

Optimal Pumping Strategies to Maximize Dissolved TCE Extraction at Mather AFB, California

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Contents

Background and Document Purpose	1
Definitions and Pumping Strategy Criteria	7
Developed Pumping Strategies and Satisfaction of Criteria	8
Sensitivity Analysis	13
Conclusions, Recommendation, and Limitations	14
Cited References	15
Appendix A. Adapted extracts from US/REMAX User's Manual, vs 2.0, 1993 (Why use a Simulation / Optimization Model: Background, Illustrative Example and Comparison with Normal Simulation Models).....	A-1
Appendix B. Maximizing Contaminant Extraction and Achieving Plume Capture with US/REMAX.....	B-1
Appendix C. Optimization Problem Formulation.....	C-1

List of Figures

1.	Mather Air Force Base vicinity map and approximate grid location	3
2.	Model grid and part of Mather Air Force Base	4
3.	Assumed initial TCE concentration, model grid, layer 1 boundary conditions, and P&T well locations	5
4.	Model grid, layer 2 boundary conditions, and supply well locations	6
5.	Initial concentration contours and those resulting from nonoptimal management and optimal pumping strategies	11
6.	Maximum concentration in aquifer versus time for selected sizes of the treatment facility	12

List of Tables

1a.	Optimal pumping rates (in gpm) for scenarios using initially assumed well locations.	
2a.	Optimal pumping rates (in gpm) for scenarios using modified well locations.	10

Background and Document Purpose

Mather Air Force Base (MAFB) is located approximately 12 miles east of Sacramento and due south of Rancho Cordova in Sacramento County, California (Figure 1). There are several areas of ground-water contamination at MAFB.

The Aircraft Control and Warning (AC&W) Site is in the east central part of MAFB. Ground surface elevations of the site range from about 107 to 134 ft above mean sea level. Surface water in the area drains into an unnamed tributary of Morrison Creek and directly into Morrison Creek.

Three main hydrogeologic units are of interest in the AC&W area (from top down): the vadose zone, the Shallow Water-Bearing Zone (SWBZ), and the Low Water-Bearing Zone (LWBZ). The top two zones are contaminated by dissolved trichloroethylene (TCE).

The ground-water flow direction in both the SWBZ and the LWBZ is toward the southwest.

An October 93 Record of Decision (ROD) stated that "The selected remedy for contaminated ground water at the AC&W Site consists of ground-water extraction, treatment via air stripping and injection of treated effluent into the SWBZ". MAFB plans to address this goal by installing a pump and treat (P&T) system. The ROD cites a 10-year planning period recommended by IT (IT, 1991). IT determined the planning period by studying several alternatives and the associated risks. They estimated that using a 200 gpm extraction/injection system would cause ground-water contaminant concentrations to drop below 5 ppb within 10 years. They felt that this approach would reduce risk from the plume more rapidly than other alternatives.

EA Engineering Science and Technology (EA) and Utah State University (USU), working under separate AFCEE contracts, cooperated in using models to determine how best to satisfy the ROD. EA calibrated aquifer parameters for a computer simulation model of the area and selected potential well locations. USU used those parameters and the potential well locations to determine optimal (maximum contaminant extraction) strategies for several sets of assumptions (scenarios).

EA calibrated the MODFLOW ground-water flow simulation model (McDonald and Harbaugh, 1988) to the study area (EA, 1994a). The model grid consisted of 52 rows and 42 columns (Figures 1,2,3,4). For model calibration, EA used ground-water monitoring data collected between 1991 and 1993. IT corporation developed a solute transport model using MT3D (Zheng, 1991). It used the solute transport model to simulate plume migration for alternative preliminary well locations and pumping strategies.

In the flow model, EA represented the aquifer as a heterogeneous two-layer aquifer. The upper layer (layer 1) is treated as unconfined. The lower layer (layer 2) is treated as confined or unconfined, depending on the position of the potentiometric surface. Layer 1 represents the SWBZ and layer 2 represents the LWBZ. All wells of the pump and treat system penetrate only layer 1.

USU used an enhanced version of US/REMAX (Peralta and Aly, 1993) to compute optimal pumping strategies for tested scenarios. US/REMAX is a simulation/optimization

(S/O) model because it incorporates both simulation ability and operations research optimization algorithms. It directly calculates the best extraction and injection rates for a given management problem. This differs from a simple simulation model that requires input of a particular pumping strategy.

EA proposed locations for extraction and injection wells. USU was assigned to: (1) utilize EA's well locations, (2) assume the 270 gpm total injection rate proposed by EA for eight injection locations, and (3) determine optimal extraction rates for eight EA-proposed extraction locations. Within these restrictions and subject to the criteria listed in the following section, USU determined optimal (maximum mass of contaminant extraction) strategies needed to achieve cleanup. USU also demonstrated the enhanced cleanup achievable by increasing treatment plant capacity. Finally, to illustrate the economic and environmental benefit of utilizing optimization as early as possible in the design process, USU tested a different extraction well configuration.

Definitions and Pumping Strategy Criteria

A pumping simulation scenario consists of a set of assumptions for which a simulation is performed. MODFLOW and MT3D are used to predict the results of using nonoptimal and optimal pumping strategies for different scenarios. The unmanaged scenario (Scenario A0) illustrates what will happen if no pumping strategy is implemented for the AC&W site.

An optimization scenario consists of a set of assumptions (management preferences, potential well locations, restrictions on pumping rates, physical system assumptions) for which an optimization is performed. A potential well location is one for which the S/O model (US/REMAX) computes a pumping rate (zero or nonzero).

There is one pumping strategy per scenario. The same scenario name is used to identify the pumping strategy assumed or developed for that scenario.

A pumping strategy consists of a spatially distributed (and possibly temporally varying) set of extraction and injection rates. In this study, a strategy computed by US/REMAX is optimal in that it maximizes the total contaminant extracted within a time horizon, while satisfying all management goals for a given scenario.

The following are common to all optimal pumping strategies developed for the AC&W site:

1. Only steady-state ground-water flow is evaluated.
2. Total extraction equals total injection.
3. An upper limit is imposed on total extraction.
4. The maximum sustained pumping from field tests of extraction wells (EA, 1994a) is the upper limit on discharge at each extraction well.
5. The goal is to maximize the mass of dissolved TCE removal during ten years.

Modelling assumptions (1 through 3 below) or requirements (4 below) common to all scenarios are:

1. No continuous source of TCE is active.
2. TCE does not degrade.
3. TCE does not adsorb to the aquifer medium.
4. The plume is captured by the extraction/injection system. Plume capture is assured if all particles placed around the 5 ppb TCE concentration contour eventually migrate to one of the extraction wells. Particles are placed halfway between the water table and the base of the aquifer. A particle tracking code is used to demonstrate capture.

The initial TCE concentrations (Figure 3) are calculated using a vertically-weighted average of observed concentrations in layer 1. The total mass of TCE in layer 1 of the model (174 lb) approximately equals the mass of TCE in the SWBZ (181 lb) estimated by IT (IT, 1992). Within the model the plume concentrations vary only horizontally although the actual TCE concentrations vary vertically and horizontally in the SWBZ. Predicted potential mass extraction of TCE is calculated by integrating the concentrations at the extraction wells over time.

Developed Pumping Strategies and Satisfaction of Criteria

USU first estimated the future TCE concentrations that would result if no pumping strategy were implemented (Figure 5, Scenario A0). Then USU used the procedure of Appendix B with the model formulation of Appendix C to compute optimal pumping strategies. In computing optimal strategies USU cycled until an arbitrary three percent contaminant mass convergence criterion was satisfied.

In overview, USU developed optimal pumping strategies for two ten-year scenarios that differ only in whether pumping was permitted to change with time. In Scenario A1 pumping was forced to be steady in time. In Scenario A2, pumping was permitted to change in each of three time periods. In Scenarios A3 and A4, USU developed optimal strategies for scenarios similar to A1, but differing in the capacity of the water treatment facility that could be employed. In Scenario A5, USU selected alternative well locations and computed an optimal steady pumping strategy for those locations.

The potential pumping locations for Scenarios A1-A4 are those provided by EA (Figure 3). Due to restrictions on the amount of time available for this project, only the extraction rates are optimized. Injection is fixed at the rates and locations previously determined by EA. The maximum capacity of the water treatment facility (270 gpm) had also been determined by EA before USU involvement. The facility capacity is the upper limit on total pumping. For the goal of maximizing contaminant extraction, the facility capacity becomes the optimal total pumping rate.

The optimal pumping strategies computed for Scenarios A1 and A2 are shown in Table 1a. The estimated mass of contaminant removed by each strategy is also listed. Figure 5 shows TCE concentration contours predicted to result from Scenarios A0 and A2. Scenarios A1 and A2 are identical for the first three years. In the first three years, both strategies require seven wells to extract a total of 270 gpm of ground water. Strategy A2 requires 6 extraction wells for the years 3-6. For the final 4 years, Strategy A2 requires only 5 extraction wells. Strategies A1 and A2 require one fewer extraction well than EA's strategy but strategy A1 yields only a two percent increase in mass extraction over that predicted to result from the EA pumping strategy (recall that the EA strategy was developed using only simulation modeling). The relatively small magnitude of improvement results because the S/O model was not given the freedom to select either facility capacity (total pumping rate) or extraction well locations.

The next two scenarios (A3 and A4) illustrate how water treatment facility capacity (540 and 810 gpm, respectively) affects potential cleanup. Contrasting the optimal strategies and mass extraction resulting from Scenarios A2, A3 and A4 (Table 1a) shows the importance of using optimization as early in the design process as possible. Optimization can help evaluate the tradeoff between facility capacity and clean-up speed. Figure 6 shows how the maximum ground-water TCE concentration changes with time for selected facility flow rates. Interpolating in Figure 6 shows that a 600 gpm capacity is needed to reduce TCE concentration below 5 ppb within 10 years. Again, this assumes no continuous source of contaminant and no degradation or adsorption (admittedly simplistic assumptions).

Scenario A5 also shows that optimization should be employed as early in the design process as possible. For Scenario A5, USU selected eight potential extraction wells (wells U1 through U8), placed along the plume centerline (Table 1b gives precise potential locations). The optimal steady pumping strategy computed for Scenario A5 (Table 1b) consists of extracting 90 gpm from wells located at (row,column) locations (17,19), (26,19), (35,19). This strategy requires only three wells versus eight for the preliminary strategy developed using simulation models alone. The optimal strategy is predicted to extract about twelve percent more contaminant mass during ten years of pumping than the nonoptimal strategy.

TABLE 1(a). Optimal Pumping Rates (in gpm) for Scenarios Using Initially Assumed Well Locations

Extraction Well			Strategy						
Well ID	Row	Col	EA	A1	A2 (time in years)			A3	A4
					0-3	3-6	6-10		
E1	26	19	35	40	40	65	45	75	0
E2	19	18	25	45	45	0	0	75	125
E3	22	19	25	30	30	30	0	0	155
E4	23	22	25	0	0	0	0	75	125
E5	32	18	30	50	50	70	145	90	155
E6	35	21	35	20	20	20	10	75	125
E7	37	19	50	50	50	50	60	75	125
E8	36	17	45	35	35	35	10	75	0
Total Extraction (gpm)			270	270	270	270	270	540	810
Estimated Removed TCE Mass (lb)			132	135	82	36	18	149	164
						(Total = 136)			

TABLE 1(b). Optimal Pumping Rates (in gpm) for Scenario Using Modified Well Locations

Extraction Well			Strategy
Well ID	Row	Col	A5
U1	15	19	0
U2	17	19	90
U3	21	19	0
U4	23	19	0
U5	26	19	90
U6	29	19	0
U7	31	19	90
U8	35	19	0
Total Extraction (gpm)			270
Estimated Removed TCE Mass (lb)			147

Sensitivity Analysis

USU analyzed how the system would respond to implementing the Scenario A1 optimal pumping strategy, given that the physical system differs from our assumptions. To do this, we made several MODFLOW and MT3D simulations. Each of these 'sensitivity runs' used the optimal pumping strategy, but assumed a different set of the top layer's hydraulic conductivity or dispersion coefficient values. After each simulation we calculated the mass of extracted TCE. No degradation or partitioning were assumed (i.e., TCE was treated as a conservative contaminant).

The mass of TCE extracted by the wells pumping at optimal pumping rates increases by 1.1% when the dispersion coefficient decreases by 90%. The TCE mass decreases by 0.5% when the dispersion coefficient increases by 100%.

The increase in TCE extraction resulting from the decrease in the dispersion coefficient can be explained as follows. When the dispersion coefficient decreases, less contaminant movement (by dispersion) takes place. Since the extraction wells are extracting contaminated water from locations with high TCE concentration, the lower dispersion coefficient will result in less contaminant movement away from the extraction wells, resulting in higher concentrations at the extraction wells. This will cause increasing contaminant mass extraction via extraction wells.

Because changes in mass extraction are relatively small for all sensitivity runs, the mass of TCE extracted by the optimal pumping strategy for Scenario A1 is considered 'robust' within the tested range of variation of the dispersion coefficient.

The mass of TCE extracted by the wells pumping at optimal pumping rates increases by 15.4% when the hydraulic conductivity decreases by 60%. TCE mass removed decreases by 2.1% when the hydraulic conductivity increases by 100%. When the hydraulic conductivity is decreased, ground-water velocities decrease and less contaminant movement (by advection) takes place. This is similar, in effect, to a decrease in the dispersion coefficient as explained before.

Conclusion, Recommendations, and Limitations

Table 1a shows the optimal pumping strategies computed for both steady (A1) and time-varying (A2) scenarios strategies requiring 270 gpm of extraction and well locations specified by EA. Both strategies require 7 wells to maximize contaminant extraction. Eight injection wells are used to recharge the aquifer with the treated water. Using the treatment plant capacity of 270 gpm and existing well locations, MAFB should consider strategy A2 to extract the maximum amount of contaminant.

In Scenarios A1 and A2, all extraction and injection well locations and the water treatment capacity were predetermined. Therefore, the S/O model did not have much freedom to optimize. There is little improvement in total mass extraction between the above optimal strategies (A1 and A2) and that proposed by EA. Strategy A2 requires one less extraction well than EA's strategy, but extracts about 2% more contaminant mass over 10 years. This very modest increase results because USU lacked freedom to: (1) select potential extraction well locations, (2) select injection well locations or change injection rates, and (3) increase total pumping rate.

The optimal strategy resulting from a different set of extraction well locations can yield about 12% more contaminant mass extraction than EA's strategy. This alternative uses the same treatment plant capacity but requires only three extraction wells (U2, U5, and U7) instead of eight. Implementing this strategy (A5) would save the construction costs of 5 extraction wells while extracting more contaminant.

Increasing treatment plant capacity and total extraction rate will speed plume cleanup. Using different extraction well locations can significantly enhance cleanup without requiring an increase in treatment plant capacity.

Head response to optimal pumping in the field is only as accurate as the calibrated simulation model used. There is always some uncertainty in ground-water flow and transport modelling. Field concentrations will also differ from simulated values because of adsorption and biodegradation. However, results of the post-optimization analysis allow us to expect that implementing any of the optimal pumping strategies will result in maximizing the mass extraction of TCE from the ground-water aquifer.

Cited References

EA Engineering, Science and Technology. Apr 1994a. Ground-water modeling technical report. USAF Contract No. F41624-92-D-8005, Delivery Order No. 002. EA Eng., Sci. & Tech., 3468 Mt. Diablo Blvd., Suite B-100, Lafayette, CA 94549. 44 p.

EA Engineering, Science and Technology. Apr 1994b. Ninety percent specifications and drawings for base boundary pump and treat system, central base area operable unit, Norton Air Force Base. USAF Contract No. F41624-92-D-8005, Delivery Order No. 002. EA Eng., Sci. & Tech., 3468 Mt. Diablo Blvd., Suite B-100, Lafayette, CA 94549. 269 p.

IT Corporation. 1991. U.S. Air Force Installation Restoration program, Final Remedial Investigation Report of the AC&W Site for Mather Air Force Base, California. March 1991, Prepared by IT Corporation for Battelle Environmental Management Operations (EMO).

IT Corporation. 1992. Preliminary Design Investigation, Mather Air Force Base, California, Aircraft Control and Warning Site. Draft Final Report. June 1992.

IT Corporation. 1993. Superfund Record of Decision: Aircraft control and Warning Site, Mather Air Force Base Sacramento County, California, October 1993.

IT Corporation. 1994. Installation Restoration program (IRP), Stage 3, Final Preliminary Engineering Report For AC&W Pump and Treat System, Air Force Base Conversion Agency (AFBCA/OL-D/EM), 19503 Kaydet Avenue, Mather, California 95655.

Kincaid D., and Cheney, W. 1991. Numerical Analysis. Brooks/Cole Publishing Co. 680p.

Peralta, R. and Aly, A. 1993. US/REMAX (Utah State Model for Optimizing Management of Stream/Aquifer Systems Using the Response Matrix Method) User's Manual. Software Engineering Division, Biological and Irrigation Engineering Department, Utah State University, Logan, Utah. 200p.

Peralta, R. and Aly, A. 1995. Optimal Pumping Strategy To Capture TCE Plume at SW Base Boundary, Norton AFB, California. Final Report. Prepared for Air Force Center for Environmental Excellence, Environmental Restoration Directorate, Consultant Operations Division, Institute for Advanced Water Studies. January 1995. 23p.

Press, W.H., Flannery, B.P., Teukolsky, S.A., and Vetterling, W.T., 1993. "Numerical Recipes in C: The Art of Scientific Computing," Cambridge University Press.

Staudte, R.G. and Sheather, S.J., 1990. "Robust Estimation and Testing," John Wiley and Sons, Inc.

Zheng, C. 1990. A modular three-dimensional transport model for simulation of advection, dispersion and chemical reactions of contaminants in ground-water systems. USEPA Robert S. Kerr Environmental Research Laboratory, Ada, Oklahoma.

Appendix A

Adapted extracts from US/REMAX User's Manual, vs 2.0, 1993

Why use a Simulation/Optimization (S/O) Model: Background, Illustrative Example and Comparison with Normal Simulation Models

Introduction and simple application of linear systems theory in groundwater management

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

To help describe what optimization is, a graphical solution of a simple steady-state ground-water optimization problem is presented here. This illustrates the problem an optimization algorithm addresses in calculating an optimal pumping and/or diversion strategy. After the example, the difference between using S/O models and the simulation (S) models currently used by over 98% of practitioners is discussed.

Response matrix (RM) S/O models utilize the multiplicative and additive properties of linear systems. The additive property permits superimposing the drawdowns due to pumping at different wells to compute the drawdown resulting at an observation well. This is commonly taught with image well theory in introductory ground water classes. The multiplicative property means that the effect of doubling a pumping rate is a doubling of drawdown (examination of the Theis Equation shows that drawdown is linearly proportional to pumping). RM models use influence coefficients that describe system response (in head, gradient, etc.) to a 'unit' pumping rate. Application to nonlinear systems is discussed later.

The following equation illustrates use of the multiplicative property in groundwater head computation. Here we assume that the initial water table is horizontal and at equilibrium. Groundwater is extracted at a single well, index number \hat{a} .

$$\Delta h(\hat{o}) = \delta^h(\hat{o}, \hat{a}) \frac{p(\hat{a})}{p^{ut}(\hat{a})} \quad (A1)$$

where

$\Delta h(\hat{o})$ = change in steady-state aquifer potentiometric surface elevation at observation location \hat{o} [L];

$\delta^h(\hat{o}, \hat{a})$ = influence coefficient describing effect of steady groundwater pumping at location \hat{a} on steady-state potentiometric surface elevation at location \hat{o} [L];

$p(\hat{a})$ = pumping rate at location \hat{a} [L^3/T]¹;

$p^{ut}(\hat{a})$ = magnitude of steady 'unit' pumping stimulus in location \hat{a} used to generate the influence coefficient [L^3/T]. This does not necessarily equal 1.

¹For clarity and ease of explaining this example, pumping to extract groundwater is treated as positive in sign, and the δ^h influence coefficients are negative. In US/REMAX those signs are reversed to be consistent with MODFLOW.

Assume that a 'unit' steady pumping extraction rate of 1 m³/min at well \hat{a} causes a drawdown of 1 m at observation point \hat{o} . In that case, $\delta^h(\hat{o}, \hat{a})$ equals (-1) and $p^u(\hat{a}) = 1$. Equation 1 shows that if $\delta^h(\hat{o}, \hat{a})$ and $p^u(\hat{a})$ are known, the change in head caused by any pumping rate can be easily computed. If pumping, $p(\hat{a})$, equals 2 m³/min, head change will equal (-1)(2)/(1) or -2. This linear response is typical of confined aquifers (or approximates behavior of unconfined aquifers where the change in transmissivity due to pumping is small by comparison with the original transmissivity).

Similarly, the effect caused by a unit pumping at location \hat{a} on the final difference in potentiometric surface elevation between locations 1 and 2, of a pair of locations, \hat{o} , can be expressed as:

$$\delta^{\Delta h}(\hat{o}, \hat{a}) = \delta^h(\hat{o}_{\hat{o},1}, \hat{a}) - \delta^h(\hat{o}_{\hat{o},2}, \hat{a}) \quad (\text{A2})$$

$\hat{o}_{\hat{o},1}$ = index referring to point 1 of pair of locations \hat{o} ;

$\hat{o}_{\hat{o},2}$ = index referring to point 2 of pair of locations \hat{o} ;

For example, if $\delta^h(\hat{o}_{1,x}, \hat{a})$ for locations $x=1$ and $x=2$ of pair 1 are (-1) and (-1.02), respectively, $\delta^{\Delta h}(\hat{o}, \hat{a})$ equals 0.02.

Assume that pumpings at M^p locations affect head at location \hat{o} . The cumulative effect at \hat{o} is simply the result of adding the effect of M^p pumping rates. The following summation expression illustrates this application of the additive property, with the same assumptions as above.

$$\Delta h(\hat{o}) = \sum_{\hat{a}=1}^{M^p} \delta^h(\hat{o}, \hat{a}) \frac{p(\hat{a})}{p^u(\hat{a})} \quad (\text{A3})$$

where

M^p = total number of locations at which water is being pumped from the aquifer.

Similarly, the additive property can be used to describe the effect on head difference due to pumping at M^p locations. The following expression is used in the subsequent example.

$$\Delta \Omega(\hat{o}) = \sum_{\hat{a}=1}^{M^p} \delta^{\Delta h}(\hat{o}, \hat{a}) \frac{p(\hat{a})}{p^u(\hat{a})} \quad (\text{A4})$$

where

$\Omega(\hat{o})$ = the difference in potentiometric surface elevation between locations 1 and 2 of pair \hat{o} , [L]. $\Delta \Omega(\hat{o})$ equals the change in the difference due to pumping.

A simple manually solved groundwater optimization problem

Both additive and multiplicative properties are illustrated in this manually solved optimization problem. Assume the study area (top right of Fig. A1) contains 2 pumping wells (P1 and P2) and 2 head-difference control locations (each location consists of a pair of observation wells). The aquifer is at steady state and the initial potentiometric surface is horizontal.

The problem statement is to compute the minimum extraction needed to cause: head difference with index 1, ($\delta = 1$), to be at least 0.2 L and head difference 2 to be at least 0.15 L (towards the pumping wells), while assuring that the sum of pumping from both wells is at least $15 \text{ L}^3/\text{T}$. Such a situation might occur if you want to assure particular speeds of contaminant movement towards the extraction wells and want to treat a pumped water flowrate of at least $15 \text{ L}^3/\text{T}$.

The four parts of the problem statement are represented by equations shown in Figure A1. The top (unnumbered) equation is the 'objective function', the value of which we wish to minimize. This contains 'decision variables' $p(1)$ and $p(2)$, pumping at wells P1 and P2, respectively. Coefficients multiplying these values are weights (sometimes these weights represent costs). Here the weights indicate that pumping at well 2 is less desirable than pumping at well 1.

Equations a-c are termed 'constraints'. Because it is an \geq constraint, all points in the graph to the right of Line (a) satisfy that equation (Fig. A1). All points to the right of Lines (b) and (c) satisfy Equations b and c, respectively.

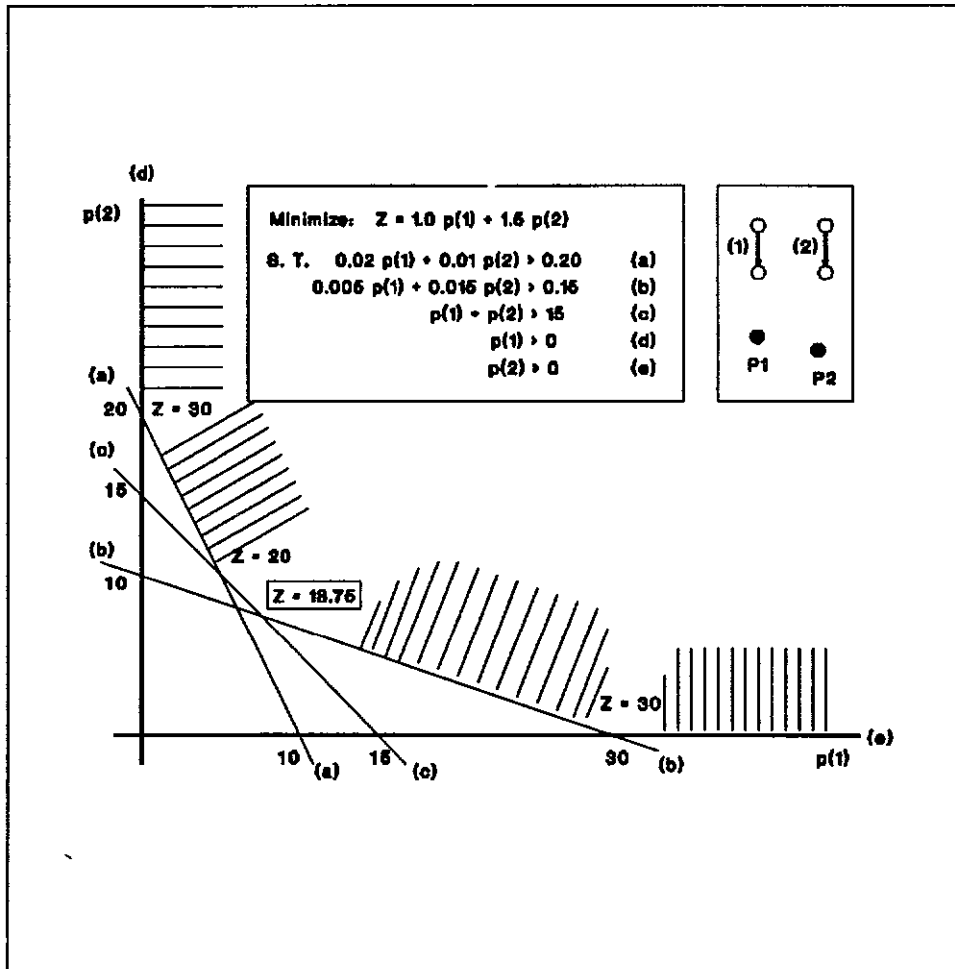
Equations a and b are applications of Equation A4 above. In Equation a, both $p^u(1)$ and $p^u(2)$ equal 1.0. Also, $\delta^{Ah}(1,1)$ and $\delta^{Ah}(1,2)$ are 0.02 and 0.01, respectively. The 0.02 coefficient describes the effect of pumping $p(1)$ on the difference in head between the two observation wells at control location 1. Each unit of $p(1)$ will cause a 0.02 increase in head difference between the two observation points of control pair 1 (i.e., an increase in gradient toward pumping well 1). Each unit of $p(2)$ will cause a 0.01 increase in head difference toward well 1 at the same location.

Equation b is similar to Equation a. It describes the effect of pumping on head difference across control pair 2.

Below the constraint equations are 'bound' Equations d and e. These prevent decision variables $p(1)$ and $p(2)$ from being negative (i.e. representing injection). Thus, only positive values of $p(1)$ and $p(2)$ are acceptable. This further defines the region of possible solutions.

Only points to the right or above all five of the constraint or bound lines satisfy all 5 equations. These points constitute the feasible 'solution space'. The optimization problem goal is to find the smallest combination of $p(1) + 1.5*p(2)$ in the solution space. That optimal combination will lie on the boundary between the feasible solution region and the infeasible region. In fact, it will be at a point where two or more lines intersect (a vertex of the solution space). For this simple problem of only 2 decision

variables, a graphical or manual solution (evaluating Z at the intersections of the lines) is simple—the minimum value of Z is 18.75, $p(1)$ and $p(2)$ both equal 7.5.²



² Note that if Equation 3 were $p(1) + p(2) \leq 15$, the feasible solution space would be the small centrally located triangle. In that case the minimum objective function value would be $Z = 18$, $(6 + 1.5 \cdot 8)$, and the optimal pumping rate would be $6 + 8 = 14$.

Also note that if, in a modification of the original problem, the weights in the objective function were both 1, there would be multiple optimal solutions of equal validity. The two points having original Z values of 18.75 and 20 would both have Z values of 15, as would all intermediate points on Line (c). However, generally this is not the case.

Optimization problems can become complex. For example, if we want to optimize 3 pumping rates in the above problem, we must solve the problem within 3-space (i.e. 3 dimensions, one for each optimizable pumping rate). Problems can rapidly become difficult or impossible to solve manually.

Formal optimization algorithms can be used to calculate optimal solutions for optimization problems having virtually unlimited dimensions (number of pumping rates) and constraint equations. These algorithms systematically search the boundaries of the feasible solution space and rapidly find the optimal solution. Generic optimization algorithms have been developed and applied to a wide range of optimization problems, including those of groundwater management. US/REMAX contains such algorithms and makes formulation and solution of groundwater optimization problems fast and easy.

An S/O model has another advantage. It will quantify for you the effect³ of each management goal (as implemented through a constraint or bound) on your objective function value. In effect, it tells you how much a constraint is costing you in terms of OF value. This shows which constraints you might want to consider changing to best improve the overall strategy.

³ This value, termed the marginal, equals the rate of improvement in the objective function, (OF), per unit change in the constraint or bound. In the original sample problem, suppose that you would like to use even less pumping than the optimal strategy indicates is necessary. Is there a reasonable way to achieve this?

You know that the optimal solution is at the intersection of Lines (b) and (c), (Fig. 1). Relaxing either constraint Equation b or c (i.e. moving their lines downward) will improve the OF value. Assume that you think you can live with relaxing Equation c, i. e. changing the 0.15 head difference constraint to 0.14. (Probably that head difference will still be adequate for our management goals.) For this problem, US/REMAX will tell us that the marginal of Equation c, $\partial Z/\partial \Omega$, equals (50). This means that the OF value will decrease in value 50 times as fast as you relax Equation c by decreasing the bound (for some finite amount of change). Proof of this value is shown below. Assume that if the right-hand side (RHS) of Eq. b is changed to 0.14, the new optimal solution will lie at the new intersection of Lines b and c. Solving for p(1) and p(2) at that point first requires rearranging Equation c.

$$p(1) = 15 - p(2)$$

Substituting for p(1) in the new Eq. b yields:

$$0.005 \{15 - p(2)\} + 0.015 p(2) = 0.14$$

$$0.075 - 0.005 p(2) + 0.015 p(2) = 0.14$$

$$0.01 p(2) = 0.065$$

$$p(2) = 6.5$$

Substituting for p(2) in Eq. c yields:

$$p(1) = 15 - 6.5 = 8.5$$

The new value of the objective function is:

$$Z = 8.5 + 1.5\{6.5\} = 18.25$$

The change in the objective function value is:

$$\Delta Z = 18.25 - 18.75 = -0.5$$

The rate of change in Z with respect to change in the restriction (i.e. RHS) of Eq. b is:

$$\partial Z/\partial \Omega = -0.5/-0.01 = 50$$

Thus, US/REMAX automatically tells you how you can best modify your management. It tells you how much objective enhancement you can expect for small changes in constraints or bounds.

A brief comparison between common simulation (S) models and simulation/optimization S/O models

If you cannot solve a given groundwater management optimization problem manually, and you have only a standard simulation (S) model available, your approach is probably as follows.

- 1) You specify the goals of the pumping strategy (ie. what system responses-- heads, gradients, etc.) are acceptable.
- 2) You assume a reasonable pumping strategy that you think might achieve these goals.
- 3) You simulate system response to the pumping strategy using the simulation model.
- 4) You evaluate acceptability of the strategy and its consequences.
- 5) Based on the evaluation of step 4) you repeat steps 2-4) until you feel you should stop.

When using an S model, the process of assuming, predicting and checking might have to be repeated many times. As the numbers of possible pumping sites and system response requirements increase, the likelihood that you have assumed an acceptable strategy decreases. Using this approach to reach the optimal strategy becomes impractical or impossible as problem complexity increases.

On the other hand, a groundwater simulation/optimization (S/O) model directly computes the pumping strategy that best satisfies your goals. The 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 (US/REMAX uses simulation equations similar to numbers A1-A4 above, plus many others). The optimization algorithm permits the specified management objective to serve as the function driving the search for an optimal strategy.

Both S and S/O models require data describing the physical system. However, other inputs differ because of their different capabilities (Table A1).

The normal S models compute aquifer responses to assumed boundary conditions and pumping values. The boundary conditions and pumping values are all used as data inputs. System response is the output.

On the other hand, S/O models directly calculate the best pumping strategies for the specified management goals. The goals and restrictions are specified via the objective function, constraint equations and bounds. Data needed to formulate these goals represent additional input required by S/O models (Table A1). Outputs include optimal pumping rates and the resulting system responses.

Although S/O models require additional data, that is only the data needed to make sure that the computed strategy indeed satisfies all your management goals. For example, upper or lower bounds of pumping rates, heads or gradients reflect the range of values which you consider acceptable. The model automatically considers those bounds while

calculating optimal pumping strategies. You might impose lower bounds on head, at a specific distance below current water levels or above the base of the aquifer. Upper bounds on head might be the ground surface or a specified distance below the ground surface.

In summary, the most important difference is that you must input a pumping strategy to an S model, while an S/O model computes it for you.

Table A1 Partial comparison between inputs and outputs of simulation (S) and simulation/optimization (S/O) models¹

Model Type	Input Values	Computed Values
Simulation (S)	Physical system parameters	
	Initial conditions	
	Some boundary flows	Some boundary flows
	Some boundary heads	Heads at 'variable' head cells
	Pumping Rates	
Simulation/ Optimization (S/O)	Physical system parameters	
	Initial conditions	
	Some boundary flows	Optimal boundary flows
	Some boundary heads	Optimal heads at 'variable' head cells
	Bounds on pumping, heads, & flows	Optimal pumping, heads, & flows
	Objective function (equation)	Objective function value

¹ Both types of models also require as input descriptors and parameters defining the physical system.

Appendix B

Maximizing Contaminant Extraction and Achieving Plume Capture with US/REMAX

Purpose:

The purpose of this appendix is to describe how to use US/REMAX to maximize extraction of contaminant in a complicated situation. Such situations might arise when the groundwater aquifer is heterogeneous and/or the initial contaminant plume has an irregular shape. Complexity can result from hydrologic features, management goals and constraints, institutional boundaries, or proximity of the plume to locations forbidden to contamination.

Tools:

- US/REMAX is used to compute optimal pumping strategies.
- MODFLOW and MT3D are used to evaluate the system response to stimuli (such as pumping).

Procedure:

To formulate the management problem, we need to express the amount of contaminant extraction as a function of the pumping rates at the 5 potential extraction locations. To accomplish this, we used iteratively re-weighted least squares (IRWLS) regression (Staudte and Sheather, 1990) to fit a linear function to the data of contaminant extraction as the response variable and the pumping rates as the explanatory variables. The integral (Appendix C, equation C1) is approximated using a 16-point gaussian quadrature rule (Kincaid and Cheney, 1991) for every 3-year period.

For practical considerations when the regression is performed, we consider the dependent variable to be the integral of concentration over time (without multiplying by the pumping rate). This approach has given a much better regression fit than fitting the regression equation to the volume of contaminant extracted. The traditional approach will suffer from the fact that the contaminant extraction from one well will be confounded by the pumping rate at that well. The procedure is outlined below.

1. Set up a matrix of sets of pumping rates to be used for regression equations. Since the optimization problem is to maximize contaminant extraction, it is expected that total optimal extraction will be 270 gpm (in magnitude).

Therefore, all the pumping rates used for calculating the regression data must sum to 270 gpm.

2. For each set of pumping rates run MODFLOW followed by MT3D and determine the contaminant extracted (integral of concentration over time) at each well. This step is done internally in US/REMAX.
3. Use IRWLS to fit a linear regression model to the data.
4. Use the fitted regression equations as constraints in the optimization model and solve the optimization problem.
5. Generate more sets of pumping rates closer to the optimal pumping rates calculated in step 4. Use the extra data (in addition to the data generated in step 2) to fit new (improved) regression equations.
6. Use the new regression equation as constraints in the optimization model and solve the optimization problem.
7. If the solution in step 6 is close (e.g., within 3%) to the solution in step 4, go to step 8. Otherwise, go to step 5. In all the considered scenarios for the presented problem, no more cycles were needed.
8. Simulate the resulting optimal pumping strategy using MODFLOW and MT3D. Check the accuracy of the predicted contaminant extraction calculated in the optimization model. If the values are close (e.g., within 3%), stop. Otherwise go to step 5. In the presented problem, the difference between the volume of contaminant extracted in the simulation (using MT3D) and that calculated in the optimization (using the regression equations) ranged between 1.0 and 3.0%.

Appendix C

Optimization Problem Formulation

A mathematical representation of the Mather AFB central base area contaminant extraction maximization problem is shown below. This considers 8 possible extraction cells. The model will compute a pumping strategy that maximizes the value of the objective function, equation C1', while simultaneously satisfying equations C2-C3 and C6. The formulation listed here is for Scenario A1. Scenario A2 is similar except it is divided into 3 separate optimization models. Each of the first two models maximizes contaminant extraction over a 3-year period. The third model maximizes contaminant extraction over a 4-year period (from year 6 to year 10) using the results from the first six years optimization as initial conditions.

$$\text{MAXIMIZE: } \sum_{\hat{a}=1}^8 \int_0^{10} (-1) p(\hat{a}, t) c(\hat{a}, t) dt \quad (\text{C1})$$

subject to:

$$200 \text{ gpm} \leq p(\hat{a}, t) \leq 0 \text{ for } \hat{a} = 1 \dots 8 \quad (\text{C2})$$

$$\sum_{\hat{a}=1}^8 p(\hat{a}, t) \geq -270 \text{ gpm} \quad (\text{C3})$$

where:

\hat{a} = Index designating location of potential groundwater extraction or injection;
 $p(\hat{a}, t)$ = magnitude of groundwater pumping rate [$L^3 T^{-1}$] from location \hat{a} at time t .

If the pumping rate, $p(\hat{a}, t)$, does not change with time, equation (C1) can be rewritten as

$$\text{MAXIMIZE: } \sum_{\hat{a}=1}^8 \left[(-1) p(\hat{a}, 1) \int_0^{10} c(\hat{a}, t) dt \right] \quad (\text{C4})$$

The integral in equation (C4) is approximated using a Gaussian quadrature rule.

We define $M(\hat{a})$ to be

$$M(\hat{a}) = \int_0^{10} c(\hat{a}, t) dt \quad (C5)$$

We rewrite the objective function (equation C1) as:

$$\text{MAXIMIZE: } \sum_{\hat{a}=1}^8 (-1) p(\hat{a}, 1) M(\hat{a}) \quad (C1')$$

A new constraint equation is introduced to relate the contaminant extraction to the pumping rates.

$$M(\hat{a}) = \beta(0) + \sum_{\hat{a}=1}^8 \beta(\hat{a}) p(\hat{a}, 1) \quad (C6)$$

Through Equation C2 the model has the freedom to select any extraction rate between 0 and 200 gpm for the cells containing extraction wells. EA's injection wells are not included in these wells, since their flow rates are assumed known.

In the objective function (equation C1'), extraction rates are multiplied by -1 because extraction rates are considered to be negative (as in MODFLOW convention). The resulting quantity will be positive and equal to the amount of contaminant removed from all wells.

No upper bounds are imposed on head because the water level is far enough below the ground surface that pressurized injection is very unlikely (a recharge mound will not reach the ground surface). No lower bounds are imposed on head because pumping extraction will be insufficient to cause unacceptable drawdowns (saturated thickness is large).

Equation C6 is a linear regression equation. The coefficients $\beta(0)$, $\beta(1)$, ..., $\beta(5)$ are calculated using an iteratively re-weighted least squares (IRWLS) fit. The predictive accuracy of this equation is tested in the post-optimization simulation. For the presented study, the prediction accuracy was always higher than 97%.

Another constraint equation is used to ensure that the computed optimal strategy also achieves capture of the contaminant plume. We use the procedure outlined in Peralta and Aly (1995) to define the lower bounds on head-difference at the control locations. For Scenario A2, the location of the head-difference constraints changes with time because the 5 ppb contour changes in response to P&T system extraction.