Optimal Pumping Strategies to Maximize Dissolved TCE Extraction at Central Base Area, Norton AFB, California

AFCEE/ERC
Water Studies Report
Number II

Final Report
Contract No. F41624-93-C-8041

United States Air Force
Air Force Center for Environmental Excellence
Environmental Restoration Directorate
Brooks Air Force Base, Texas 78235-5000

Consulting Operations Division (ERC)
Lt. Col. Darrel Cornell, Chief

Media Branch-
James Williams, Chief
Tel. 800-821-4528 x5246

Technical Project Manager
Philip Hunter
Tel. 800-821-4528 x5281

Prepared By
Richard C. Peralta and Alaa H. Aly
Professor and Research Assistant
Systems Simulation/Optimization Lab.
Dept. Of Biological and Irrigation
Engineering & Coop. Extension Svc.
Utah State University
Logan, Utah 84322-4105
Tel. 801-797-2786
Fax. 801-797-1248

August 1995

Contents

Background and Document Purpose 1

Pumping Strategy Criteria 8

Developed Pumping Strategy and Satisfaction of Criteria 9

Sensitivity Analysis 11

Conclusions and Recommendation 13

References 14

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 with US/REMAX . . B-1

Appendix C. Optimization Problem Formulation C-1

List of Figures

1. Ground-water basin and geologic faults near Norton AFB, California 2
2. Central Base Area and Southwestern Boundary Area, Norton AFB 3
3. Central Base Area and approximate grid location 4
4. Model grid and Central Base Area 5
5. Assumed initial TCE concentration and finite difference grid 7
6. Initial concentration contours and those resulting from nonoptimal management and optimal pumping strategies 10
7. Cleanup ratios for selected sizes of the treatment facility 12

Background and Document Purpose

Norton Air Force Base (NAFB) is located in the San Bernardino Valley, part of the California Peninsular Range geomorphic province (Figure 1). The elevation at NAFB is about 1,100 feet above mean sea level (msl). The ground slopes gradually to the southwest.

The San Bernardino Valley is a graben lying between the San Andreas and San Jacinto faults (Figure 1). The graben is filled with deep unconsolidated alluvial material, comprising what is termed the Bunker Hill hydrologic basin.

Three ground-water bearing zones, and two semiconfining zones (aquitards) exist in the vicinity of NAFB. The top ground water-bearing zone is contaminated by dissolved trichloroethylene (TCE), which is migrating from NAFB toward the southwest and wells which supply Riverside, California.

A 24 November 1993 Record of Decision (ROD) mandates that NAFB is to "maintain hydraulic control to the extent possible of the plume while extracting contaminated ground water, and reinjecting treated ground water into the contaminant plume or the clean portion of the aquifer" (EA, Apr 1994a, p. 1). NAFB plans to address this goal by installing two pump and treat (P&T) systems--one in the central base area (CBA) near the TCE plume source and the other near the southwestern base boundary (Figure 2).

EA Engineering Science and Technology (EA) and Utah State University (USU) are responsible for designing the P&T system for the southwestern boundary area. Earth Technology Corporation (ETC) and USU are responsible for the design of the CBA P&T system. Currently, the CBA P&T system is extracting 200 gpm. This system is to be augmented to extract up to 400 gpm (the capacity of the existing treatment unit).

ETC and USU, working under separate AFCEE contracts, cooperated in using models for this purpose. In overview, ETC 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 the optimal (maximum contaminant extraction) strategy.

ETC calibrated the MODFLOW ground-water flow simulation model (McDonald and Harbaugh, 1988) to the study area (EA, 1994a). The model's grid consisted of 60 rows and 55 columns (Figures 3 and 4). For model calibration, ETC used ground-water monitoring data collected in June 1992 by Camp, Dresser and McKee, Inc. (CDM, 1993). ETC used MOC (Konikow and Bredhoeft, 1984) to simulate plume migration for alternative preliminary well locations and pumping strategies.

In its model, ETC represented the aquifer as a heterogeneous single-layer unconfined aquifer. This single layer represents only the uppermost ground-water bearing zone. All wells of the pump and treat systems will penetrate this layer.

USU utilized the aquifer parameters resulting from EA's calibration, but used MT3D (Zheng, 1991) for simulating plume migration for different pumping strategies.

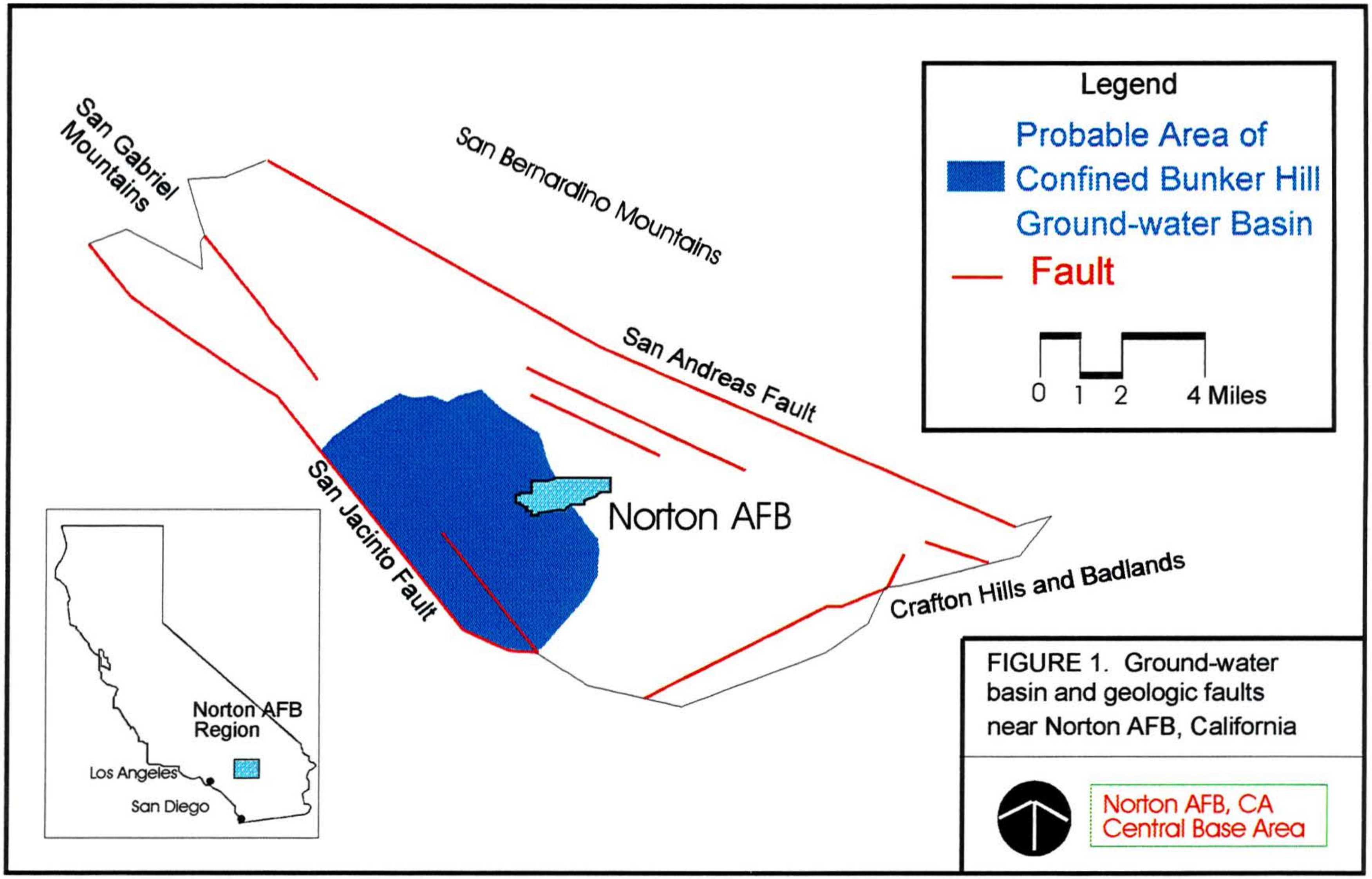


FIGURE 1. Ground-water basin and geologic faults near Norton AFB, California

Modified from Hardt and Hutchinson, 1980
and Earth Technology, 1994

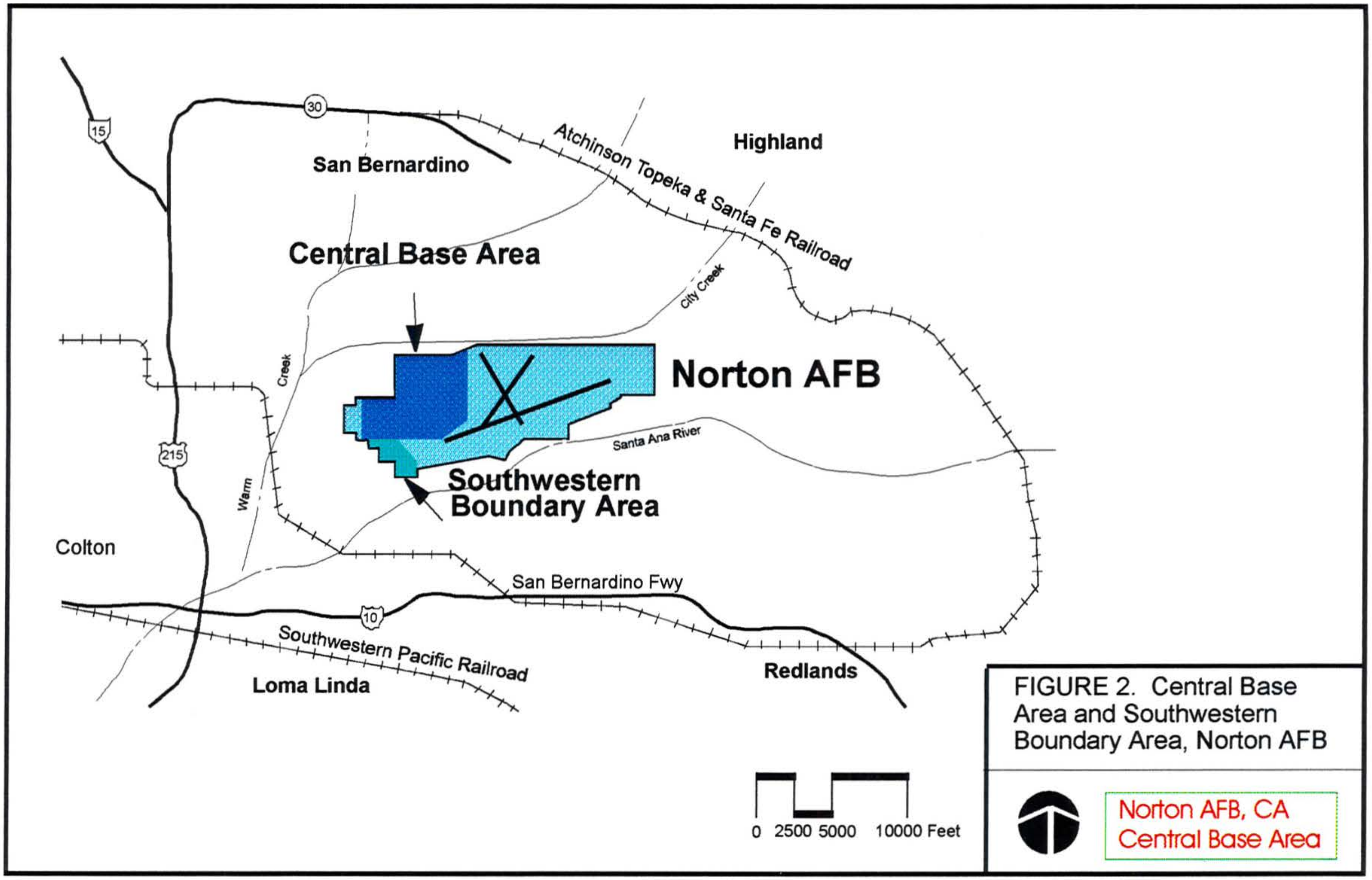


FIGURE 2. Central Base Area and Southwestern Boundary Area, Norton AFB

Modified from Earth Technology, 1994

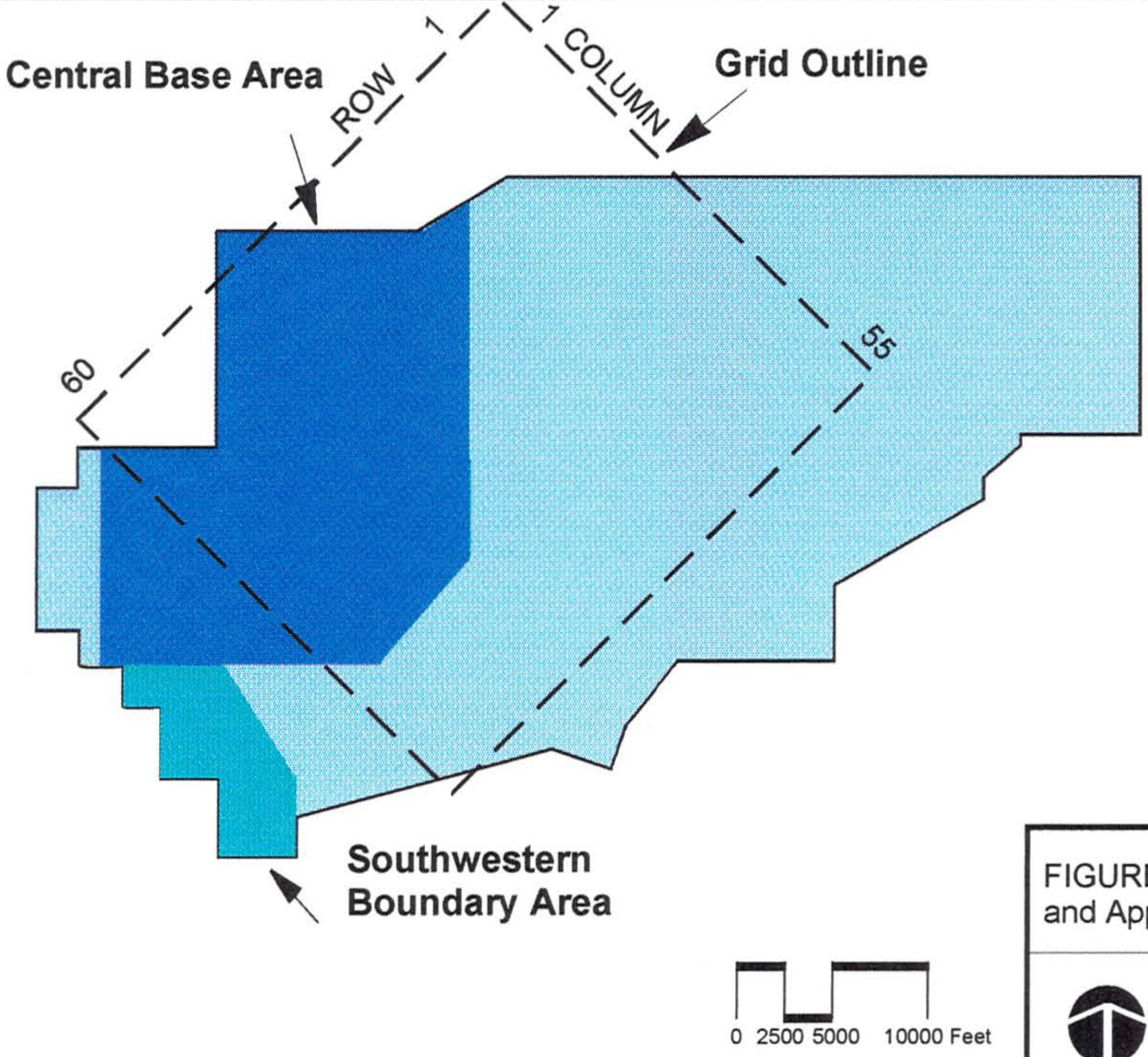


FIGURE 3. Central Base Area and Approximate Grid Location

Norton AFB, CA
Central Base Area

Modified from Earth Technology, 1994

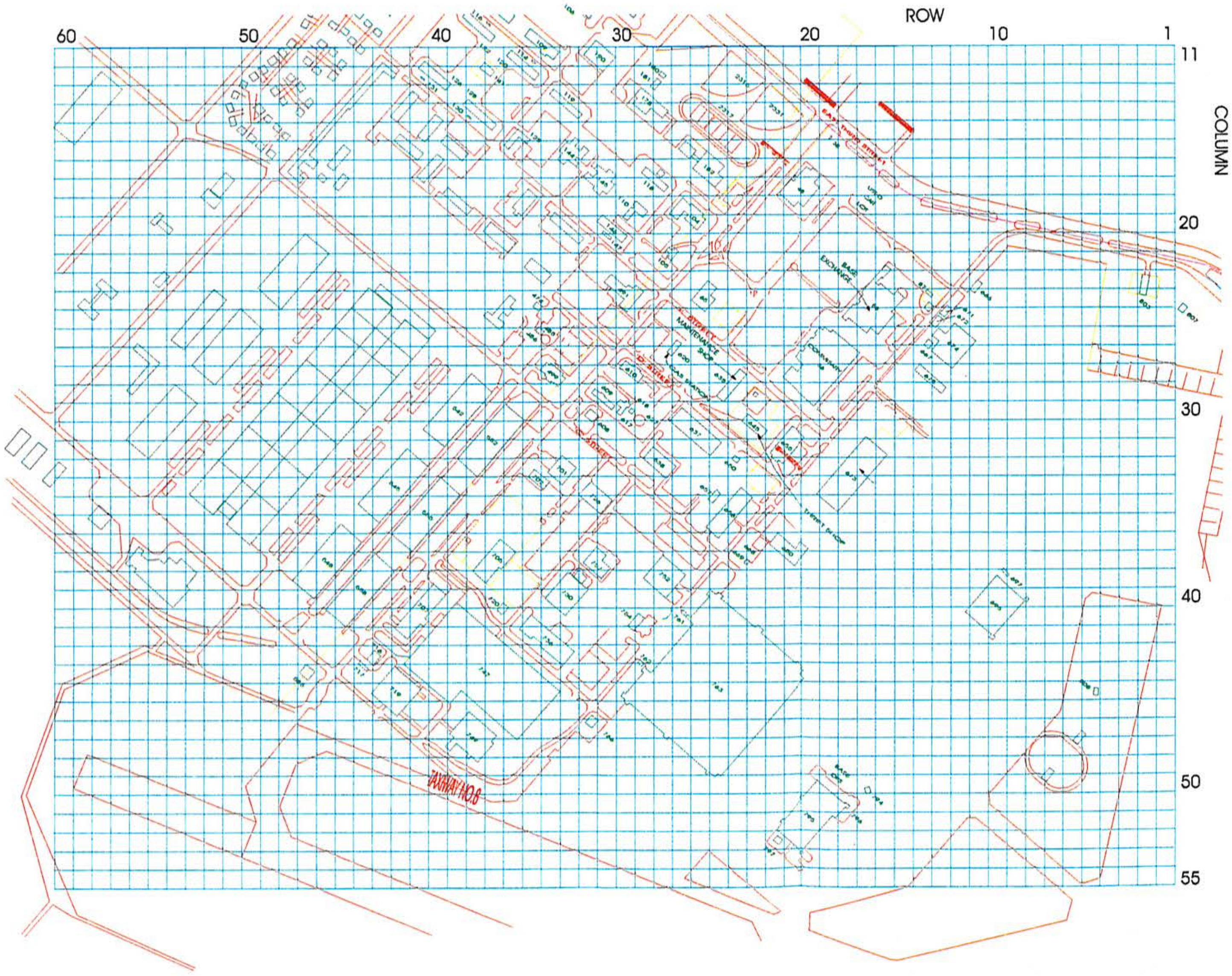


Figure 4. Model Grid and Central Base Area

Norton AFB, CA
Central Base Area

USU used an enhanced version of US/REMAX (Peralta and Aly, 1993) to compute optimal pumping strategies for posed scenarios. US/REMAX is termed 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 posed management problem. This differs from the action of a simulation model that requires input of an assumed pumping strategy.

ETC specified fixed injection well locations to be placed along existing pipelines. ETC also proposed locations and preliminary pumping rates for extraction wells. ETC developed their preliminary pumping strategy using a normal simulation model (i.e., without S/O modeling). ETC expected to modify these rates later based on field-observed response to pumping.

Due to the time restrictions on accomplishing this optimization effort, USU was assigned to: (1) utilize ETC's well locations, (2) assume 100 gpm injection rate at each of ETC proposed 4 injection locations, and (3) determine optimal extraction rates for 5 ETC proposed extraction locations. USU determined the optimal (maximum mass of contaminant extraction) strategies needed to achieve cleanup. Figure 5 shows the boundary conditions used by USU for the study area and the assumed initial TCE plume configuration.

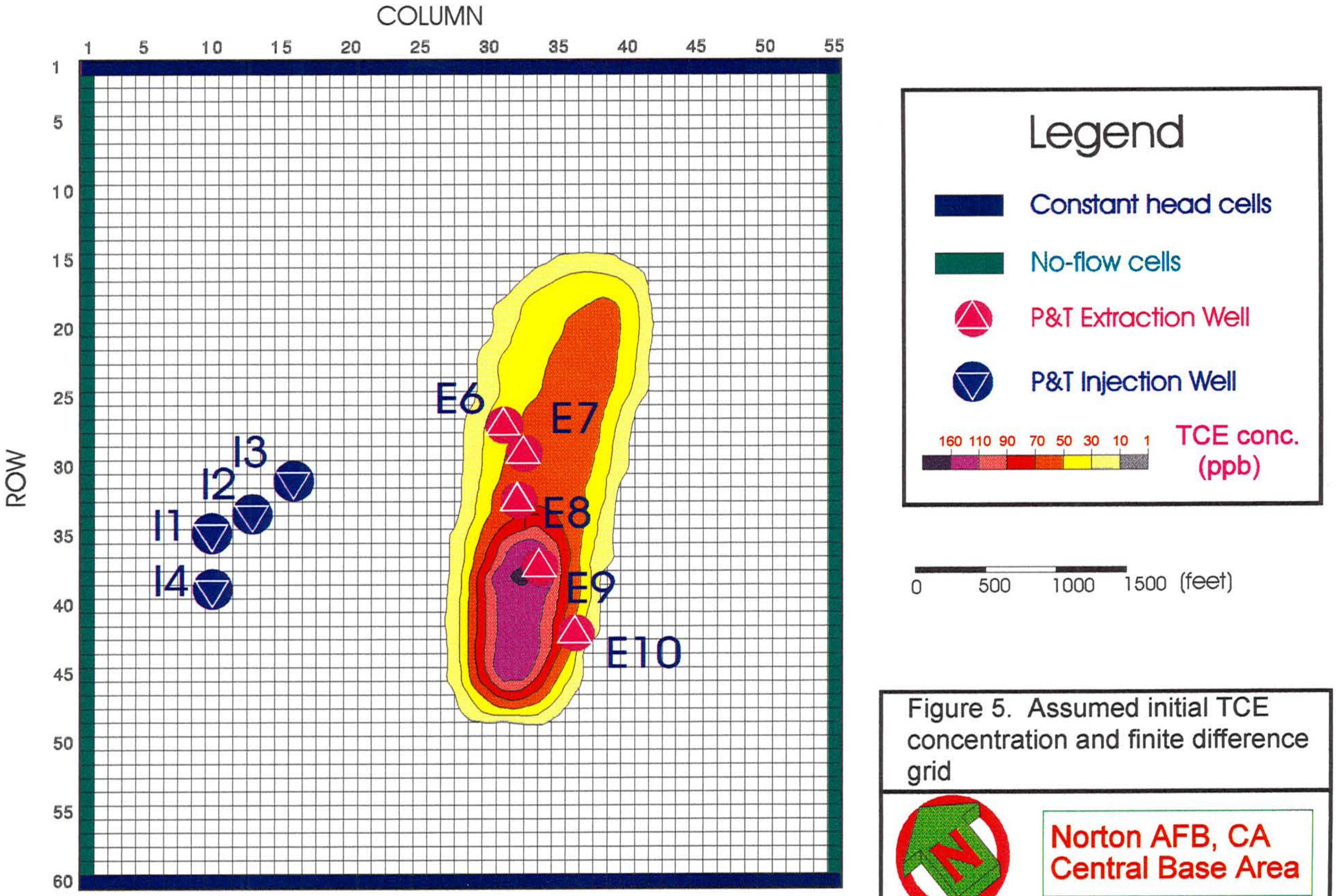


Figure 5. Assumed initial TCE concentration and finite difference grid

Pumping Strategy Criteria

The following characteristics are considered as being essential (^{E}) or desirable (^{D}) for developing pumping strategies.

1^E. steady-state ground-water flow evaluation.
2^E. total extraction must equal total injection.
3^E. utilize 400 gpm as the upper limit on total extraction.
4^E. use 100 gpm as the injection at each injection well, and 200 gpm as the upper limit on discharge at each extraction well.
5^E. use 150 ppb as the upper limit on the time average concentration of total extracted water.
6^D. utilize currently existing base extraction well E6, if practical.

Two sets of scenarios (A and B) are considered. Each scenario consists of an unmanaged scenario (A0 or B0) and an optimally managed scenario (A1 or B1). The unmanaged scenario illustrates what will happen if no optimal pumping strategy is implemented. The optimal scenario illustrates the results of implementing (using) an optimal pumping strategy computed by US/REMAX.

The first set (A0 and A1) assumes no continuous source of TCE is active. The second set (B0 and B1) assumes that a TCE source introduces about 53 lb. of TCE per year for the first 2 years and none thereafter. The optimal pumping strategies for both sets are those computed to maximize total contaminant extraction during a 3-year period. For scenario set 1, the calculated pumping strategy uses constant pumping rates for 3 years. For scenario set 2, optimal pumping rates are calculated first for the first 2 years and then are calculated for the third year (after the TCE source is inactive).

Developed Pumping Strategies and Satisfaction of Criteria

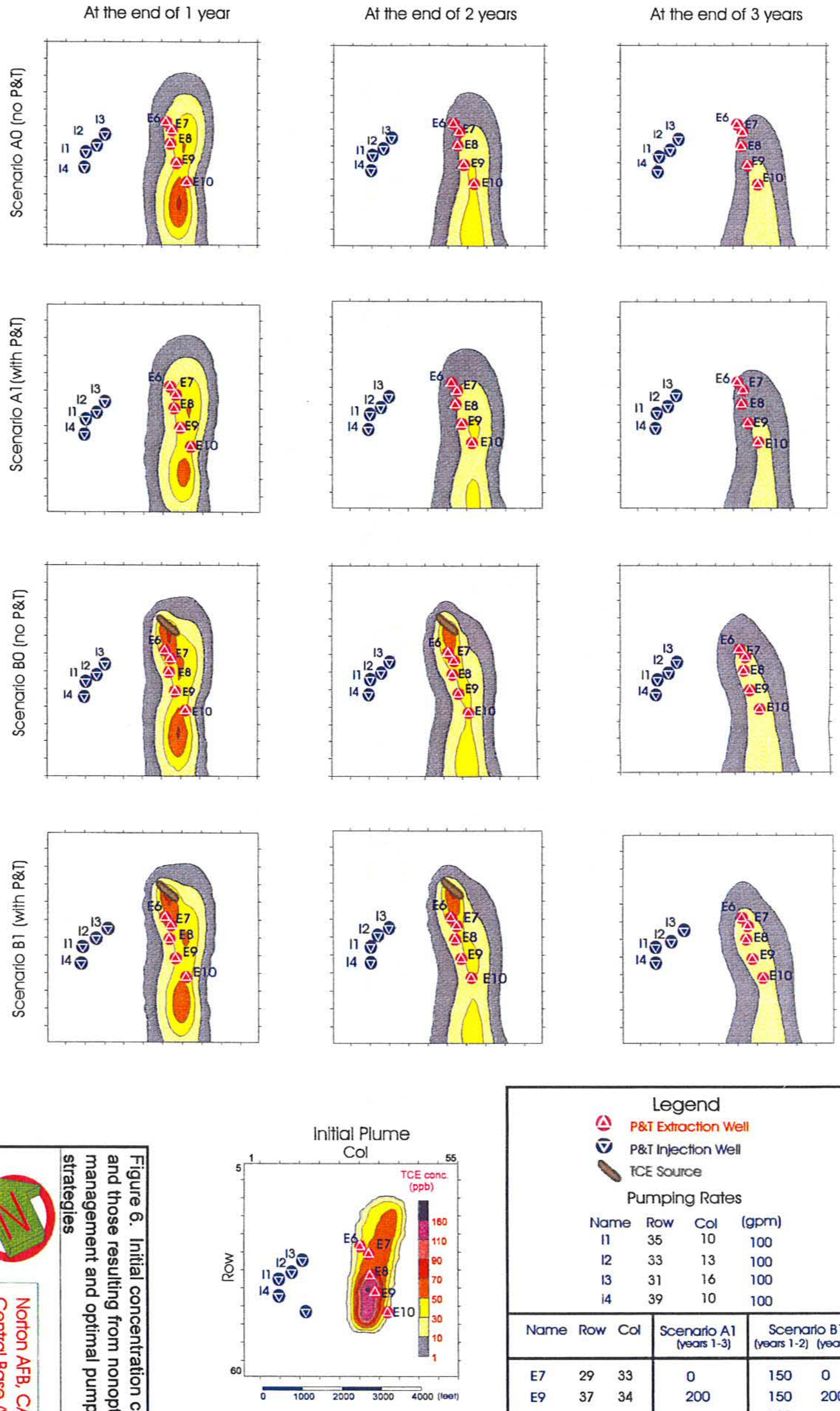
USU used the procedure outlined in Appendix B to develop optimal pumping strategies. A steady pumping strategy consists of a spatially distributed set of extraction and injection rates. A strategy computed by US/REMAX is optimal in that it maximizes the total contaminant extraction over the considered time horizon while satisfying all management goals for a posed management situation (scenario). A scenario consists of a set of assumptions (management preferences, potential well locations, maximum total pumping rates, assumed physical system) which are input into US/REMAX. A potential well location is one for which the model will compute a pumping rate (zero or nonzero). There is one optimal pumping strategy per posed scenario. As explained earlier, two sets of scenarios were examined.

Appendix C summarizes the optimization model formulation. Figure 6 shows the potential pumping locations. Due to restrictions on the amount of time for this project, only the extraction rates are optimized. The injection rates are fixed at 100 gpm at each of the four injection wells (USU was given these values by ETC).

Figure 6 shows the TCE concentrations projected to result with and without optimal pumping for both scenario sets A and B. According to post-optimization simulation using MODFLOW and MT3D, the optimal pumping strategies satisfy all specified criteria.

The optimal pumping strategy for Scenario A1 consists of extracting TCE-contaminated ground water at 200 gpm from each of two wells (Figure 6) (compared to five extraction wells needed by ETC's preliminary strategy). Scenario A1 is predicted to extract about 160% more contaminant mass over the 3-year period than the strategy developed without the S/O model.

The optimal pumping strategy for Scenario B1 consists of extracting TCE-contaminated ground water from three wells in the first two years. Two of the wells pump at 150 gpm and one well pumps at 100 gpm. In the third year, two of the three wells each pump at 200 gpm.



Legend

△ P&T Extraction Well

▽ P&T Injection Well

TCE Source

Pumping Rates

Name	Row	Col	(gpm)
I1	35	10	100
I2	33	13	100
I3	31	16	100
I4	39	10	100

Name	Row	Col	Scenario A1 (years 1-3)	Scenario B1 (years 1-2)	(year 3)
E7	29	33	0	150	0
E9	37	34	200	150	200
E10	42	37	200	100	200

Figure 6. Initial concentration contours and those resulting from nonoptimal management and optimal pumping strategies

Norton AFB, CA
Central Base Area

Sensitivity Analysis

We analyzed how the system would respond to implementing the optimal pumping strategy for Scenario A2, if the physical system differs significantly from our assumptions. To do this, we made several MODFLOW and MT3D simulations. Each of these 'sensitivity runs' used the optimal pumping strategy for Scenario A2, but assumed a different set of values for layer one hydraulic conductivity, dispersion coefficient, or porosity. Zero degradation and partitioning was assumed (i.e.,TCE was treated as a conservative contaminant). After each simulation we calculated the mass of extracted TCE.

The mass of TCE extracted by the wells pumping at optimal pumping rates increases by 8.4% when the dispersion coefficient decreases by 90%. The TCE mass decreases by 3% when the dispersion coefficient increases by 60%. 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 thus resulting in higher concentrations at the extraction wells. This will result in increasing the mass of contaminant extracted via the extraction wells. Because changes in mass extraction are relatively small among these sensitivity runs, the mass of TCE extracted for the optimal pumping strategy for Scenario A2 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 11.9% when the hydraulic conductivity decreases by 70%. The TCE mass decreases by 14.1% when the hydraulic conductivity increases by 60%. The increase in mass extraction resulting from the decrease in hydraulic conductivity can be explained as follows. When the hydraulic conductivity decreases, the 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.

Determining the treatment facility size was not part of the USU effort. The facility maximum flow rate had been selected before USU involvement. However, USU did evaluate the sensitivity of aquifer cleanup to selected treatment facility size. We selected a range of sizes between 400 and 2400 gpm. For each size, the maximum mass of TCE that can be extracted using the extraction wells is determined using the optimization procedure described previously. Cycling was performed until an arbitrary 3% contaminant mass convergence criterion was satisfied. Figure 7 shows the optimum cleanup ratios for the selected maximum facility flow rate. Cleanup ratio is defined as the ratio of TCE mass extracted by the extraction wells during three years to the initial mass of the TCE plume. USU estimates the initial mass of TCE in the plume as 4120 lb. For the largest tested treatment facility (size = 2400 gpm), the maximum potential extracted TCE mass is calculated to be 2225 lb.

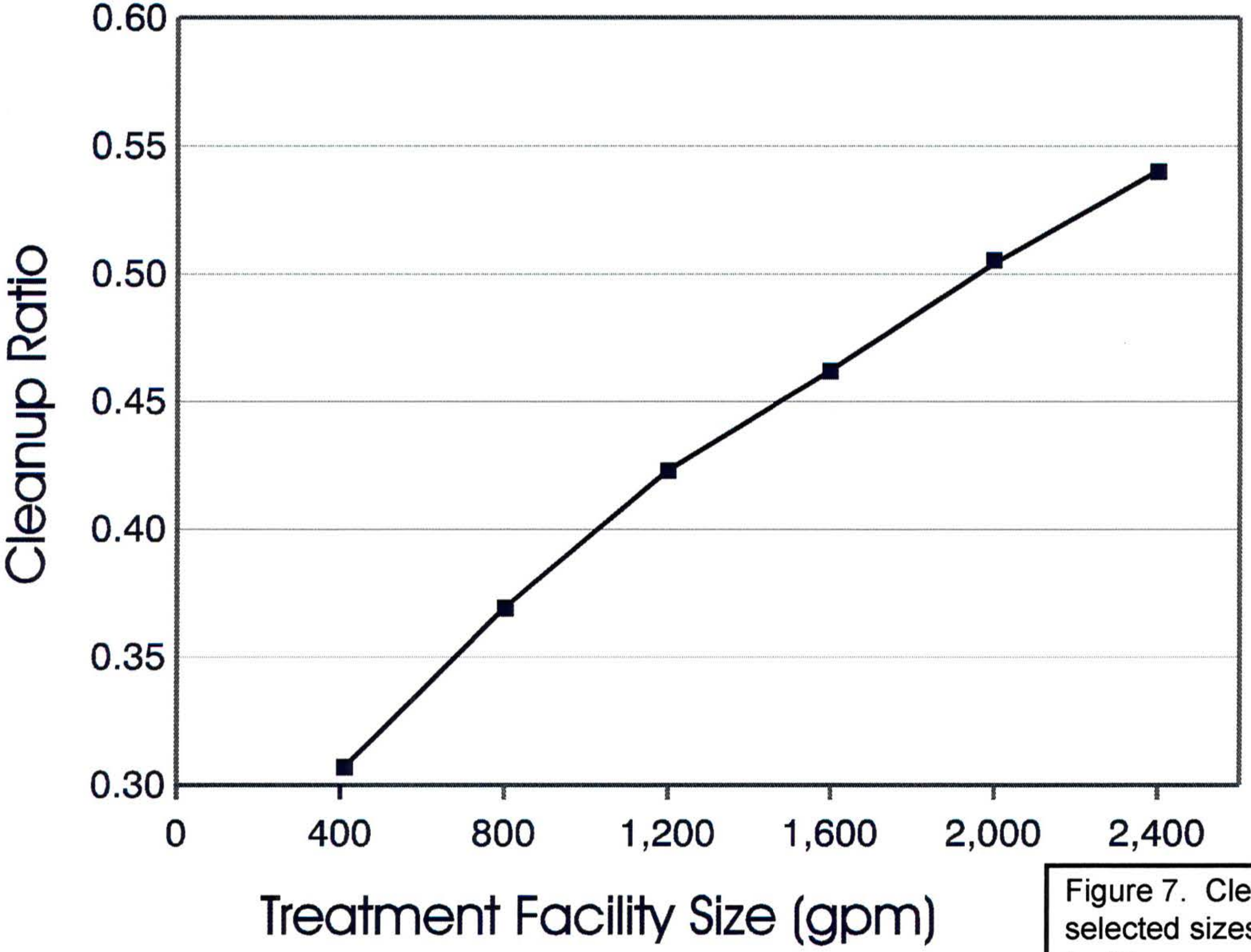


Figure 7. Cleanup ratios for selected sizes of the treatment facility

Norton AFB, CA
Central Base Area

Conclusions, Recommendations, and Limitations

The presented optimal pumping strategies satisfy all the stated criteria. Each proposed optimal strategy requires 400 gpm of extraction to maximize contaminant extraction while keeping the resulting flow concentration into the treatment facility below 150 ppb.

NAFB should consider two proposed pumping strategies for implementation. One optimal strategy assumes no continuing source of contamination and requires two extraction wells and four injection wells. A second optimal strategy assumes two years of continued source, three extraction wells and four injection wells for the first two years. In the third year, only two of the three extraction wells "should be" used.

More TCE mass can be extracted if the flow capacity of the treatment facility is increased. At 400 gpm extraction, up to 31% of the original mass can be removed. At 2000 gpm, 50% removal can be obtained (assuming no natural degradation or adsorption).

Developed pumping strategies are only as accurate as the calibrated simulation model upon which they are based. There is always some uncertainty in ground-water modelling. 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 for their respective situations.

Cited References

CDM Federal Programs Corporation. 27 Sep 1993. Draft ground water data trends report for Norton AFB, San Bernardino, CA. CDM Fed. Programs Corp., 301 Howard St., Ste 910, San Francisco, CA 94105.

CDM Federal Programs Corporation. 26 Apr 1994. Technical Memorandum, Jan 1994, ground water sampling, data results summary report; Comprehensive ground water monitoring program, Norton AFB, San Bernardino, CA. CDM Fed. Programs Corp., 301 Howard St., Ste 910, San Francisco, CA 94105.

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.

Konikow, L.F. and Bredhoeft, J.D. 1984. Computer model of two-dimensional solute transport and dispersion in ground water. Techniques of water-resources investigations of the USGS, Chap. 2, Book 7.

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.

Additional References

CDM Federal Programs Corporation. February 1994. Technical Memorandum, November 1993 Ground water Sampling Data Results Summary Report Comprehensive Ground water Monitoring Program. USAF Contract No. F41624-92-D-8005, Document Control No. 7900-027-TM-CJZZ. CDM Federal Programs Corporation, 301 Howard Street, Suite 910, San Francisco, CA 94105. 33 p.

EA Engineering. October 1993. Draft Preliminary Engineering Report Base Boundary Pump and Treat System, Norton AFB. USAF Contract No. F41624-92-D-8005, Delivery Order No. 0003. EA Eng., Sci. & Tech., 3468 Mt. Diablo Blvd., Suite B-100, Lafayette, CA 94549. 45 p.

EA Engineering, Science and Technology. March 1994. Ninety Percent Specifications and Drawings for Base Boundary Pump and Treat System Central Base Area Operable Unit Norton AFB. USAF Contract No. F41624-92-D-8005, Delivery Order No. 0002. EA Eng., Sci. & Tech., 3468 Mt. Diablo Blvd., Suite B-100, Lafayette, CA 94549. 44 p.

EA Engineering, Science and Technology. April 1994a. Ground water modeling technical report. USAF Contract No. F41624-92-D-8005, Delivery Order No. 0002. EA Eng., Sci. & Tech., 3468 Mt. Diablo Blvd., Suite B-100, Lafayette, CA 94549. 44 p.

EA Engineering, Science and Technology. April 1994b. Ninety Percent Specifications and Drawings for Base Boundary Pump and Treat System Central Base Area Operable Unit Norton AFB. USAF Contract No. F41624-92-D-8005, Delivery Order No. 0002. EA Eng., Sci. & Tech., 3468 Mt. Diablo Blvd., Suite B-100, Lafayette, CA 94549. 44 p.

Earth Technology Corporation. July 1993. Final Norton Air Force Base Central Base Area Operable Unit Aquifer Testing Southwestern Base Boundary Report. USAF Contract No. F41624-92-D-8005. Earth Tech. Corp., 1420 King Street, Suite 600, Alexandria, Virginia 22314. 70 p.

Earth Technology Corporation. October 1993. Draft Norton AFB, Central Base Area Operable Unit Remedial Investigation Report Supplement, Off-Base Trichloroethylene, Plume Investigation, Phase II Report. USAF Contract No. F41624-92-D-8005. Earth Tech. Corp., 1461 Dast Cooley Drive, Suite 100, Colton, CA 92324. 79 p.

Earth Technology Corporation. January 1994a. Water Wells in the Off-Base TCE Plume Area Norton AFB, CA. USAF Contract No. F41624-92-D-8005. Earth Tech. Corp. 1461 Dast Cooley Drive, Suite 100, Colton, CA 92324. 29 p.

Earth Technology Corporation. January 1994b. Final Norton AFB, Central Base Area

Operable Unit Remedial Investigation Report Supplement, Off-Base Trichloroethylene, Plume Investigation, Phase II Report. USAF Contract No. F41624-92-D-8005. Earth Tech. Corp., 1461 Dast Cooley Drive, Suite 100, Colton, CA 92324. 100 p.

Earth Technology Corporation. March 1994. Installation Restoration Program (IRP) Remedial Action Work Plan Addendum The Pump-And-Treat System Expansion Central Base Area, Norton AFB, CA. USAF Contract No. F41624-92-D-8005. Earth Tech. Corp., 1461 Dast Cooley Drive, Suite 100, Colton, CA 92324. 38 p.

WASTEBASKET

It is important to note that determining the size of the treatment facility was not part of our effort. The treatment facility has been already installed before USU was tasked with designing the pump and treat system.

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 groundwater 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 an 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 groundwater 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 â.

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

where

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

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

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

Assume that a 'unit' steady pumping extraction rate of 1 m^3/min at well â causes a drawdown of 1 m at observation point ô. In that case, $\delta^h(\hat{o},\hat{a})$ equals (-1) and $p^{ut}(\hat{a}) = 1$. Equation 1 shows that if $\delta^h(\hat{o},\hat{a})$ and $p^{ut}(\hat{a})$ are known, the change in head caused by any pumping rate can be easily computed. If pumping, $p(\hat{a})$, equals 2 m^3/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 â on the final difference in potentiometric surface elevation between locations 1 and 2, of a pair of locations, ò, can be expressed as:

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

$\hat{o}_{\grave{o},1}$ = index referring to point 1 of pair of locations ò;
$\hat{o}_{\grave{o},2}$ = index referring to point 2 of pair of locations ò;

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, $\delta^{\Delta h}(\grave{o},\hat{a})$ equals 0.02.

Assume that pumpings at M^p locations affect head at location ô. The cumulative effect at ô 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.

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

For 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.

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.

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

where

$\Omega(\grave{o})$ = the difference in potentiometric surface elevation between locations 1 and 2 of pair ò, [L]. Here, since the initial steady-state potentiometric surface is horizontal, $\Omega(\grave{o})$ also equals the change in the difference due to pumping, $\Delta\Omega(\grave{o})$.

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 and 2 head-difference control locations (each such 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 1, (ò = 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 L^3/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 L^3/T.

The 4 parts of the problem statement are represented by the 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 $p^{ut}(1)$ and $p^{ut}(2)$ equal 1.0. Also, $\delta^{\Delta h}(1,1)$ and $\delta^{\Delta h}(1,2)$ 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]

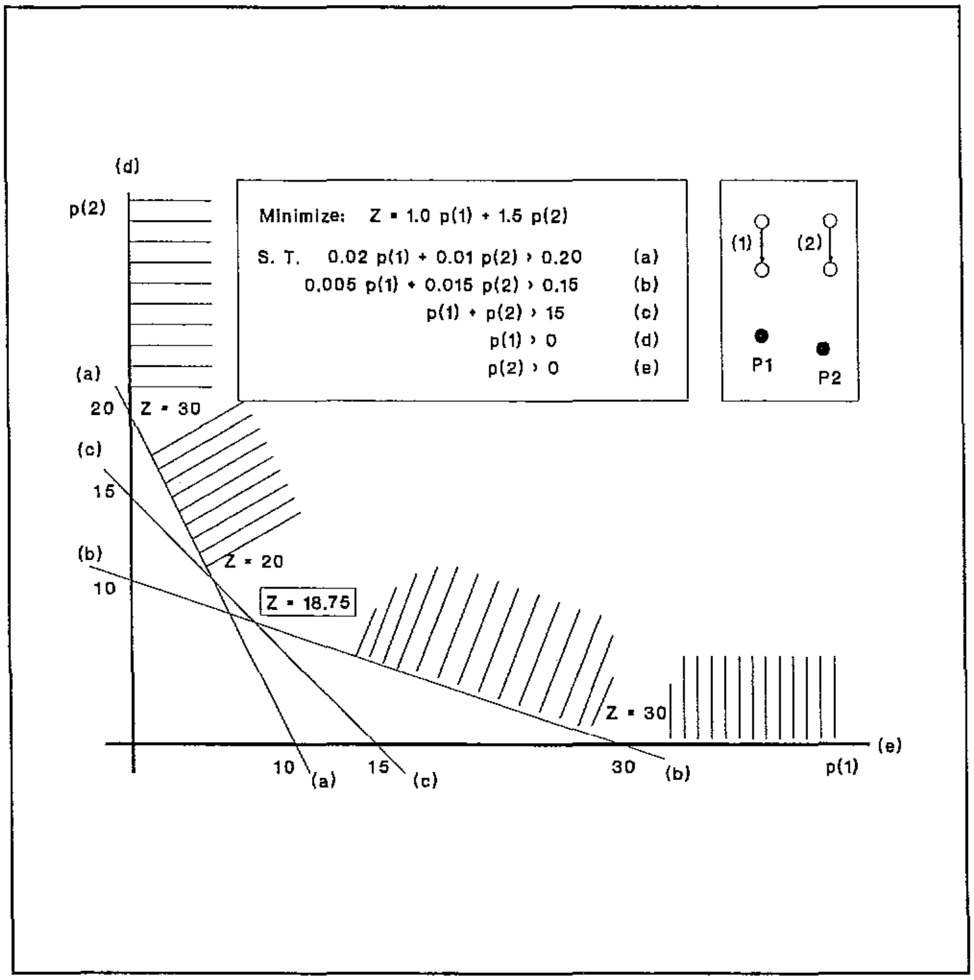


FIGURE A1.Graphical representation of simple pumping optimization problem.

---

[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*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 (ie. 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 effect[3] 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 consting 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:

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

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

$0.01 \quad p(2) = 0.065$

$p(2) = 6.5$

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 using common simulation models and S/O models

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

■1) You specify what you want the pumping strategy to achieve (ie. what system responses-- heads, gradients, etc.) are acceptable.

■2) You assume a reasonable pumping strategy that you think might achieve those 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. Assuming an 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 A1-4 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 1). 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 and Simulation/Optimization (S/O) models[1]

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 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 (equation C1) is approximated using an alternating extended Simpson's rule (Press et. al., 1993). 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 400 gpm (in magnitude). Therefore, all the pumping rates used for calculating the regression data must sum to 400 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 calculated in the simulation (using MT3D) and that calculated in the optimization (using the regression equations) ranged between 0.4 and 2.8%.

Appendix C

Optimization Problem Formulation

A mathematical representation of the Norton AFB central base area contaminant extraction maximization problem is shown below. This considers 5 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-C4 and C7. The formulation listed here is for Scenario 1. Scenario 2 is similar to this one except it is divided into two seperate optimization models. The first one maximizes contaminant extraction over 2 years. The second maximizes contaminant extraction over 1 year using the results from the 2-year optimization as initial conditions.

$$\text{MAXIMIZE:} \quad \sum_{\hat{a}=1}^{5} \int_{0}^{3} (-1)\, p(\hat{a},t)\, c(\hat{a},t)\; dt \qquad \text{(C1)}$$

subject to:

$$-\,200 \text{ gpm} \le p(\hat{a},t) \le 0 \quad \text{for } \hat{a} = 1 \ldots \qquad \text{(C2)}$$

$$\sum_{\hat{a}=1}^{5} p(\hat{a},t) \ge -400 \text{ gpm} \qquad \text{(C3)}$$

$$\frac{\sum_{\hat{a}=1}^{5} p(\hat{a},t)c(\hat{a},t)}{\sum_{\hat{a}=1}^{5} p(\hat{a},t)} \le 150 \text{ ppb} \qquad \text{(C4)}$$

where:

$\hat{a}$ =Index designating location of potential groundwater extraction or injection;

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

If the pumping rate, p(â,t), does not change with time, equation (C1) can be re-written as

$$\text{MAXIMIZE} \sum_{\hat{a}=1}^{5} \left[(-1)\, p(\hat{a}, 1) \int_{0}^{3} c(\hat{a}, t) \quad dt \right] \qquad (C5)$$

The integral in equation (C5) is approximated using an alternating extended Simpson's rule.

We define M(â) to be

$$M(\hat{a}) = \int_{0}^{3} c(\hat{a},t) \quad dt \qquad (C6)$$

We rewrite the objective function (equation C1) as:

$$\text{MAXIMIZE:} \sum_{\hat{a}=1}^{5} (-1)p(\hat{a},1)\, M(\hat{a}) \qquad (C1')$$

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

$$M(\hat{a}) = \beta(0) + \sum_{\hat{a}=1}^{5} \beta(\hat{a})\, p(\hat{a},1) \qquad (C7)$$

Through Equation C2 the model has the freedom to select any extraction rate between 0 and 200 gpm for the cells containing extraction wells. ETC'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.

Equation C4 states that the (average) concentration of all extracted water must be below 150 ppb. This condition is posed by the capabilities of the treatment facility. 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 C7 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 prediction accuracy of this equation is tested in the post-optimization simulation. For the presented study, the prediction accuracy was always higher than 97%.