35.56	40.00	0.000
12	30.00	35.54	40.00	0.000
13	30.00	35.56	40.00	0.000
14	30.00	35.66	40.00	0.000
15	30.00	35.74	40.00	0.000
16	30.00	35.64	40.00	0.000

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OPTIMAL HEADS AT EXTRACTION WELLS

FIRST TIME PERIOD

Well No	L.Bound	Optimal	U.Bound	Marginal
1	30.00	35.09	40.00	0.000
2	30.00	35.29	40.00	0.000
3	30.00	35.29	40.00	0.000
4	30.00	35.09	40.00	0.000
5	30.00	35.61	40.00	0.000
6	30.00	35.62	40.00	0.000
7	30.00	35.61	40.00	0.000

SECOND TIME PERIOD

Well No	L.Bound	Optimal	U.Bound	Marginal
1	30.00	35.69	40.00	0.000
2	30.00	35.72	40.00	0.000
3	30.00	35.73	40.00	0.000
4	30.00	35.70	40.00	0.000
5	30.00	35.24	40.00	0.000
6	30.00	34.90	40.00	0.000
7	30.00	35.25	40.00	0.000

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OPTIMAL HEADS AT INJECTION WELLS

FIRST TIME PERIOD

Well No	L.Bound	Optimal	U.Bound	Marginal
1	30.00	35.90	40.00	0.000
2	30.00	36.03	40.00	0.000
3	30.00	36.46	40.00	0.000
4	30.00	36.47	40.00	0.000
5	30.00	35.83	40.00	0.000

SECOND TIME PERIOD

Well No	L.Bound	Optimal	U.Bound	Marginal
1	30.00	35.65	40.00	0.000
2	30.00	35.88	40.00	0.000
3	30.00	36.33	40.00	0.000
4	30.00	36.08	40.00	0.000
5	30.00	35.67	40.00	0.000

OPTIMAL HYDRAULIC GRADIENTS

FIRST TIME PERIOD

From	To	L.Bound	Optimal	U.Bound	Marginal
1 ->	11	0.00000	0.00055	0.01000	0.000
3 ->	12	0.00000	0.00003	0.01000	0.000
5 ->	13	0.00000	0.00019	0.01000	0.000
6 ->	14	0.00000	0.00000	0.01000	1.17E+7
7 ->	14	0.00000	0.00157	0.01000	0.000
8 ->	15	0.00000	0.00000	0.01000	3.26E+7
9 ->	16	0.00000	0.00087	0.01000	0.000
10 ->	16	0.00000	0.00000	0.01000	1.17E+7

SECOND TIME PERIOD

From	To	L.Bound	Optimal	U.Bound	Marginal
1 ->	11	0.00000	0.00082	0.01000	0.000
3 ->	12	0.00000	0.00241	0.01000	0.000
5 ->	13	0.00000	0.00027	0.01000	0.000
6 ->	14	0.00000	0.00014	0.01000	0.000
7 ->	14	0.00000	0.00115	0.01000	0.000
8 ->	15	0.00000	0.00000	0.01000	2.88E+8
9 ->	16	0.00000	0.00081	0.01000	0.000
10 ->	16	0.00000	0.00000	0.01000	0.000

Figure 2 Continued.

B. US/REMAX^B for Heterogeneous Multilayer Systems

1. Model Background

For optimizing management of complex heterogeneous systems, one would rather use US/REMAX^B [16] than US/WELLS^D. This is the basic version of the Utah State response matrix model. To develop influence coefficients, it uses code modified from MODFLOW, a modular finite-difference groundwater flow simulation model [4], and STR, a related stream routing module [17]. The physical system data needed by US/REMAX^D can be input in the same format as is used by MODFLOW and STR. Internally, US/REMAX^B also uses a portion of PLUMAN, a decision support system for optimal groundwater contaminant plume management [18], and other code.

The optimization model formulation capabilities are similar to those of US/WELLS^D (Table 2). For steady state, the generic objective is to minimize

$$\sum_{j=1}^{J} W_j E_j + \sum_{k=1}^{K} W_k I_k \tag{3}$$

where W_j is the weight assigned to pumping in cell j, dimensionless or [$\$\cdot T/L^3$]. US/REMAX^B can employ constraints 1–3 of US/WELLS^D for multiple layers. Similar to the US/WELLS^D constraint 4, US/REMAX^B can force total extraction to exceed, equal, or be less than total injection. Again, via the sign on the weighting coefficients, one can perform maximization. One can also achieve multiobjective optimization by the weighting method. Whereas in US/WELLS^D the same weight must be applied to all extraction wells in a time step (and a different weight can be used for injection wells, but the same must be applied to all such wells in a particular time step), in US/REMAX^B each well can employ a different weight.

2. Application and Results

Introduction. For illustration, we discuss addressing a contaminant plume in a representative study area. First, the study area is described and the results of continuing current management are predicted, using MODFLOW+STR for flow simulation and MOC [19] for transport simulation. Then an approach to developing an optimal strategy is discussed, the S/O model is applied, and an optimal strategy is computed. Next, the system response to implementing the optimal strategy is verified using MODFLOW+STR and MOC. Finally, slight variations in the management goal or situation are assumed and new optimal strategies are developed. Computed optimal strategies are compared. Suguino [20] first addressed this study area using PLUMAN. Some of the discussion below follows his development.

Study Area Description and Situation. The area (Figure 3) measures about 4.3 km by 4.3 km. It is bounded on the north by a large saltwater body; on the south, east, and northwest by impermeable material; and on the west by a lake. A river transects the area from south to north. Aquifer parameters of this example study area were obtained from ranges reported by Todd [21].

For the unconfined upper layer (layer 1), parameters are as follows.

Hydraulic conductivity:

1st zone: 45 m/day (coarse sand) from lake to contaminant spill area (columns 1–36 and 57–58)
2nd zone: 30 m/day (medium sand) in irrigated area (columns 51–56)
3rd zone: 450 m/day (fine gravel) in contaminant spill area (columns 37–50).

Specific yield:

1st zone: 0.27 (coarse sand)
2nd zone: 0.28 (medium sand)
3rd zone: 0.25 (fine gravel)

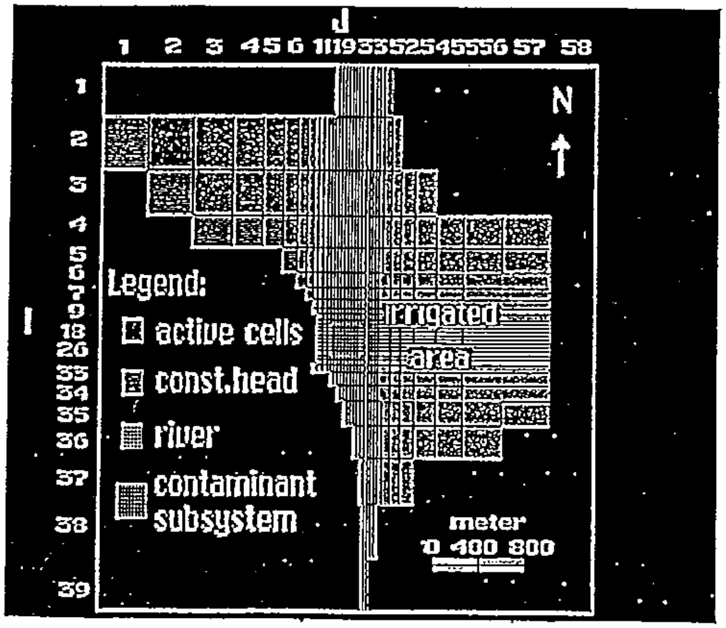

Figure 3 Finite-difference grid for the area addressable with US/REMAX[B].

Recharge by deep percolation and/or irrigation:

1.167×10^{-8} m/sec in nonirrigated area
1.928×10^{-8} m/sec in irrigated area

In the confined lower layer (layer 2):

Transmissivity:	0.1564 m^2/sec
Saturated thickness:	30.0 m
Storage coefficient:	0.0001

Finite-difference models are to be used in this study. This requires system discretization. The resulting block-centered cell grid (Figure 3) has 58 columns and 39 rows. Cell side lengths range from 3 to 400 m. Because MOC will be used for transport simulation near the plume, cells of uniform size are specified for that region. The resulting 17 row by 20 column region (subsystem) near the plume has square cells of 15.2 m (50 ft) side length.

A conservative (nonreactive) contaminant is assumed to be spilled in the top aquifer layer (layer 1) of cell (22, 18) or (11_s, 3_s). (The subscript "s" after a cell row or column index indicates that the cell is in the subsystem.) This cell is treated as a continuous source during the management period.

Initially, pumping for water supply occurs in two cells between the plume and the river. One well is in layer 1 of (23, 15) or (12_s, 15_s). The other well is in layer 2 of (18, 18) or (7_s, 18_s). There is immediate concern about the potential for contamination reaching the supply well in layer 1.

Nonoptimal System Response Determination (Step 1). Before one attempts to develop an optimal strategy, one usually demonstrates the need for such a strategy. This requires predicting system response if no optimal strategy is implemented. Frequently, simulation models are used for this action. Here, MODFLOW+STR computes the potentiometric surface that will result from assumed steady-state conditions (Figure 4).

Because of the gradient, the contaminant will tend to migrate toward the supply wells. MOC is used to quantify the migration resulting in the subsystem from the steady flow. Figure 5 shows the 210 ppb contour expected to result 60 days after contamination begins. Furthermore, concentration in the cell containing the drinking well (12_s, 15_s) reaches 317 ppb 8 months after the spill. We assume that this concentration level exceeds the health advisory for human consumption and that developing a plume capture strategy is desirable.

Management Goals Specification and S/O Model Formulation for Scenario 1 (Step 2). The assumed goal is to minimize the steady pumping (extraction and injection) needed to capture the plume. Plume capture will presumably be achieved when hydraulic gradients, just outside the plume boundary, all point toward the plume interior. We also want the head at extraction wells not to drop too far (to avoid reducing saturated thickness by more than about 10%) or the head at injection wells not to rise to the ground surface. These criteria identify the example problem termed Scenario 1.

The S/O model formulation for this scenario is shown below. The model computes the pumping strategy that minimizes the value of the objective function, subject to the stated constraints and bounds. Locations of potential injection and extraction wells to be considered by the model are shown in Figure. 5. Figure 6 identifies head difference (gradient) control cell pairs and shows the direction that will be imposed on the hydraulic gradient by any computed optimal strategy. These are placed to enclose the plume projected to exist by day 60. A modeler can select potential well locations on the basis of practical experience. For example, the closer the injection wells are to the head gradient control locations, the less pumping is needed to

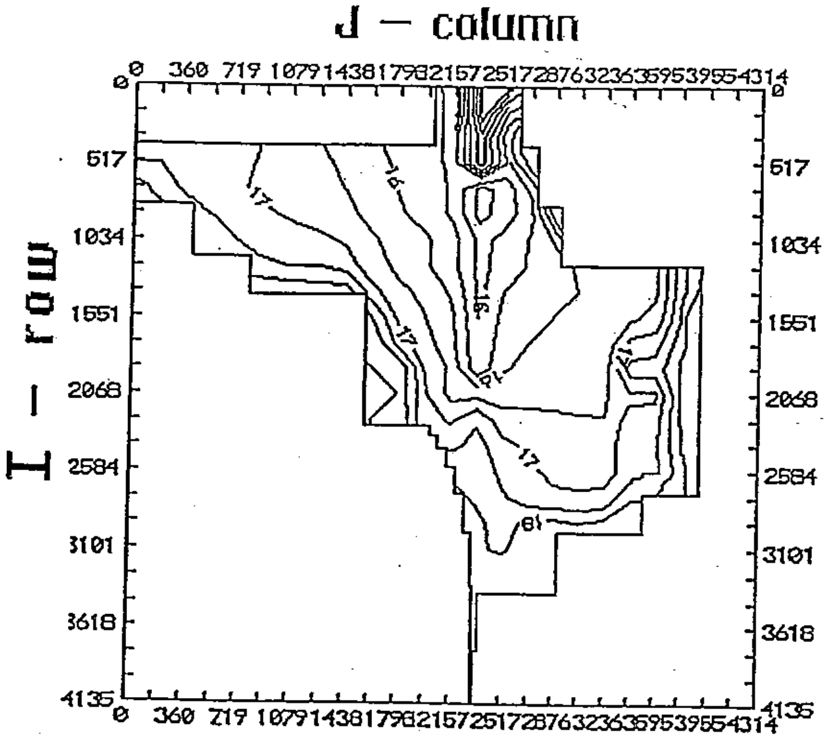

Figure 4 Nonoptimal (unmanaged) steady-state potentiometric surface contour map for the study area of Scenario 1 (meters above MSL).

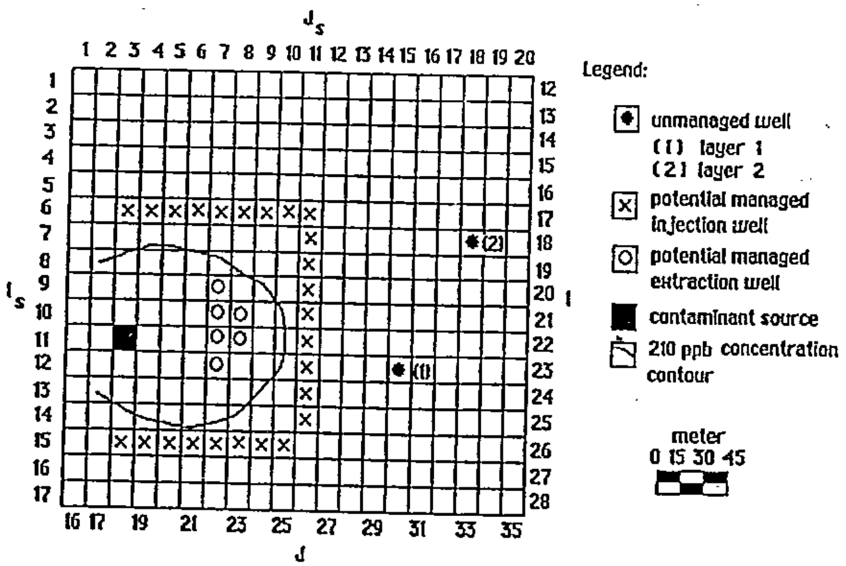

Figure 5 Subsystem discretization, potential well locations for Scenario 1, and 210 ppm contour, 60 days after contamination begins.

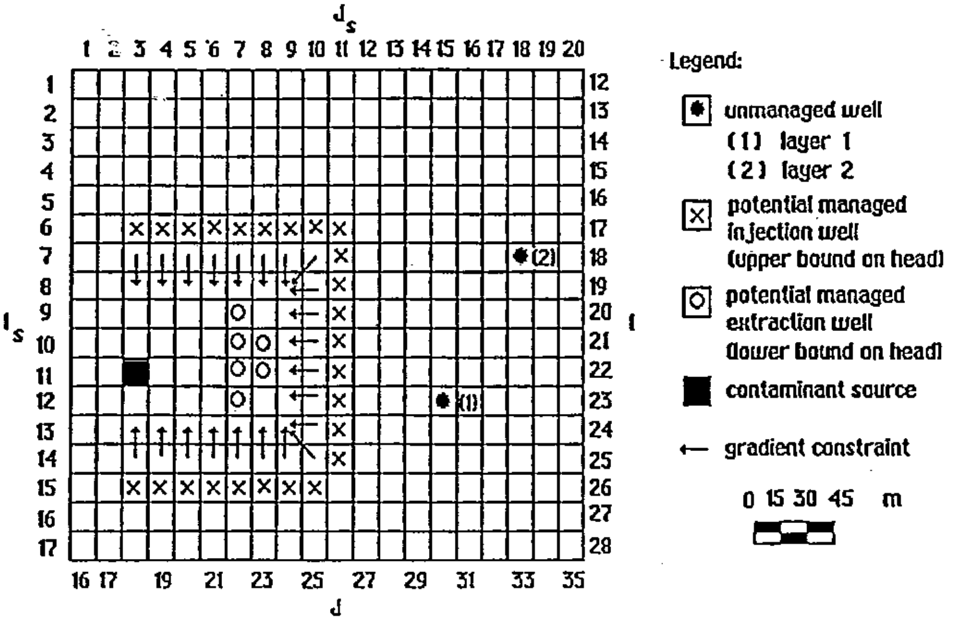

Figure 6 Head-difference constraint locations applied within the S/O model in Scenario 1.

satisfy the head-difference constraint. Thus, the modeler might want the model to consider pumping sites near the location where heads need most to be affected.

The model objective is to minimize the value of Equation (3), using weights of 1, subject to

$$G_{\bar{o}} \geq 0.01, \qquad \text{for } \bar{o} = 1, \ldots, 22 \tag{4}$$

$$h_{\hat{e}} \geq 15.0, \qquad \text{for } \hat{e} = 1, \ldots, 6 \tag{5}$$

$$h_{\hat{e}} \leq 25.0, \qquad \text{for } \hat{e} = 1, \ldots, 25 \tag{6}$$

where $G_{\bar{o}}$ is the difference in head between a pair of cells, the first located farther from the plume. A positive value denotes a higher head farther from the plume, [L]; $h_{\hat{e}}$ is the hydraulic head just outside the casing of pumping well $\hat{e}$ located in the center of a pumping cell, [L]; $\bar{o}$ is the index denoting pair of cells head-difference (gradient) control pair; and $\hat{e}$ is the index denoting pumping well at the center of cell j or k. Here $j = 6$ and $k = 25$.

Note that identifying the location of potential extraction and injection wells for the model (Figure 5) does not mean that the model will choose to pump at those locations. Via the optimization process, the model might choose to pump at only a few of the potential sites. The computed strategy will require less total pumping than any other strategy possible for the specified potential well locations and imposed bounds and constraints. Furthermore, since this is a steady-state problem, steady-state system response to implementing the strategy computed by the model will satisfy all those bounds and constraints. This is verified in the next step.

Optimal Strategy Computation and Verification for Scenario 1 (Step 3). The optimal strategy computed for Scenario 1 is shown in Table 3. Because the model is minimizing pumping only for plume containment in layer 1, no extraction is shown for layer 2. The original unmanaged pumping does continue from original supply wells in both layers (Figure 3) but is not included in Table 3 because the model is not optimizing that pumping.

Table 3 Pumping Results for the Sample Scenarios

Scenario	Constraints	g(extr) 1st Layer	g(extr) 2nd Layer	b(inj.) (m³/sec)	(g + b) total (gpm)
1	Gradient constraint on heads located on the same layer, head constraint on injection and extraction well.	0.01338 (212.05)	— —	0.02020 (320.13)	0.03358 (532.18)
2	Added pumping constraint: total sum of extraction = total sum of injection.	0.01702 (269.74)	— —	0.01702 (269.74)	0.03404 (539.48)
3	Gradient constraint on heads located on the same and on different layers, head constraint on injection and extraction wells.	0.00300 (47.54)	0.00329 (52.14)	0.03786 (600.03)	0.04415 (699.69)

Figure 7 shows the locations of wells that will pump, according to the optimal strategy. It also shows the head-difference constraints [Equation (4)] that will be tight. Tight constraints are those that are satisfied exactly. The other gradient constraints are also satisfied, but the model had no difficulty in doing so. These latter head-difference constraints are "loose" (there is more than 0.01 m difference between the heads at the two cells coupled by an arrow in Figure 6 but not shown at all in Figure 7). No heads are against their bounds. Therefore neither Equation (5) nor (6) is tight.

It is appropriate to verify that the computed strategy accomplished its goal of plume capture. MODFLOW+STR can be used to demonstrate how quickly the optimal steady pumping

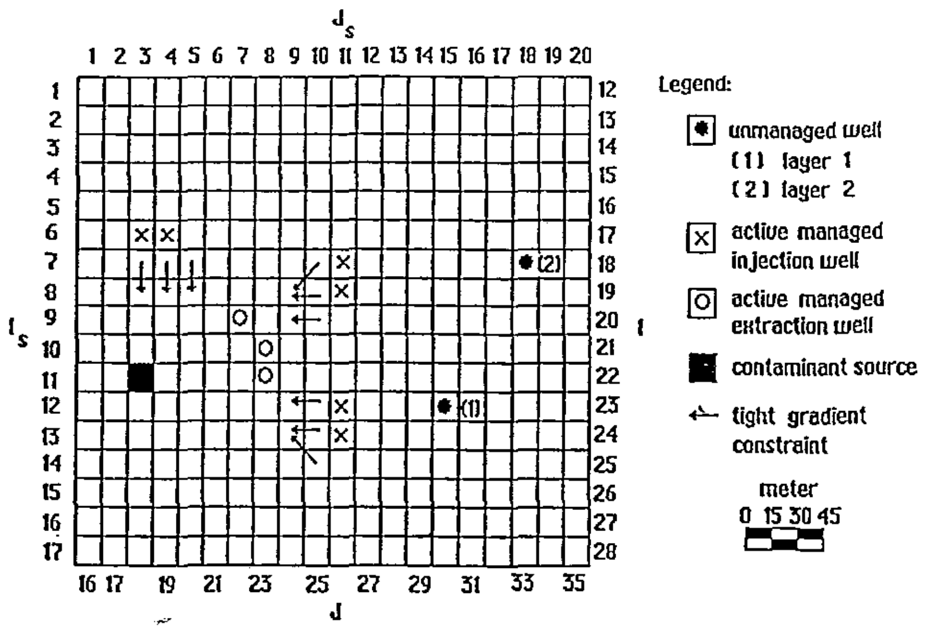

Figure 7 Location of optimal pumping wells and tight head-difference (gradient) constraints for Scenario 1.

strategy will cause the desired gradients to occur. Transient simulation demonstrated that the gradient constraints would be satisfied 30 days after implementing the optimal pumping strategy (Figure 8). Figures 9 and 10 show the ultimate steady-state surface resulting from strategy implementation. Clearly, a groundwater divide has been formed between the plume and the supply well.

MOC is used to predict the pollutant transport that would result from strategy implementation. No contaminant moved past the injection wells.

Theoretical verification of the optimality of the computed strategy is beyond the scope of this document. However, many texts on operations research and linear programming assure the optimality of solutions to models having a linear objective function and constraints.

Alternative Scenarios.

Scenario 2. This scenario differs from the previous in the addition of a constraint forcing total injection to equal total extraction around the plume. Again, pumping from the two supply wells is not included in the total.

```
aquifer  optimal  all gradients                    check of
contam.  pumping  constraints                      cont.conc.
         begins    achieved

   I--------I--------I--------------------------------I

   0        60       90                              240   days
```

Figure 8 Time scale of Scenario 1.

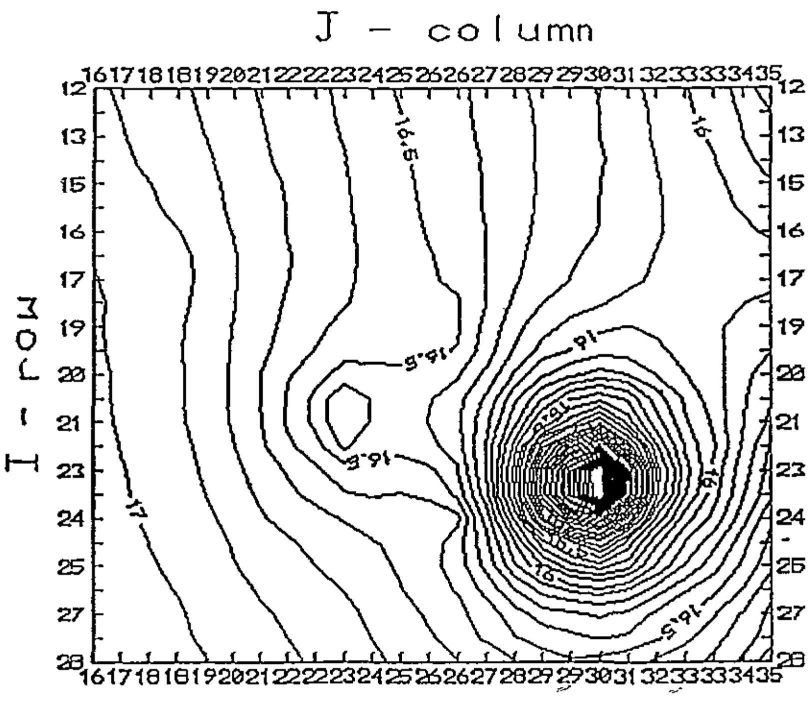

Figure 9 Subsystem potentiometric surface resulting from implementing the optimal pumping strategy for Scenario 1 (meters above MSL).

Well	lps	gpm	Well	lps	gpm
1	1.36	21.56	6	−3.09	−49.02
2	0.62	9.89	7	5.02	79.53
3	−0.60	−9.49	8	4.46	70.67
4	−9.69	−153.55	9	7.88	124.96
5	0.85	13.46	10	−100.00	−1584.82

(+) recharge (−) withdrawal

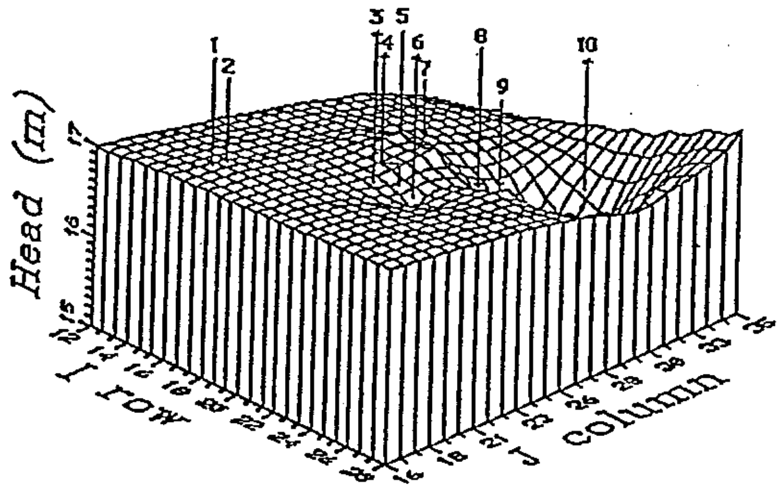

Figure 10 Subsystem potentiometric surface resulting after 6 months of optimal pumping for Scenario 1 (meters above MSL).

Results in Table 3 show an increase in extraction and a decrease in injection. Total pumping needed for plume containment increased slightly (1.4%). This illustrates the phenomenon—increasing the number or restrictiveness of constraints does not improve the value of the objective function.

Although total pumping increased, one less extraction well is used in this strategy than in the previous (Table 4). The same number of gradient constraints are tight, but the locations of the tight gradient constraints differ slightly.

Scenario 3. This scenario demonstrates what might happen if involved managers have conflicting goals. It differs slightly from Scenario 1. In addition to controlling the plume, the agency wishes to extract more from layer 2 for water supply. Three new potential extraction wells are located in cells (19, 25), (20, 25), and (21, 25), as if along a nearby road. Pumping is not permitted to change at the two initial supply wells.

Table 4 Numbers of Managed Wells that Will Pump Under the Optimal Strategies for the Tested Scenarios

	g(extr.)			
Scenario	1st Layer	2nd Layer	b(inj.)	$(g + b)$ total
1	3	—	6	9
2	2	—	6	8
3	4	3	14	21

As a result, the objective function is altered to maximize new extraction from layer 2 while still minimizing the pumping in layer 1 needed to capture the plume. This is achieved by assigning a negative sign to extraction from the supply wells, and minimizing:

$$\sum_{j=1}^{J} (E_j)_{1st\ layer} - (E_j)_{2nd\ layer} + \sum_{k=1}^{K} (I_k)_{1st\ layer} \tag{7}$$

Since minimizing a negative number is the same as maximizing a positive number, minimizing negative extraction in layer 2 means maximizing that extraction.

Also added are new constraints imposed on vertical flow in cells (21, 21) and (22, 21). There, the head in the lower layer is forced to exceed that in the upper layer by 0.01 m, preventing the downward migration of contaminant.

Figure 11 shows the resulting optimal injection and extraction well locations and tight gradient constraints. The optimal pumping strategy includes seven extraction wells and 14 injection wells. Although extraction of polluted water decreases, injection increases with respect to Scenario 1 (Table 3). Extraction of water for public supply increases by 31% above the unmanaged rate.

Although the gradient constraints are all satisfied by the optimal strategy, subsequent simulation demonstrated that the vertical gradient is reversed in some plume-containing cells in which the gradient was unconstrained. This illustrates that one must be careful in placing head or gradient control in appropriate locations. In practice, another optimization would be performed, using additional vertical head-difference or gradient constraints.

Processing Considerations. It is useful to consider the resources required to address optimization problems. First, the total computer time needed to solve an optimization problem is of

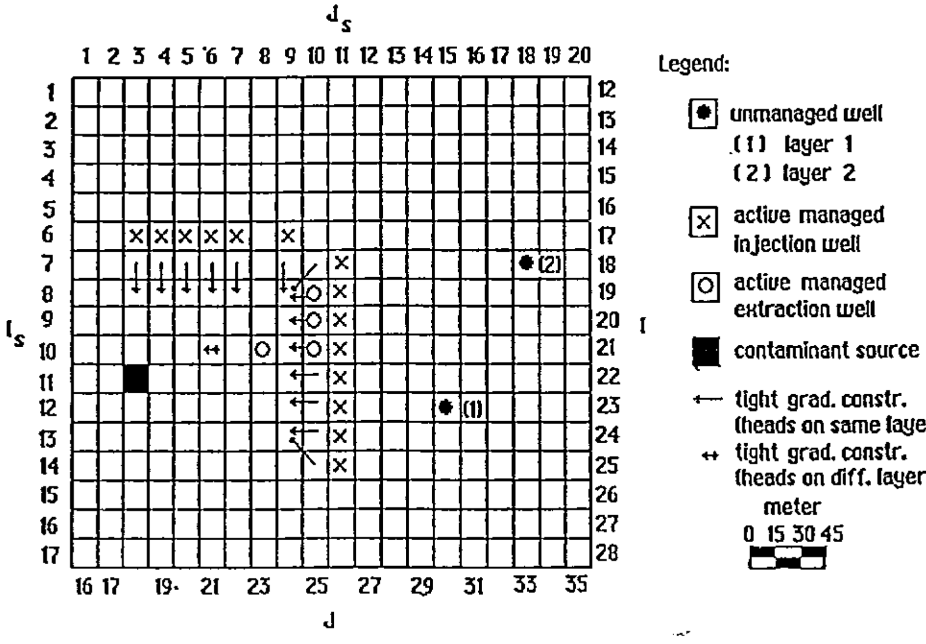

Figure 11 Location of optimal pumping wells and tight head-difference (gradient) constraints for Scenario 3.

interest. Table 5 illustrates the time needed to address Scenario 1. Included stages use either the discussed simulation models or the PLUMAN code on a 386 PC running at 33 MHz and having 4 MB RAM. Time required for US/REMAX^{B} is comparable to that of PLUMAN, since it uses many of the same solution procedures.

Clearly, the stage of computing influence coefficients, arranging the optimization model, and calculating an optimal strategy is the most computationally intensive. For this scenario and stage, two steps can be distinguished. The first involves computing influence coefficients. The second is model organization and optimization problem solution.

Here, the step of generating influence coefficients requires by far the most time. This results because this act essentially involves one simulation of a modified MODFLOW+STR per potential pumping location. Since there are 31 potential pumping locations, 31 simulations are performed to develop the influence coefficients needed for the response matrix. The more decision variables (potential pumping rates), the more computer time involved in this step.

The step involving model formulation and calculation of the optimal strategy is fairly short. The time needed to perform the optimization is a function of the number of decision variables (potential pumping rates) and state variables (heads or gradients that must be constrained within the optimization model). The larger these numbers, the more time required.

Second, the size of the optimization problem being solved is of interest. For example, the special versions of US/WELLS^{D} and US/REMAX^{B} that are released in shortcourses are limited in the number of nonzero values they can have in the optimization formulation. (Even optimization algorithms that are not part of water management models are commonly limited either in the number of nonzeros or in the number of rows and columns in their constraint equations.)

By way of explanation, there is one row in the response matrix per head or gradient constraint equation per time step of constraint. There is one column in the matrix per decision variable. For a steady-state problem, total matrix size is the product of the number of control locations and the number of decision variables. The matrix contains one nonzero coefficient for each potential pumping location–head control location pair (per time step of active constraint).

For the steady-state Scenario 1, there are $31 \times (22 + 31)$, or 1643, nonzeros due to influence coefficients. There are also 31 nonzeros due to the weighting coefficients (even if they are 1 in value) assigned to decision variables in the objective function. Thus, the optimization model formulation for Scenario 1 employs almost 1700 nonzeros. (That of Scenario A using US/WELLS^{D} includes 919 nonzeros.) This number can be reduced significantly by considering injection in only every other cell on the plume periphery rather than in each cell. For example, if only 12 injection wells were considered, the number of nonzeros would be about $18 \times (22 + 18) + 18$, or 738. In addition to reducing problem size, this would significantly reduce computational time.

Table 5 Computer Time Required to Perform Each Activity for Scenario 1

Step	Software used	Time (min)
1	MODFLOW+STR (compute nonoptimal head)	5.0
2	MOC (predict solute transport in a nonoptimal potent surface)	35.0
3	PLUMAN (compute influence coefficients, formulate management model and determine optimal pumping strategy)	150.0
4	MODFLOW+STR (compute transient head response to optimal pumping)	1.3
5	MOC (compute head and solute transport response to optimal pumping)	8.0

Reducing the number of nonzeros below 1000 is important because that is the upper limit on problem size in the inexpensive "special" versions of US/REMAX[B] and US/WELLS[D]. If problem size increases beyond that, software price increases dramatically. The full professional versions of the software can address problems of virtually unlimited size.

V. SUMMARY

Use of simulation/optimization models can significantly aid management of groundwater contamination. It can speed the design process and reduce manpower costs. It can improve the produced remediation designs and reduce remediation costs. It can easily address problems previously considered very difficult.

S/O modeling methods for groundwater flow management have been well established in research literature. Now, generally applicable S/O models are available for use on PCs. The discussed models, US/WELLS[D] and US/REMAX[B], use linear systems theory, influence coefficients, and superposition. These models can address a wide range of problems. Easy to use, they include all simulation and optimization algorithms needed to compute optimal strategies.

US/WELLS[D] and US/REMAX[B] are perfectly applicable to linear (confined) aquifer systems and can be applied to nonlinear systems. The former is most appropriate for fairly homogeneous aquifer and stream-aquifer systems. The latter can address complex heterogeneous multilayer stream-aquifer systems.

Increasing use of these PC-based S/O models is anticipated, especially as user-friendly options increase. Even the special versions of these models (released at shortcourses), can solve important real-world problems.

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1. Page 600: replace "depletion" with "pumping" in the 10^{th} line from the bottom of the page.

2. Page 601: replace "0.X" with "1.X" in Table 2.

3. Page 606: change "US/REMAX^{D}" to be "US/REMAX^{B}", i.e., change the superscript (first paragraph).

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PC Software for Optimizing Groundwater Contaminant Plume Capture and Containment

Richard C. Peralta, Herminio H. Suguino, and Alaa H. Aly
Utah State University
Logan, Utah

I. INTRODUCTION

Simulation/optimization (S/O) models can be used to speed the process of computing desirable groundwater pumping strategies for plume management. They make the process of computing optimal strategies fairly straightforward and can help minimize the labor and cost of groundwater contaminant cleanup.

Differences between S/O models and the simulation (S) models currently used by over 98% of practitioners are discussed in Section II [1], followed by an overview of the two most common forms of groundwater management S/O models, their strengths and limitations, in Section III. In Section IV, currently available PC-based S/O models are discussed, and the ways in which they would be applied to representative situations are illustrated. Included is US/WELLS^D, an easy-to-use deterministic model that requires minimal data but will address aquifer and stream-aquifer systems where the analytical solutions of Theis [2] and Glover and Balmer [3] are appropriate. Also included is US/REMAX^B, appropriate for heterogeneous, multilayer systems. To ease use, that code accepts data in format readable by MODFLOW [4], the most widely used flow simulation model in the United States today.

These two S/O models are selected because they are the only ones we are aware of that (1) are available for use on PCs, (2) include with them the optimization algorithms necessary for solution, and (3) use superposition. As explained later, these characteristics make them especially useful for plume management by consultants and water resource managers.

II. COMPARISON BETWEEN COMMONLY USED SIMULATION MODELS AND SIMULATION/OPTIMIZATION MODELS

A simulation/optimization (S/O) model contains both simulation equations and an operations research optimization algorithm. The simulation equations permit the model to appropriately represent aquifer response to hydraulic stimuli and boundary conditions. The optimization algorithm permits the specified management objective to serve as the function driving the search for an optimal strategy. The model computes a pumping strategy that minimizes (or maximizes) the value of the objective function.

Table 1 shows generic inputs and outputs of the generally used simulation (S) model and those of an S/O model. The normal S models compute aquifer responses to assumed (input) boundary conditions and pumping values. Using such models to develop acceptable pumping strategies can be tedious and involve much trial and error. For example, simulated system response to an assumed pumping strategy might cause unacceptable consequences. In that case, the user must assume another pumping strategy, reuse the model to calculate aquifer response, and recheck for acceptability of results. This process of assuming, predicting, and checking might have to be repeated many times. The number of repetitions increases with the number of pumping locations and control locations (places where acceptability of system response must be evaluated and ensured).

When using an S model, as the number of possible pumping sites increases the likelihood that the user has assumed an "optimal" strategy decreases. Also, as the number of restrictions on acceptable system response to pumping increases, the ability of the user to assume an optimal strategy also decreases. Assuming a truly optimal strategy becomes impractical or nearly impossible as problem complexity increases. There are too many different possible combinations of pumping values. Furthermore, even if the computation process is automated in a computer program, the act of checking and ensuring strategy acceptability becomes increasingly painful as the number of control locations becomes large. In essence, it becomes impossible to compute mathematically optimal strategies for complicated groundwater management problems using S models.

Alternatively, S/O models directly calculate the best pumping strategies for the specified management objectives and ensure that the resulting heads and flows lie within prespecified limits or bounds (Table 1). The upper and lower bounds reflect the range of values that the user considers acceptable for cell pumping rates and resulting heads. The model automatically considers the bounds while calculating optimal pumping strategies. The user might choose to use lower bounds on pumping at currently operating public supply wells. He/she might choose to limit pumping at the upper end of the range, depending on hardware availability or legal restrictions. The user might impose lower bounds on head, at a specific distance below current water levels or above the base of the aquifer. Upper bounds might be the ground surface or a specified distance below the ground surface.

Assume, for example, a situation in which a planning agency is attempting to determine the least amount of groundwater pumping needed to capture a contaminant plume and the locations where it should be pumped, i.e., the spatial distribution of the withdrawals and injections. If a pumping strategy is not implemented to achieve capture, the contaminant will reach public supply wells, resulting in litigation and undesirable costs.

Table 1 Comparison Between Simulation and Simulation/Optimization Models

Model type	Input values	Computed values
Simulation (S)	Some boundary flows Some boundary heads Pumping	Some boundary flows Heads at "variable" head cells
Simulation/optimization (S/O)	Some boundary flows Some boundary heads Bounds on pumping, heads, flows	Optimal boundary flows Optimal heads at "variable" head cells Optimal pumping

An S/O model can be used to directly calculate an optimal pumping strategy for the goal of minimizing the pumping needed to capture the plume without causing unacceptable consequences. For example, assume that no injection mounds should reach the ground surface and that no drawdowns should exceed 2 m. In addition, assume that potentiometric surface gradients near the plume should be toward the plume source.

The S/O model will directly calculate the minimum total pumping rate needed and will identify how much should be pumped from each pumping location. The potentiometric surface heads and gradients that will result from the optimal pumping will lie within the bounds specified initially (Table 1). In other words, future heads will not reach the ground surface, future heads will not be more than 2 m below current heads, and final gradients will be toward the contaminant source. Thus, the very first optimal pumping strategy computed by an S/O model will satisfy all specified management goals.

III. COMMON S/O MODELING APPROACHES AND LIMITATIONS

Most S/O models employ either an embedding or a response matrix approach for representing system (head) response to pumping [5]. Embedding models contain finite-difference or finite-element equations embedded directly as constraints. In a finite-difference embedding model, head and pumping values (or other flows) must be computed for each time step at each cell. This is a very useful approach for those situations in which (1) pumping should be a decision variable at most cells, (2) head must be constrained in a high proportion of cells, and (3) either a steady-state strategy should be developed or there need be very few time steps. It is not as desirable if there are relatively few pumping cells and control points or if many time steps are needed. Thus, embedding models have been mainly used for steady-state regional planning and for small hypothetical problems.

Response matrix S/O models use linear systems theory and superposition with influence coefficients (e.g., [6]–[14] and many others). The matrix containing the influence coefficients and superposition (summation equations) is termed the response matrix. Response matrix (RM) models use a two-step process. First, normal simulation (analytical or numerical) is used to calculate system response to assumed unit stimuli. Then optimization is performed by an S/O model that includes summation equations (discretized forms of the convolution integral).

Response matrix models are ideal for transient management situations. They require constraint equations for only those specific cells and time steps at which head or flow (other than pumping) must be restricted during the optimization. To predict system response to the optimal strategy at locations and times other than those constrained in the S/O model, an external simulation model is used after the optimization.

Regardless of the simulation approach used, S/O models share some of the limitations of standard simulation models. Poor physical system representation or inadequate data will cause error. One cannot properly optimize management of system processes that one cannot correctly simulate. Useful simulation/optimization modeling presupposes that aquifer parameters are appropriate and that actual boundary conditions are represented adequately within the model.

Both embedding and RM S/O models generally assume system linearity during at least some part of their processing operation. Confined aquifers are linear, unless they become unconfined. Unconfined aquifers are nonlinear, but frequently the change in transmissivity is insignificant, and they can be treated as if they were linear. Most commonly, system nonlinearity is addressed by cycling. Cycling involves (1) assuming aquifer parameters (and computing influence coefficients for RM models), (2) calculating an optimal strategy, (3) recalculating system parameters, (4) comparing assumed and newly calculated parameter values, and (5) either stopping or returning to step 2 and repeating the process (if the assumed parameter values are still inappropriate for the problem or if the optimal strategy is still changing with cycling). Frequently, three cycles are sufficient for this convergence process. Thus, although both types of models are completely applicable for confined aquifers, some adjustments must be made to accurately apply them to unconfined aquifers.

Within S/O models, plume capture is generally achieved by controlling hydraulic gradients and thus controlling advective transport. Generally, nonlinear transport equations are not included. This approach permits the modeler to retain use of the characteristics of linear systems (superposition, etc.). All of the RM model applications presented below achieve capture via gradient control.

Concerning data input, S/O models require all of the data needed by simulation models, plus information on lower and upper bounds on decision variables (pumping rate, location) and state variables (head, gradient, etc.). Although the same sort of information should be required when using an S model, the forced codification of these data as S/O model input is helpful. It causes the modeler to specify strategy acceptability criteria earlier than he/she might otherwise.

Concerning model results, an S/O model might tell a user that the posed problem is infeasible. This means that the user has posed a problem for which all the constraints cannot be satisfied simultaneously. For example, the user might have instructed the model to cause the head near an injection cell to reach at least 100 m above mean sea level and simultaneously told it that the upper bound on injection in 50 m^3/day. If that injection rate is inadequate to cause the required change in head, the model will declare the problem to be infeasible. The model will be unable to determine even one pumping rate that can satisfy both conditions.

Of course, if there is more than one potential injection well, the same problem might be feasible. In that case, the model can compute an optimal pumping strategy (probably the user would have requested a strategy that minimizes the total pumping needed to achieve that head).

Fortunately, S/O model users rapidly get beyond the stage wherein they try to develop impossible pumping strategies (force the model to achieve goals that are impossible or mutually exclusive when considering both the laws of nature and the goals of humans). Experience brings the S/O modeler great ability to address common management problems.

IV. PC-BASED S/O MODELS AND SAMPLE APPLICATIONS

A. US/WELLS^D for Systems Addressable Using Analytical Solutions

1. Model Background

US/WELLS^D (Utah State extraction/injection well system for optimal groundwater management) is a deterministic version of an RM model. It uses influence coefficients based on analytical equations for potentiometric surface response to pumping and river depletion resulting from depletion. It is appropriate for systems where those analytical approaches are appropriate—presumably relatively homogeneous systems. (Of course, in the management and consulting arena, such approaches are commonly applied to heterogeneous systems, with acceptable error.)

pumping

Characteristics of US/WELLS^D are summarized in Table 2. The overview below is derived from the user's manual [15].

The objective function of the optimization module in US/WELLS is generally applicable and easily used for a variety of situations. The user can select either a linear or a quadratic form. The linear objective function is to minimize

$$\sum_{x=1}^{2} [W_{E,x} \sum_{j=1}^{J} E_{j,x} + W_{I,x} \sum_{k=1}^{K} I_{k,x}] \tag{1}$$

Table 2 Characteristics of US/WELLS^D and US/REMAX^B

	US/WELLS^D	US/REMAX^B
Systems addressed	One Layer, homogeneous Stream/aquifer Stream stage not affected by pumping	Multilayer heterogeneous Stream/aquifer Stream stage affected by pumping
Management period	One or two stress periods of equal or unequal duration Steady state or transient Can rep. transient evolutionary era with terminal steady-state conditions.	One or multiple stress periods of equal duration Steady state or transient
Influence coefficients	Deterministic Based on analytical expressions by Theis and Glover and Balmer	Deterministic Based on finite-difference simulation (MODFLOW+STR)
Objective function	Min or max pumping or combination Time-varying weight for extraction and injection	Min or max pumping or combination Diff. weight for each pumping location
Bounds and constraints	$g^L \le g \le g^U$ $h^L \le h \le h^U$ $G^L_{1,2} \le G_{1,2} \le G^U_{1,2}$ $\frac{\Sigma\,(\text{Ext})}{\Sigma\,(\text{Inj})} \le 0.X$ 1.X $= 1.0$ $\ge 1.X$ $d^L \le d \le d^U$	$g^L \le g \le g^U$ $h^L \le h \le h^U$ $\Delta h^L_{1,2} \le \Delta h_{1,2} \le \Delta h^U_{1,2}$ $G^L_{1,2} \le G_{1,2} \le G^U_{1,2}$ $V^L_{1,2} \le V_{1,2} \le V^U_{1,2}$ $\frac{\Sigma\,(\text{Ext})}{\Sigma\,(\text{Inj})} \le 1.0$ $= 1.0$ ≥ 1.0 $\Sigma(\text{Ext})^L \le \Sigma(\text{Ext}) \le \Sigma(\text{Ext})^U$

Notes: Superscripts L and U refer to lower and upper bounds; g = extraction or injection, [L^3/T]; h = head.; Δh, $G_{1,2}$, $V_{1,2}$ = head-difference, gradient, and velocity, respectively, between any two locations, [L], dimensionless, or [L/T]; Σ (Ext), Σ (Inj) = total extraction or injection, [L^3/T]; d = stream depletion, [L^3/T].

where $W_{E,x}$ and $W_{I,x}$ are the cost coefficient or weight assigned to extraction (E) or injection (I) rates in the x_{th} time period, [\$/(L^3·T)] or dimensionless; $E_{j,x}$ and $J_{k,x}$ are extraction (E) or injection (I) rate at well j (or k) in the x_{th} time period, [L^3/T]; and J and K are number of extraction (J) or injection (K) wells.

Potential constraints are the following.

1. Hydraulic gradient between any gradient control pair of wells at any time period must be within user-specified bounds. This can ensure that water is moving only in the desired direction. The maximum value can differ for each gradient control pair and time period. This constraint is useful, for example, when US/WELLS^D is used for groundwater contaminant plume immobilization or for any situation where hydraulic gradient control is desired.
2. Extraction or injection rate at any well must be within user-specified bounds (lower and upper limits). If the user cannot decide if a certain well should be used for extraction or injection, he can locate one of each at the same location. The model will then determine either an extraction or an injection rate, or neither, for that location.

3. Hydraulic head at any injection, extraction, or observation well must be within user-specified lower and upper bounds. For example, a lower bound may be used to maintain adequate saturated thickness. An upper bound may be used to prevent surface flooding or to eliminate the need for pressurized injection. These lower and upper bounds can differ for different locations. The bounds are the same for both time periods.
4. Total import or export of water can be controlled to be within a user-specified range. The user can also completely prevent import or export of water or both. If no import or export of water is allowed, the total optimal extraction must equal the total optimal injection.
5. Depletion from the river must be within user-specified bounds (lower and upper limits). This is applicable only if a river exists in the considered system.
6. Constraint 3 is modified such that the probability that the actual change in head at any point in the groundwater system is not less than the change calculated by the model or is not greater than the change calculated by the model and is at least equal to the reliability level specified by the user. (This ability is found only in an alpha-test chance-constrained version of the model, US/WELLS^S, which considers the stochastic nature of hydraulic conductivity. The utilized chance constraint is more accurate than previously reported formulations.)

Optionally, US/WELLS^D can use a quadratic objective function to minimize

$$\sum_{x=1}^{2} [WW_{E,x} \sum_{j=1}^{J} E_{j,x} H_{j,x} + W_{E,x} \sum_{j=1}^{J} E_{j,x} + W_{I,x} \sum_{k=1}^{K} I_{k,x}] \tag{2}$$

where $H_{j,x}$ is the dynamic lift, the difference between ground surface elevation and optimal potentiometric head resulting at extraction well j at the end of the x_{th} time period, [L]; and $WW_{E,x}$ is the weight assigned to the power used for extraction in the x_{th} time period, [\$/L·T)].

The weighting factors can be used to emphasize different criteria and different time periods. For example, assume a problem of minimizing the total extraction using the linear objective function. If the second time period is chosen to be much longer than the first time period and the weights assigned to extraction and injection in the second time period are larger than those used for the first time period, then the solution will tend to minimize steady-state extraction/injection rates, and less attention will be given to the short-term transient rates. Through the weighting factors, US/WELLS^D can also be used for maximizing pumping rates for water supply problems.

2. Application and Results

Here we illustrate the use of US/WELLS^D to determine the optimal time-varying sequence of extraction and injection of water in prespecified locations needed for first immobilizing and then extracting a groundwater contaminant plume. In this example, the user specifies *potential* locations of extraction and injection wells around the contaminant plume (Figure 1). US/WELLS^D then determines optimal extraction and injection rates for different time periods.

To illustrate model flexibility, four potential extraction wells and five potential injection wells are considered for placement outside the contaminant plume during the first period. In the second time period, three extraction wells are considered for placement inside the plume (to extract contaminated water) and five potential downgradient injection wells are considered. During both periods, the resulting hydraulic gradients (between 10 pairs of head observation locations) must be toward the center of the plume. Alternatively, the user could choose to minimize the pumping needed to capture the plume using only internal extraction wells in one or both periods.

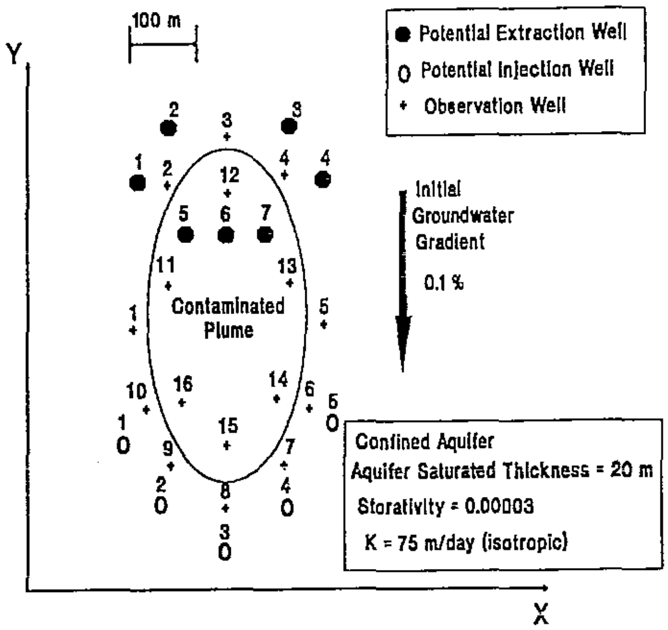

Figure 1 Hypothetical study area for Example A, addressable with US/WELLS^D.

Here, the quadratic objective function is used and employs greater weights for the second time period than the first period. This supports the fact that the second period is much longer than the first. In addition, neither export nor import of water is allowed—total injection must equal total extraction in each period. All the above considerations are incorporated within the model via the input data [15]. The user also specifies lower and upper bounds on head and pumping rates.

Figure 2 shows US/WELLS^D output, in meters and m^3/day. This contains, in addition to the input bounds (L. Bound and U. Bound), the optimal values of the decision variables (pumping), state variables (head and gradient), and marginal values.

The marginal is defined as the value by which the objective function will change if a tightly bounded variable changes one unit. If a variable's optimal value is not equal to either its lower or upper bound, its marginal will be zero. That is, the marginal will be nonzero only if the optimal value of the variable equals one of its bounds. In this case, the marginal shows the improvement of the value of the objective function resulting from relaxing this bound by one unit. Marginals are valid only as long as no other variable also changes in value. Thus they might be valid for only a small range of change in the bound.

To illustrate, the output file (Figure 2) shows that the marginal of the optimal injection rate in the first time period at injection well 3 is −45.3. The objective function value was 334,668.1. If the upper bound on injection in the first time period is relaxed by one unit at the mentioned well (that is, the new upper bound is 901 instead of 900), one would expect the value of the objective function to change by about −45.3 to 334,622.8. If this change is actually made and the model is rerun, the resulting change in objective function value is −45.4.

Marginals are useful in determining how to refine an optimal strategy. They help one to decide which bounds or constraints should be looked at more closely and perhaps relaxed. They also indicate the trade-off between that bound and objective achievement. They show how much one is giving up in terms of objective attainment to satisfy that restriction.

MODEL STATUS : OPTIMAL SOLUTION FOUND
VALUE OF OBJECTIVE FUNCTION 334668.1

OPTIMAL EXTRACTION RATES

FIRST TIME PERIOD

Well No	L.Bound	Optimal	U.Bound	Marginal
1	0.00	745.42	900.00	0.000
2	0.00	447.60	900.00	0.000
3	0.00	448.71	900.00	0.000
4	0.00	747.86	900.00	0.000
5	0.00	0.00	0.00	0.000
6	0.00	0.00	0.00	0.000
7	0.00	0.00	0.00	0.000

SECOND TIME PERIOD

Well No	L.Bound	Optimal	U.Bound	Marginal
1	0.00	0.00	0.00	81.955
2	0.00	0.00	0.00	81.627
3	0.00	0.00	0.00	81.605
4	0.00	0.00	0.00	81.913
5	0.00	426.53	900.00	0.000
6	0.00	883.77	900.00	0.000
7	0.00	428.90	900.00	0.000

OPTIMAL INJECTION RATES

FIRST TIME PERIOD

Well No	L.Bound	Optimal	U.Bound	Marginal	
1	0.00	211.66	900.00	0.000	
2	0.00	328.89	900.00	0.000	
3	0.00	900.00	900.00	-45.342	<=== *explained in text*
4	0.00	900.00	900.00	0.000	
5	0.00	49.04	900.00	0.000	

SECOND TIME PERIOD

Well No	L.Bound	Optimal	U.Bound	Marginal
1	0.00	0.00	900.00	132.584
2	0.00	293.53	900.00	0.000
3	0.00	900.00	900.00	-4.3E+2
4	0.00	545.67	900.00	0.000
5	0.00	0.00	900.00	132.583

OPTIMAL HEADS AT OBSERVATION WELLS

FIRST TIME PERIOD

Well No	L.Bound	Optimal	U.Bound	Marginal
1	30.00	35.69	40.00	0.000
2	30.00	35.54	40.00	0.000
3	30.00	35.60	40.00	0.000
4	30.00	35.55	40.00	0.000
5	30.00	35.70	40.00	0.000
6	30.00	35.79	40.00	0.000
7	30.00	35.92	40.00	0.000
8	30.00	35.88	40.00	0.000
9	30.00	35.84	40.00	0.000
10	30.00	35.77	40.00	0.000
11	30.00	35.65	40.00	0.000
12	30.00	35.60	40.00	0.000
13	30.00	35.65	40.00	0.000
14	30.00	35.79	40.00	0.000
15	30.00	35.88	40.00	0.000
16	30.00	35.77	40.00	0.000

Figure 2 US/WELLS^D output file for Example A.

SECOND TIME PERIOD

Well No	L.Bound	Optimal	U.Bound	Marginal
1	30.00	35.62	40.00	0.000
2	30.00	35.62	40.00	0.000
3	30.00	35.68	40.00	0.000
4	30.00	35.62	40.00	0.000
5	30.00	35.63	40.00	0.000
6	30.00	35.66	40.00	0.000
7	30.00	35.75	40.00	0.000
8	30.00	35.74	40.00	0.000
9	30.00	35.71	40.00	0.000
10	30.00	35.64	40.00	0.000
11	30.00	35.56	40.00	0.000
12	30.00	35.54	40.00	0.000
13	30.00	35.56	40.00	0.000
14	30.00	35.66	40.00	0.000
15	30.00	35.74	40.00	0.000
16	30.00	35.64	40.00	0.000

==

OPTIMAL HEADS AT EXTRACTION WELLS

FIRST TIME PERIOD

Well No	L.Bound	Optimal	U.Bound	Marginal
1	30.00	35.09	40.00	0.000
2	30.00	35.29	40.00	0.000
3	30.00	35.29	40.00	0.000
4	30.00	35.09	40.00	0.000
5	30.00	35.61	40.00	0.000
6	30.00	35.62	40.00	0.000
7	30.00	35.61	40.00	0.000

SECOND TIME PERIOD

Well No	L.Bound	Optimal	U.Bound	Marginal
1	30.00	35.69	40.00	0.000
2	30.00	35.72	40.00	0.000
3	30.00	35.73	40.00	0.000
4	30.00	35.70	40.00	0.000
5	30.00	35.24	40.00	0.000
6	30.00	34.90	40.00	0.000
7	30.00	35.25	40.00	0.000

==

OPTIMAL HEADS AT INJECTION WELLS

FIRST TIME PERIOD

Well No	L.Bound	Optimal	U.Bound	Marginal
1	30.00	35.90	40.00	0.000
2	30.00	36.03	40.00	0.000
3	30.00	36.46	40.00	0.000
4	30.00	36.47	40.00	0.000
5	30.00	35.83	40.00	0.000

SECOND TIME PERIOD

Well No	L.Bound	Optimal	U.Bound	Marginal
1	30.00	35.65	40.00	0.000
2	30.00	35.88	40.00	0.000
3	30.00	36.33	40.00	0.000
4	30.00	36.08	40.00	0.000
5	30.00	35.67	40.00	0.000

Figure 2 Continued.

OPTIMAL HYDRAULIC GRADIENTS

FIRST TIME PERIOD

From	To	L.Bound	Optimal	U.Bound	Marginal
1 ->	11	0.00000	0.00055	0.01000	0.000
3 ->	12	0.00000	0.00003	0.01000	0.000
5 ->	13	0.00000	0.00019	0.01000	0.000
6 ->	14	0.00000	0.00000	0.01000	1.17E+7
7 ->	14	0.00000	0.00157	0.01000	0.000
8 ->	15	0.00000	0.00000	0.01000	3.26E+7
9 ->	16	0.00000	0.00087	0.01000	0.000
10 ->	16	0.00000	0.00000	0.01000	1.17E+7

SECOND TIME PERIOD

From	To	L.Bound	Optimal	U.Bound	Marginal
1 ->	11	0.00000	0.00082	0.01000	0.000
3 ->	12	0.00000	0.00241	0.01000	0.000
5 ->	13	0.00000	0.00027	0.01000	0.000
6 ->	14	0.00000	0.00014	0.01000	0.000
7 ->	14	0.00000	0.00115	0.01000	0.000
8 ->	15	0.00000	0.00000	0.01000	2.88E+8
9 ->	16	0.00000	0.00081	0.01000	0.000
10 ->	16	0.00000	0.00000	0.01000	0.000

Figure 2 Concluded.

B. US/REMAX^B for Heterogeneous Multilayer Systems

1. Model Background

For optimizing management of complex heterogeneous systems, one would rather use US/REMAX^D [16] than US/WELLS^D. This is the basic version of the Utah State response matrix model. To develop influence coefficients, it uses code modified from MODFLOW, a modular finite-difference groundwater flow simulation model [4], and STR, a related stream routing module [17]. The physical system data needed by US/REMAX^D can be input in the same format as is used by MODFLOW and STR. Internally, US/REMAX^B also uses a portion of PLUMAN, a decision support system for optimal groundwater contaminant plume management [18], and other code.

The optimization model formulation capabilities are similar to those of US/WELLS^D (Table 2). For steady state, the generic objective is to minimize

$$\sum_{j=1}^{J} W_j E_j + \sum_{k=1}^{K} W_k I_k \tag{3}$$

where W_j is the weight assigned to pumping in cell j, dimensionless or [$\$\cdot T/L^3$]. US/REMAX^B can employ constraints 1–3 of US/WELLS^D for multiple layers. Similar to the US/WELLS^D constraint 4, US/REMAX^B can force total extraction to exceed, equal, or be less than total injection. Again, via the sign on the weighting coefficients, one can perform maximization. One can also achieve multiobjective optimization by the weighting method. Whereas in US/WELLS^D the same weight must be applied to all extraction wells in a time step (and a different weight can be used for injection wells, but the same must be applied to all such wells in a particular time step), in US/REMAX^B each well can employ a different weight.

2. Application and Results

Introduction. For illustration, we discuss addressing a contaminant plume in a representative study area. First, the study area is described and the results of continuing current management are predicted, using MODFLOW+STR for flow simulation and MOC [19] for transport simulation. Then an approach to developing an optimal strategy is discussed, the S/O model is applied, and an optimal strategy is computed. Next, the system response to implementing the optimal strategy is verified using MODFLOW+STR and MOC. Finally, slight variations in the management goal or situation are assumed and new optimal strategies are developed. Computed optimal strategies are compared. Suguino [20] first addressed this study area using PLUMAN. Some of the discussion below follows his development.

Study Area Description and Situation. The area (Figure 3) measures about 4.3 km by 4.3 km. It is bounded on the north by a large saltwater body; on the south, east, and northwest by impermeable material; and on the west by a lake. A river transects the area from south to north. Aquifer parameters of this example study area were obtained from ranges reported by Todd [21].

For the unconfined upper layer (layer 1), parameters are as follows.

Hydraulic conductivity:

1st zone: 45 m/day (coarse sand) from lake to contaminant spill area (columns 1–36 and 57–58)
2nd zone: 30 m/day (medium sand) in irrigated area (columns 51–56)
3rd zone: 450 m/day (fine gravel) in contaminant spill area (columns 37–50).

Specific yield:

1st zone: 0.27 (coarse sand)
2nd zone: 0.28 (medium sand)
3rd zone: 0.25 (fine gravel)

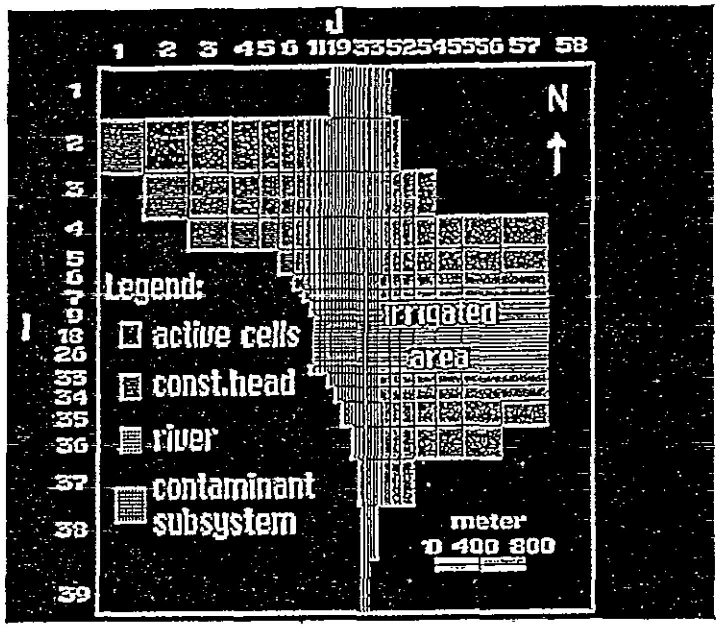

Figure 3 Finite-difference grid for the area addressable with US/REMAX[B].

Recharge by deep percolation and/or irrigation:

1.167×10^{-8} m/sec in nonirrigated area
1.928×10^{-8} m/sec in irrigated area

In the confined lower layer (layer 2):

Transmissivity:	0.1564 m^2/sec
Saturated thickness:	30.0 m
Storage coefficient:	0.0001

Finite-difference models are to be used in this study. This requires system discretization. The resulting block-centered cell grid (Figure 3) has 58 columns and 39 rows. Cell side lengths range from 3 to 400 m. Because MOC will be used for transport simulation near the plume, cells of uniform size are specified for that region. The resulting 17 row by 20 column region (subsystem) near the plume has square cells of 15.2 m (50 ft) side length.

A conservative (nonreactive) contaminant is assumed to be spilled in the top aquifer layer (layer 1) of cell (22, 18) or (11_s, 3_s). (The subscript "s" after a cell row or column index indicates that the cell is in the subsystem.) This cell is treated as a continuous source during the management period.

Initially, pumping for water supply occurs in two cells between the plume and the river. One well is in layer 1 of (23, 15) or (12_s, 15_s). The other well is in layer 2 of (18, 18) or (7_s, 18_s). There is immediate concern about the potential for contamination reaching the supply well in layer 1.

Nonoptimal System Response Determination (Step 1). Before one attempts to develop an optimal strategy, one usually demonstrates the need for such a strategy. This requires predicting system response if no optimal strategy is implemented. Frequently, simulation models are used for this action. Here, MODFLOW+STR computes the potentiometric surface that will result from assumed steady-state conditions (Figure 4).

Because of the gradient, the contaminant will tend to migrate toward the supply wells. MOC is used to quantify the migration resulting in the subsystem from the steady flow. Figure 5 shows the 210 ppb contour expected to result 60 days after contamination begins. Furthermore, concentration in the cell containing the drinking well (12_s, 15_s) reaches 317 ppb 8 months after the spill. We assume that this concentration level exceeds the health advisory for human consumption and that developing a plume capture strategy is desirable.

Management Goals Specification and S/O Model Formulation for Scenario 1 (Step 2). The assumed goal is to minimize the steady pumping (extraction and injection) needed to capture the plume. Plume capture will presumably be achieved when hydraulic gradients, just outside the plume boundary, all point toward the plume interior. We also want the head at extraction wells not to drop too far (to avoid reducing saturated thickness by more than about 10%) or the head at injection wells not to rise to the ground surface. These criteria identify the example problem termed Scenario 1.

The S/O model formulation for this scenario is shown below. The model computes the pumping strategy that minimizes the value of the objective function, subject to the stated constraints and bounds. Locations of potential injection and extraction wells to be considered by the model are shown in Figure. 5. Figure 6 identifies head difference (gradient) control cell pairs and shows the direction that will be imposed on the hydraulic gradient by any computed optimal strategy. These are placed to enclose the plume projected to exist by day 60. A modeler can select potential well locations on the basis of practical experience. For example, the closer the injection wells are to the head gradient control locations, the less pumping is needed to

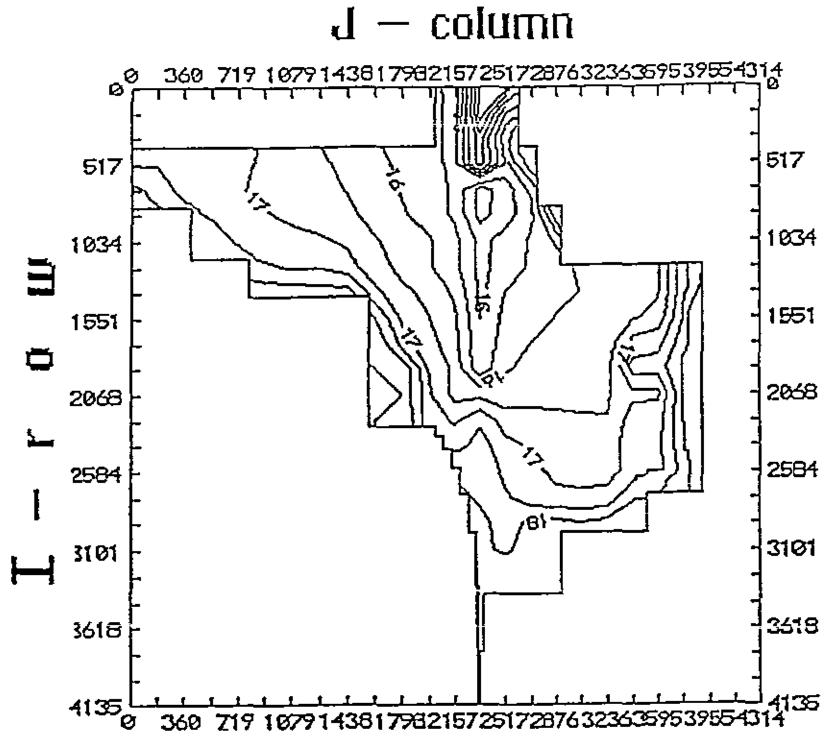

Figure 4 Nonoptimal (unmanaged) steady-state potentiometric surface contour map for the study area of Scenario I (meters above MSL).

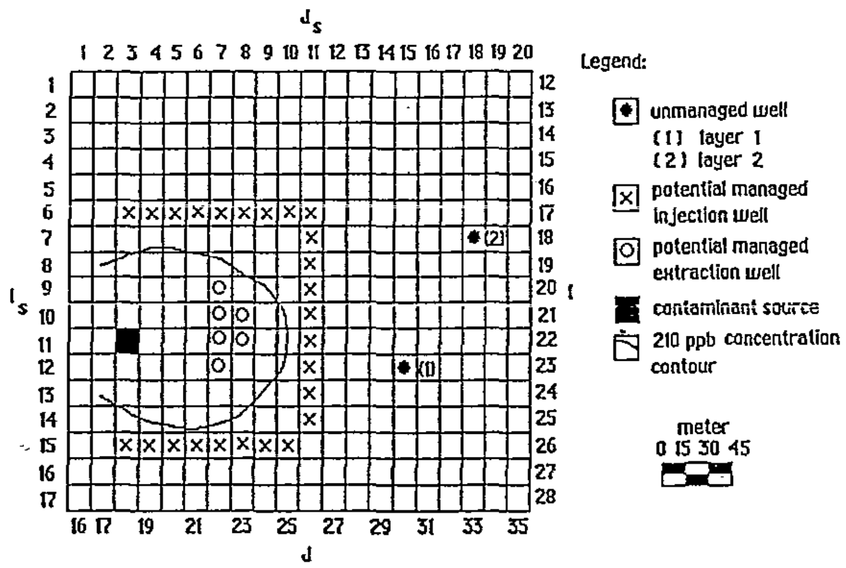

Figure 5 Subsystem discretization, potential well locations for Scenario 1, and 210 ppm contour, 60 days after contamination begins.

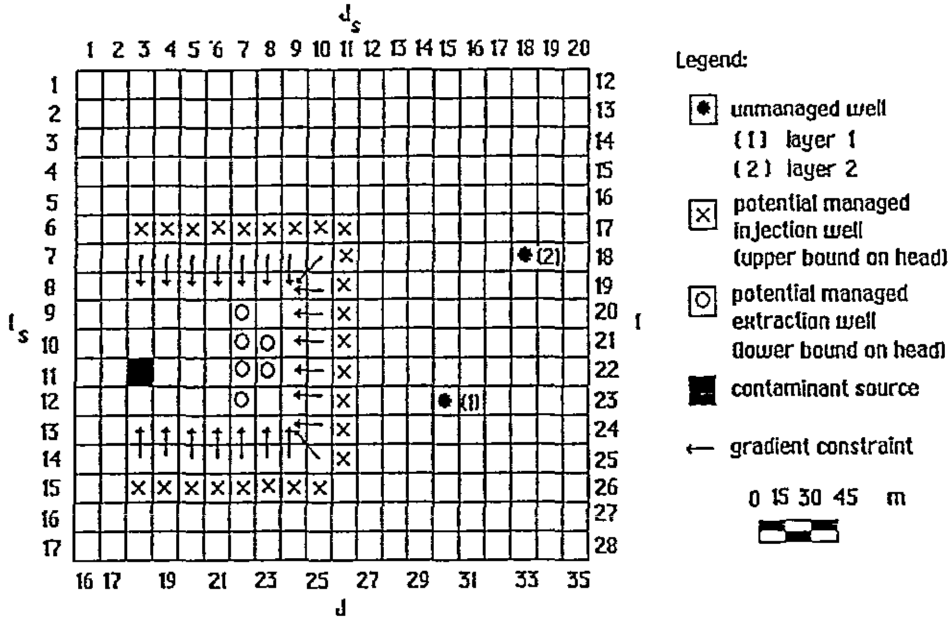

Figure 6 Head-difference constraint locations applied within the S/O model in Scenario 1.

satisfy the head-difference constraint. Thus, the modeler might want the model to consider pumping sites near the location where heads need most to be affected.

The model objective is to minimize the value of Equation (3), using weights of 1, subject to

$$G_{\bar{o}} \geq 0.01, \qquad \text{for } \bar{o} = 1, \ldots, 22 \tag{4}$$

$$h_{\hat{e}} \geq 15.0, \qquad \text{for } \hat{e} = 1, \ldots, 6 \tag{5}$$

$$h_{\hat{e}} \leq 25.0, \qquad \text{for } \hat{e} = 1, \ldots, 25 \tag{6}$$

where $G_{\bar{o}}$ is the difference in head between a pair of cells, the first located farther from the plume. A positive value denotes a higher head farther from the plume, [L]; $h_{\hat{e}}$ is the hydraulic head just outside the casing of pumping well $\hat{e}$ located in the center of a pumping cell, [L]; $\bar{o}$ is the index denoting pair of cells head-difference (gradient) control pair; and $\hat{e}$ is the index denoting pumping well at the center of cell j or k. Here $j = 6$ and $k = 25$.

Note that identifying the location of potential extraction and injection wells for the model (Figure 5) does not mean that the model will choose to pump at those locations. Via the optimization process, the model might choose to pump at only a few of the potential sites. The computed strategy will require less total pumping than any other strategy possible for the specified potential well locations and imposed bounds and constraints. Furthermore, since this is a steady-state problem, steady-state system response to implementing the strategy computed by the model will satisfy all those bounds and constraints. This is verified in the next step.

Optimal Strategy Computation and Verification for Scenario 1 (Step 3). The optimal strategy computed for Scenario 1 is shown in Table 3. Because the model is minimizing pumping only for plume containment in layer 1, no extraction is shown for layer 2. The original unmanaged pumping does continue from original supply wells in both layers (Figure 3) but is not included in Table 3 because the model is not optimizing that pumping.

Table 3 Pumping Results for the Sample Scenarios

Scenario	Constraints	g(extr) 1st Layer	g(extr) 2nd Layer	b(inj.) (m^3/sec)	($g + b$) total (gpm)
1	Gradient constraint on heads located on the same layer, head constraint on injection and extraction well.	0.01338 (212.05)	— —	0.02020 (320.13)	0.03358 (532.18)
2	Added pumping constraint: total sum of extraction = total sum of injection.	0.01702 (269.74)	— —	0.01702 (269.74)	0.03404 (539.48)
3	Gradient constraint on heads located on the same and on different layers, head constraint on injection and extraction wells.	0.00300 (47.54)	0.00329 (52.14)	0.03786 (600.03)	0.04415 (699.69)

Figure 7 shows the locations of wells that will pump, according to the optimal strategy. It also shows the head-difference constraints [Equation (4)] that will be tight. Tight constraints are those that are satisfied exactly. The other gradient constraints are also satisfied, but the model had no difficulty in doing so. These latter head-difference constraints are "loose" (there is more than 0.01 m difference between the heads at the two cells coupled by an arrow in Figure 6 but not shown at all in Figure 7). No heads are against their bounds. Therefore neither Equation (5) nor (6) is tight.

It is appropriate to verify that the computed strategy accomplished its goal of plume capture. MODFLOW+STR can be used to demonstrate how quickly the optimal steady pumping

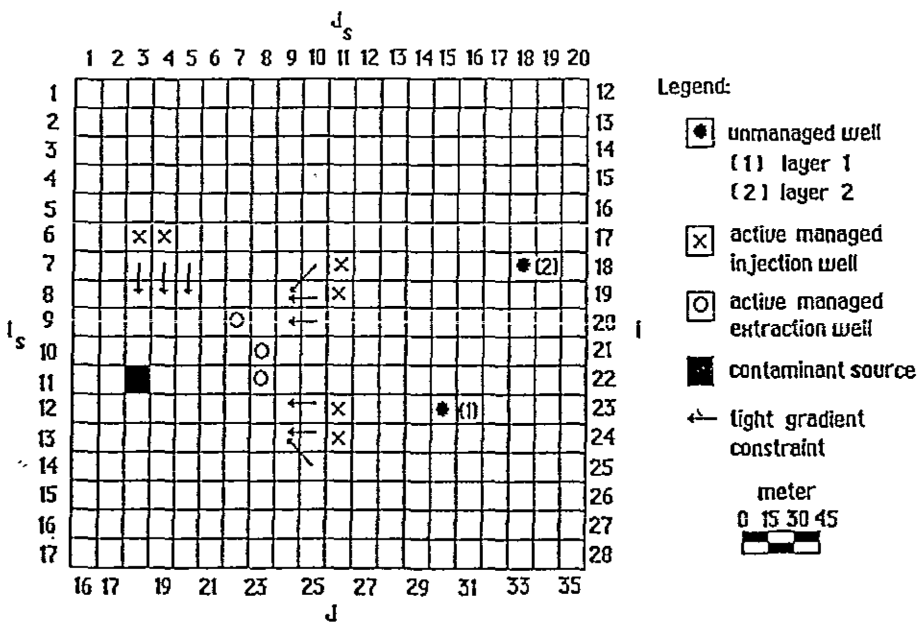

Figure 7 Location of optimal pumping wells and tight head-difference (gradient) constraints for Scenario 1.

strategy will cause the desired gradients to occur. Transient simulation demonstrated that the gradient constraints would be satisfied 30 days after implementing the optimal pumping strategy (Figure 8). Figures 9 and 10 show the ultimate steady-state surface resulting from strategy implementation. Clearly, a groundwater divide has been formed between the plume and the supply well.

MOC is used to predict the pollutant transport that would result from strategy implementation. No contaminant moved past the injection wells.

Theoretical verification of the optimality of the computed strategy is beyond the scope of this document. However, many texts on operations research and linear programming assure the optimality of solutions to models having a linear objective function and constraints.

Alternative Scenarios.

Scenario 2. This scenario differs from the previous in the addition of a constraint forcing total injection to equal total extraction around the plume. Again, pumping from the two supply wells is not included in the total.

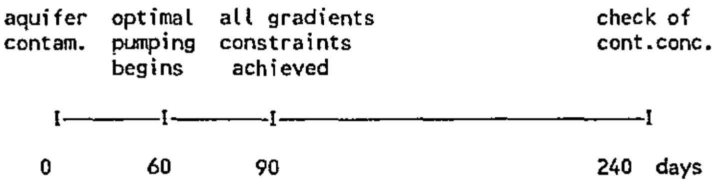

Figure 8 Time scale of Scenario 1.

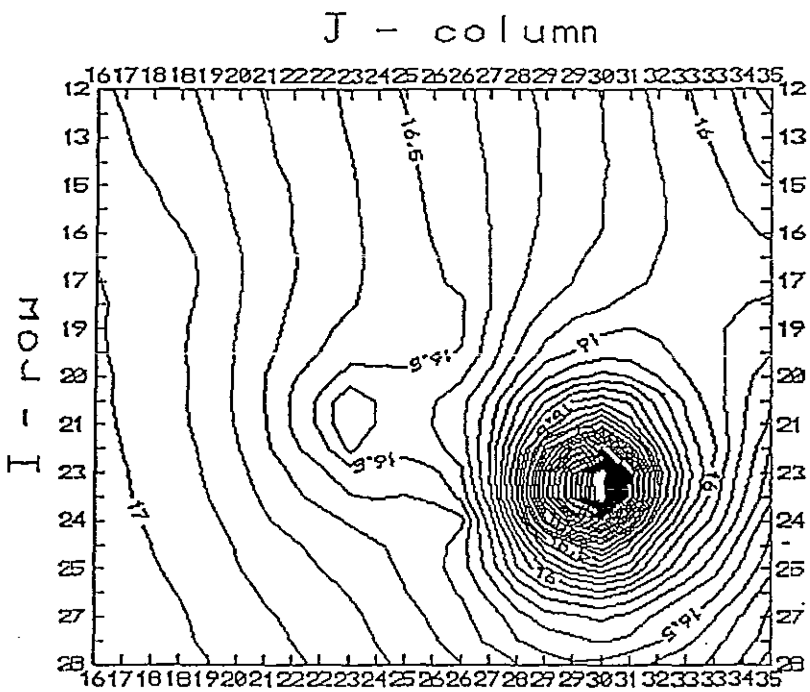

Figure 9 Subsystem potentiometric surface resulting from implementing the optimal pumping strategy for Scenario 1 (meters above MSL).

Well	lps	gpm	Well	lps	gpm
1	1.36	21.56	6	−3.09	−49.02
2	0.62	9.89	7	5.02	79.58
3	−0.60	−9.49	8	4.46	70.67
4	−9.69	−153.55	9	7.88	124.96
5	0.85	13.46	10	−100.00	−1584.82

(+) recharge (−) withdrawal

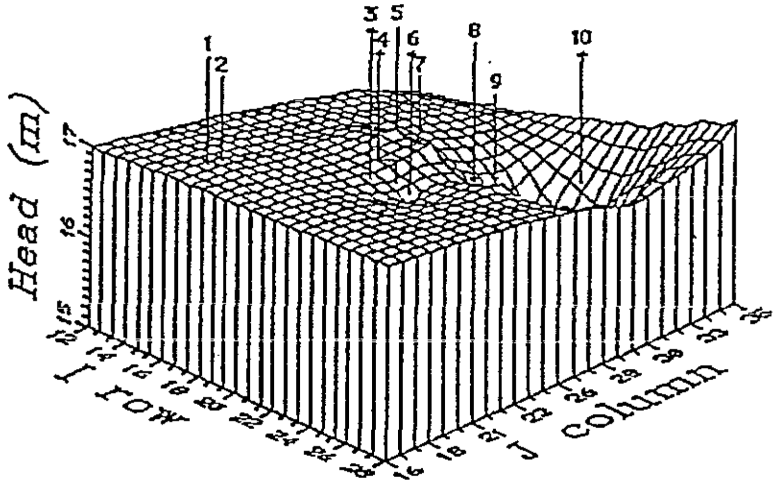

Figure 10 Subsystem potentiometric surface resulting after 6 months of optimal pumping for Scenario 1 (meters above MSL).

Results in Table 3 show an increase in extraction and a decrease in injection. Total pumping needed for plume containment increased slightly (1.4%). This illustrates the phenomenon—increasing the number or restrictiveness of constraints does not improve the value of the objective function.

Although total pumping increased, one less extraction well is used in this strategy than in the previous (Table 4). The same number of gradient constraints are tight, but the locations of the tight gradient constraints differ slightly.

Scenario 3. This scenario demonstrates what might happen if involved managers have conflicting goals. It differs slightly from Scenario 1. In addition to controlling the plume, the agency wishes to extract more from layer 2 for water supply. Three new potential extraction wells are located in cells (19, 25), (20, 25), and (21, 25), as if along a nearby road. Pumping is not permitted to change at the two initial supply wells.

Table 4 Numbers of Managed Wells that Will Pump Under the Optimal Strategies for the Tested Scenarios

	g(extr.)			
Scenario	1st Layer	2nd Layer	b(inj.)	$(g + b)$ total
1	3	—	6	9
2	2	—	6	8
3	4	3	14	21

As a result, the objective function is altered to maximize new extraction from layer 2 while still minimizing the pumping in layer 1 needed to capture the plume. This is achieved by assigning a negative sign to extraction from the supply wells, and minimizing:

$$\sum_{j=1}^{J} (E_j)_{1st\ layer} - (E_j)_{2nd\ layer} + \sum_{k=1}^{K} (I_k)_{1st\ layer} \tag{7}$$

Since minimizing a negative number is the same as maximizing a positive number, minimizing negative extraction in layer 2 means maximizing that extraction.

Also added are new constraints imposed on vertical flow in cells (21, 21) and (22, 21). There, the head in the lower layer is forced to exceed that in the upper layer by 0.01 m, preventing the downward migration of contaminant.

Figure 11 shows the resulting optimal injection and extraction well locations and tight gradient constraints. The optimal pumping strategy includes seven extraction wells and 14 injection wells. Although extraction of polluted water decreases, injection increases with respect to Scenario 1 (Table 3). Extraction of water for public supply increases by 31% above the unmanaged rate.

Although the gradient constraints are all satisfied by the optimal strategy, subsequent simulation demonstrated that the vertical gradient is reversed in some plume-containing cells in which the gradient was unconstrained. This illustrates that one must be careful in placing head or gradient control in appropriate locations. In practice, another optimization would be performed, using additional vertical head-difference or gradient constraints.

Processing Considerations. It is useful to consider the resources required to address optimization problems. First, the total computer time needed to solve an optimization problem is of

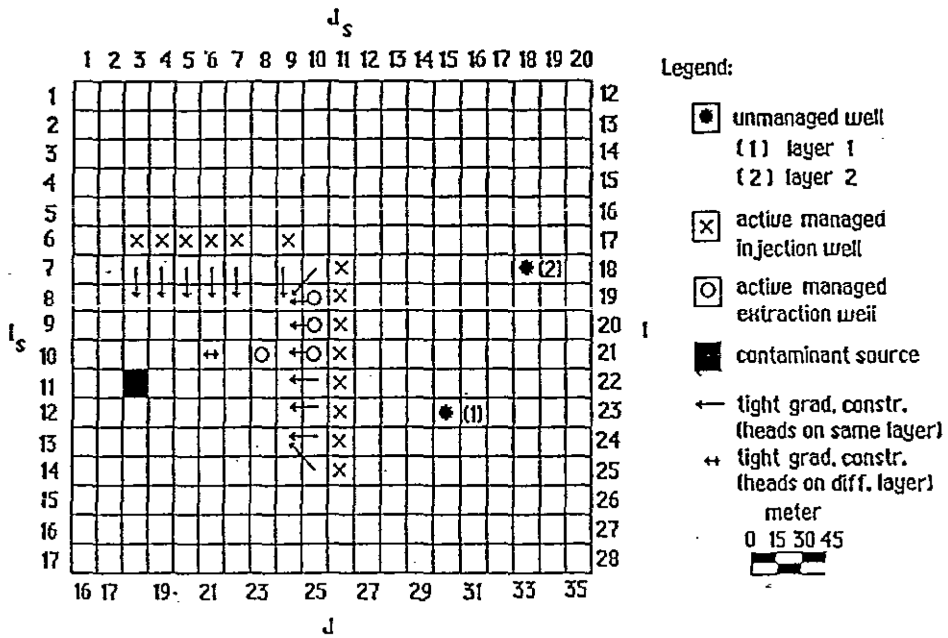

Figure 11 Location of optimal pumping wells and tight head-difference (gradient) constraints for Scenario 3.

interest. Table 5 illustrates the time needed to address Scenario 1. Included stages use either the discussed simulation models or the PLUMAN code on a 386 PC running at 33 MHz and having 4 MB RAM. Time required for US/REMAX^B is comparable to that of PLUMAN, since it uses many of the same solution procedures.

Clearly, the stage of computing influence coefficients, arranging the optimization model, and calculating an optimal strategy is the most computationally intensive. For this scenario and stage, two steps can be distinguished. The first involves computing influence coefficients. The second is model organization and optimization problem solution.

Here, the step of generating influence coefficients requires by far the most time. This results because this act essentially involves one simulation of a modified MODFLOW+STR per potential pumping location. Since there are 31 potential pumping locations, 31 simulations are performed to develop the influence coefficients needed for the response matrix. The more decision variables (potential pumping rates), the more computer time involved in this step.

The step involving model formulation and calculation of the optimal strategy is fairly short. The time needed to perform the optimization is a function of the number of decision variables (potential pumping rates) and state variables (heads or gradients that must be constrained within the optimization model). The larger these numbers, the more time required.

Second, the size of the optimization problem being solved is of interest. For example, the special versions of US/WELLS^D and US/REMAX^B that are released in shortcourses are limited in the number of nonzero values they can have in the optimization formulation. (Even optimization algorithms that are not part of water management models are commonly limited either in the number of nonzeros or in the number of rows and columns in their constraint equations.)

By way of explanation, there is one row in the response matrix per head or gradient constraint equation per time step of constraint. There is one column in the matrix per decision variable. For a steady-state problem, total matrix size is the product of the number of control locations and the number of decision variables. The matrix contains one nonzero coefficient for each potential pumping location–head control location pair (per time step of active constraint).

For the steady-state Scenario 1, there are $31 \times (22 + 31)$, or 1643, nonzeros due to influence coefficients. There are also 31 nonzeros due to the weighting coefficients (even if they are 1 in value) assigned to decision variables in the objective function. Thus, the optimization model formulation for Scenario 1 employs almost 1700 nonzeros. (That of Scenario A using US/WELLS^D includes 919 nonzeros.) This number can be reduced significantly by considering injection in only every other cell on the plume periphery rather than in each cell. For example, if only 12 injection wells were considered, the number of nonzeros would be about $18 \times (22 + 18) + 18$, or 738. In addition to reducing problem size, this would significantly reduce computational time.

Table 5 Computer Time Required to Perform Each Activity for Scenario 1

Step	Software used	Time (min)
1	MODFLOW+STR (compute nonoptimal head)	5.0
2	MOC (predict solute transport in a nonoptimal potent surface)	35.0
3	PLUMAN (compute influence coefficients, formulate management model and determine optimal pumping strategy)	150.0
4	MODFLOW+STR (compute transient head response to optimal pumping)	1.3
5	MOC (compute head and solute transport response to optimal pumping)	8.0

Reducing the number of nonzeros below 1000 is important because that is the upper limit on problem size in the inexpensive "special" versions of US/REMAX^B and US/WELLS^D. If problem size increases beyond that, software price increases dramatically. The full professional versions of the software can address problems of virtually unlimited size.

V. SUMMARY

Use of simulation/optimization models can significantly aid management of groundwater contamination. It can speed the design process and reduce manpower costs. It can improve the produced remediation designs and reduce remediation costs. It can easily address problems previously considered very difficult.

S/O modeling methods for groundwater flow management have been well established in research literature. Now, generally applicable S/O models are available for use on PCs. The discussed models, US/WELLS^D and US/REMAX^B, use linear systems theory, influence coefficients, and superposition. These models can address a wide range of problems. Easy to use, they include all simulation and optimization algorithms needed to compute optimal strategies.

US/WELLS^D and US/REMAX^B are perfectly applicable to linear (confined) aquifer systems and can be applied to nonlinear systems. The former is most appropriate for fairly homogeneous aquifer and stream-aquifer systems. The latter can address complex heterogeneous multilayer stream-aquifer systems.

Increasing use of these PC-based S/O models is anticipated, especially as user-friendly options increase. Even the special versions of these models (released at shortcourses), can solve important real-world problems.

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