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Optimal Pumping Strategy To Capture TCE Plume at SW Base Boundary, Norton AFB, California

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Environmental Restoration Directorate
Consultant Operations Division
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Executive Summary

Ground water contaminated by trichloroethylene (TCE) at Norton AFB (NAFB) has reached off-base supply wells. Utah State University (USU) computed an optimal steady pumping strategy to eventually halt off-base migration of TCE exceeding 5 ppb. (A steady pumping strategy is a spatially distributed set of extraction and injection rates.)

USU utilized: calibrated aquifer parameters and data provided by another contractor; the US/REMAX simulation / optimization (S/O) model; and MODFLOW and MODPATH simulation codes. A S/O model incorporates both simulation ability and operations research optimization algorithms. It directly calculates the best extraction and injection rates for a defined management problem. This differs from the action of a normal simulation model (such as MODFLOW), which is to predict system response to an assumed pumping strategy. For example, in one optimization here, the S/O model computed the least total pumping needed at all potential injection and extraction wells to capture the plume. The model indicated that NAFB should only extract at three and inject at seven of the 50 potential wells simultaneously considered.

The 2250 gpm computed optimal strategy satisfies the following prerequisite design criteria (the last two are verified via post-optimization simulation): (1) total extraction equals total injection, and does not exceed 2500 gpm; (2) all extraction and injection wells lie within NAFB boundaries; (3) currently existing base extraction wells are utilized to the extent practical; (4) TCE-contaminated ground water is prevented from reaching lower water-bearing strata; and (5) TCE (greater than 5 ppb) is eventually prevented from reaching public supply wells, even assuming summer (maximum) pumping rates for the downgradient public supply wells.

Sensitivity analyses show that the optimal pumping strategy will capture the contaminant if the actual hydraulic conductivity values of the contaminated layer range from 60% to 180% of the values used in computing the optimal strategy (i.e., of the best calibrated values). The strategy is robust (insensitive to error in assumptions) within this range of variation of conductivity.

The optimal strategy requires 2250 gpm of extraction. Two of the three proposed extraction wells are already in place. The strategy requires less total pumping and fewer wells than the strategy originally expected to be implemented. The result is a present value savings of about $5.8 M over a 15 year project life, assuming a 5% discount factor. This savings is achieved by reducing the number of extraction wells by one and the number of injection wells by one, reductions of 25% and 12.5% respectively. Also reduced is the expense of auxiliary construction and operation and maintenance costs.

The coupled use of simulation / optimization and pathline modeling has proven effective for this study. Injection is used to split the plume and direct contaminated water toward extraction wells. Without S/O modeling and the coordinated application of injection and extraction, much more extraction would be required.

Background and Document Purpose

Norton AFB (NAFB) is located in the north-central portion of the San Bernardino Valley area, approximately 65 miles east of Los Angeles, California (Fig. 1). The western portion of NAFB is situated over the Bunker Hill Ground-water Basin. The basin is bounded by the San Andreas Fault and the San Bernardino Mountains to the northeast, the San Jacinto Fault to the southwest, the San Gabriel Mountains to the northwest, and the Crafton Hills and Badlands to the south and southeast (Fig. 2.)

Drilling logs near NAFB indicate materials of five hydrostatigraphic layers. Three layers which yield ground water are separated by two semiconfining layers. The top layer is contaminated by dissolved TCE, which is migrating from NAFB toward water wells which supply Riverside, California (Figures 3-6).

A Record of Decision (ROD) dated November 24, 1993 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 will 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.

Earth Technology Corporation (ETC) has designed a small P&T system to extract dissolved phase TCE near the plume source. EA Engineering Science and Technology (EA) is responsible for designing the second P&T system.

EA and USU, working under separate Air Force Center for Evironmental Excellence (AFCEE) contracts, cooperated in developing and using ground-water models to help satisfy the ROD. EA calibrated aquifer parameters for a computer simulation model of the area. EA determined the background pumping rates and the water levels for which a P&T strategy is needed. USU determined the optimal (least pumping) strategy needed to achieve plume capture for the situation posed by EA.

EA calibrated the MODFLOW ground-water flow simulation model (McDonald and Harbaugh, 1988) to the study area (EA, 1994a). They used ground-water monitoring data collected in June 1992 by Camp, Dresser and McKee, Inc. (CDM, 1993). EA used hydraulic parameters derived from aquifer tests at the base boundary by ETC and at the CBA by CDM. EA also modeled the ground-water surface upon which the effects of a P&T strategy were to be superimposed by USU.

In their model, EA represented only the top three layers. Layers 1 and 3 are water bearing formations. Layer 2 is relatively impermeable and semi-confining. Layer 1 is unconfined. Layers 2 and 3 are confined. It was assumed that only Layer 1 is appreciably contaminated with TCE. All wells of the pump and treat systems will penetrate only Layer 1.

USU utilized the aquifer parameters resulting from EA's calibration, and other EA data. However, USU developed a finer grid mesh near plume capture wells. For increased resolution, USU partitioned each of the 150x150 ft cells used by EA in the plume vicinity into 4 cells of 75x75 ft. Aquifer parameters from a single large cell were assigned to all 4 daughter cells without interpolation. Figures 7a & 7b show the resulting grid discretization used by USU for this study.

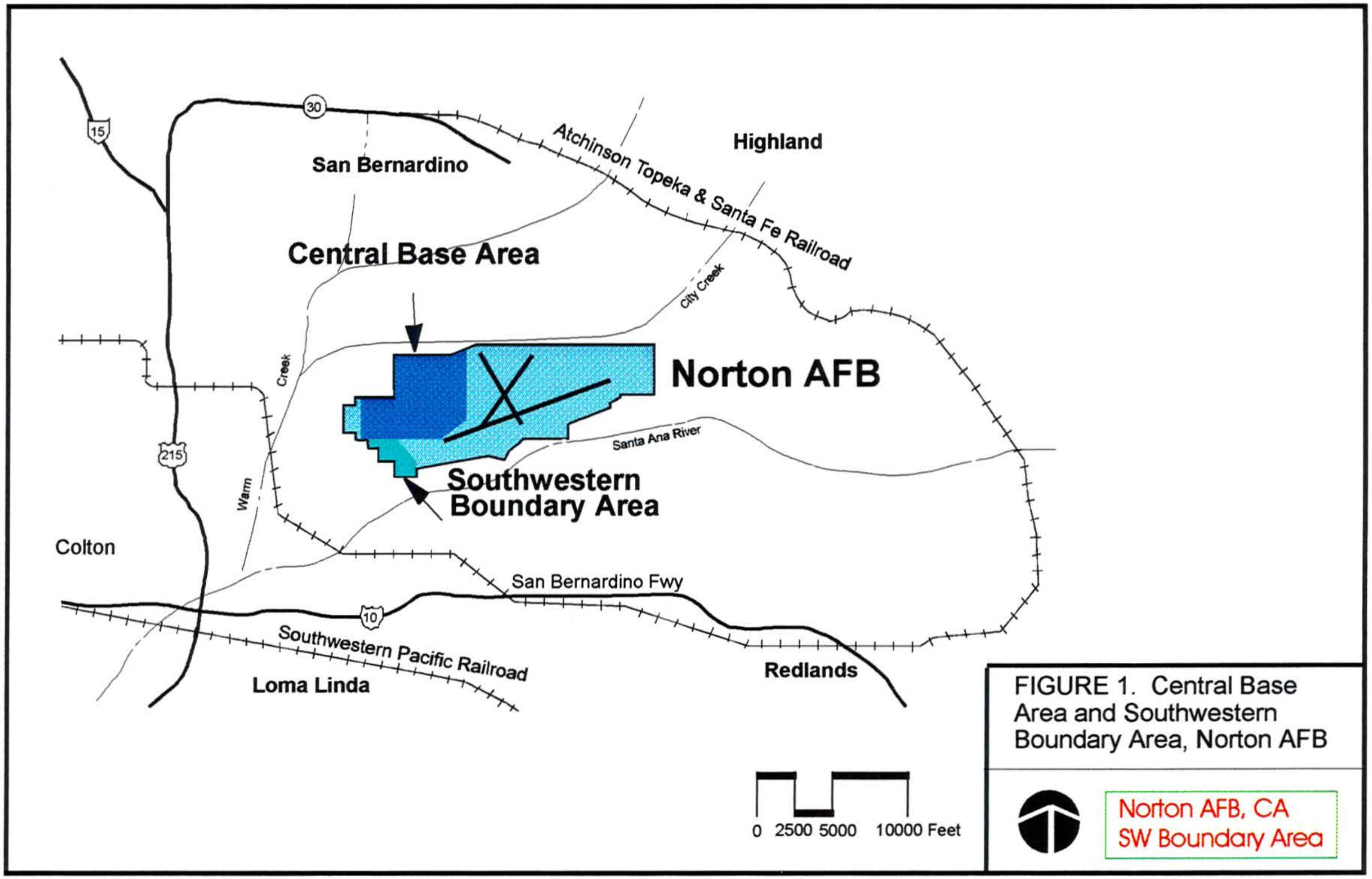


FIGURE 1. Central Base Area and Southwestern Boundary Area, Norton AFB

Modified from Earth Technology, 1994

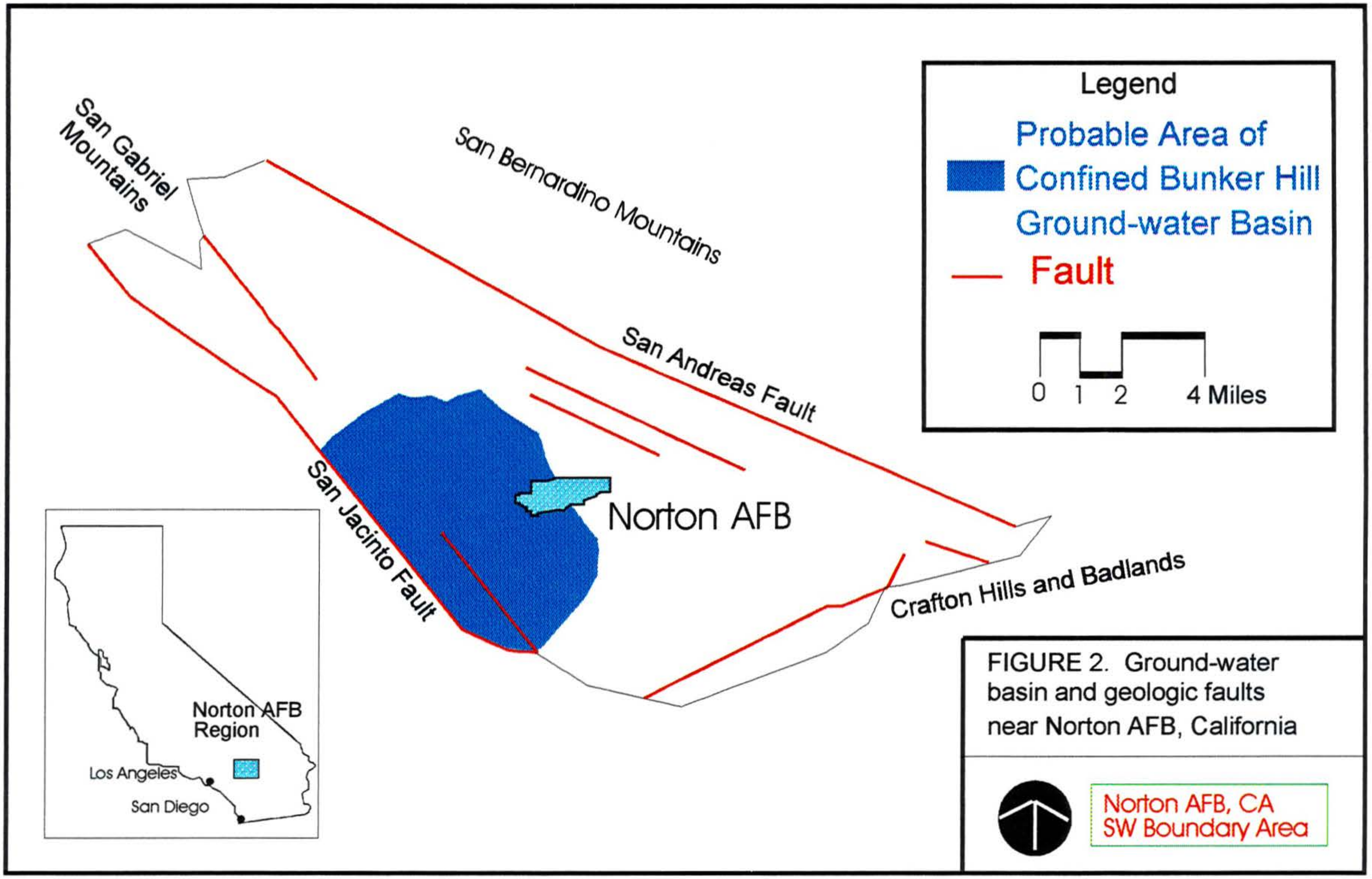
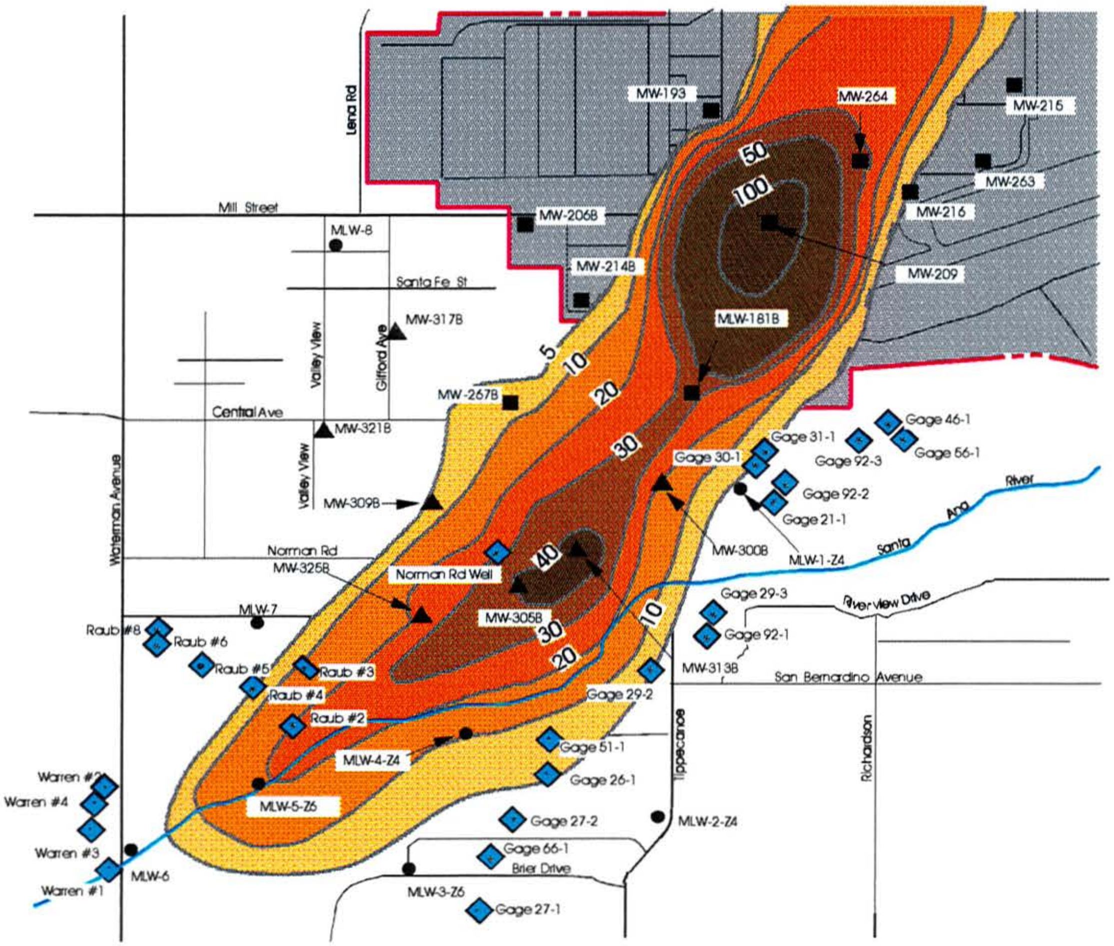


FIGURE 2. Ground-water basin and geologic faults near Norton AFB, California

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



Legend

- Phase II Multi-Level Monitoring Well
- Off-Base Monitoring Well
- CDM Monitoring Well
- Off-Base Production Well
- 50 TCE Concentration (PPB) (100-150 ft below ground surface, Aug. 1993, dashed where approximate)
- NORTON AFB

0 400 800 1600 Feet

FIGURE 3. Southwestern Boundary well location map and TCE plume, Norton AFB

Norton AFB, CA
SW Boundary Area

Modified from Earth Technology, 1994

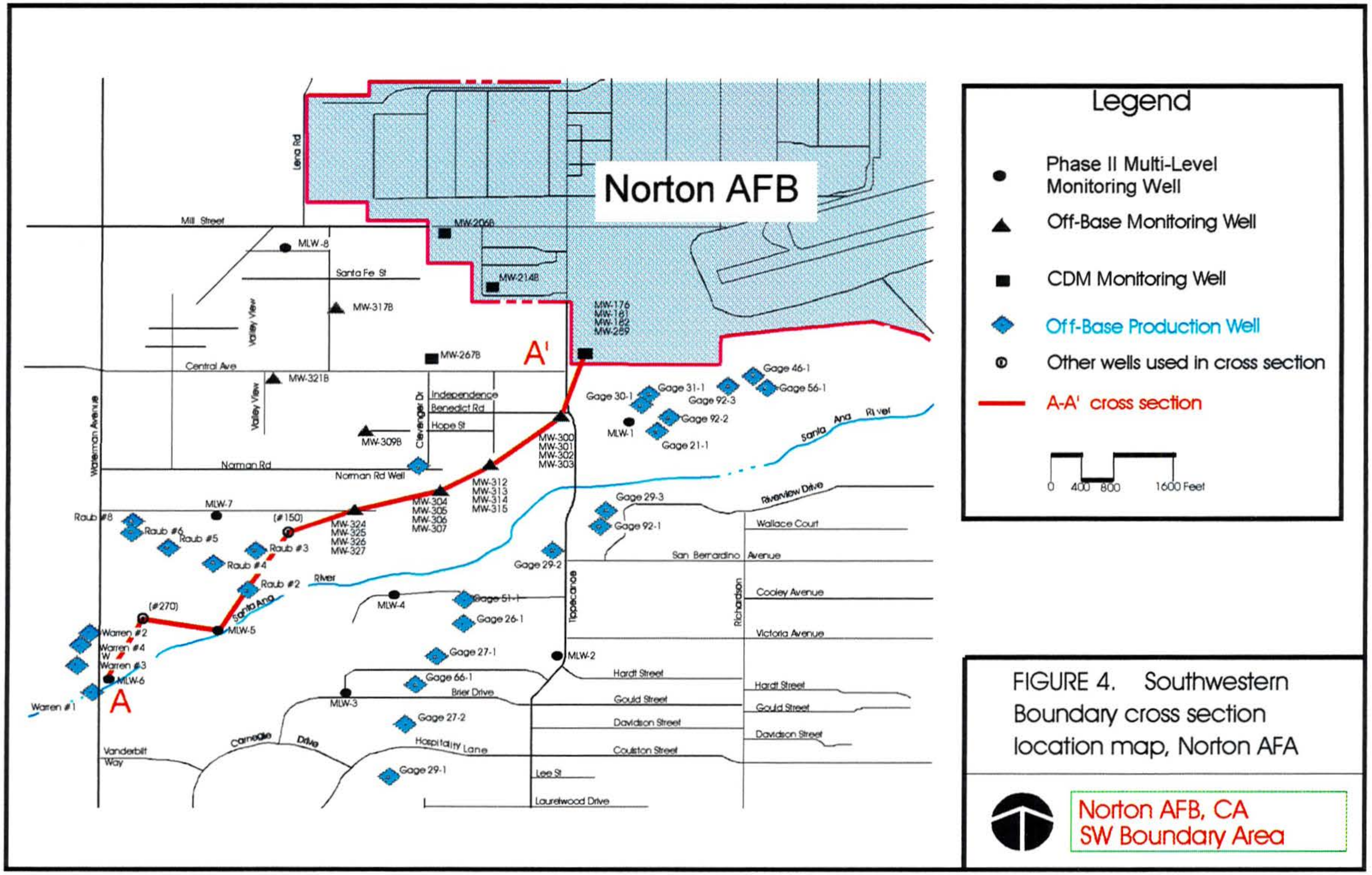


FIGURE 4. Southwestern Boundary cross section location map, Norton AFA

Modified from Earth Technology, 1994

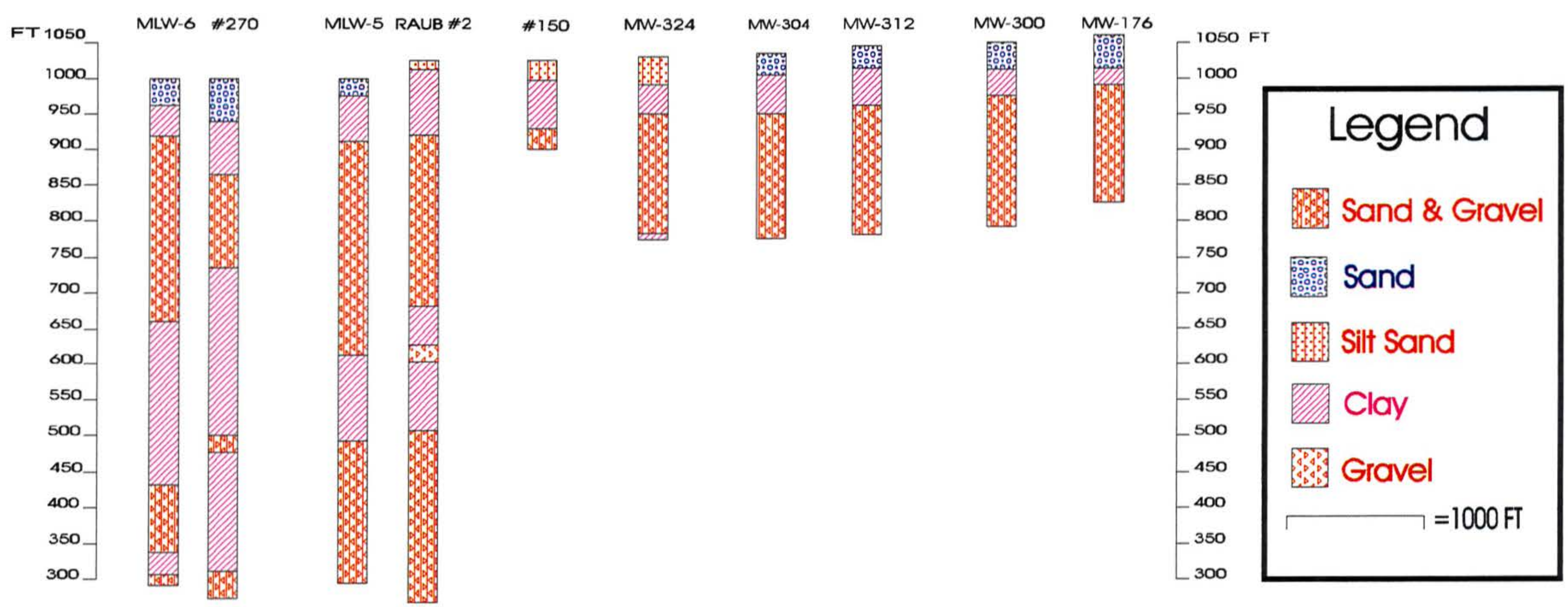


FIGURE 5. Borehole logs along cross section A-A'

Norton AFB, CA
SW Boundary Area

Modified from Earth Technology, 1994

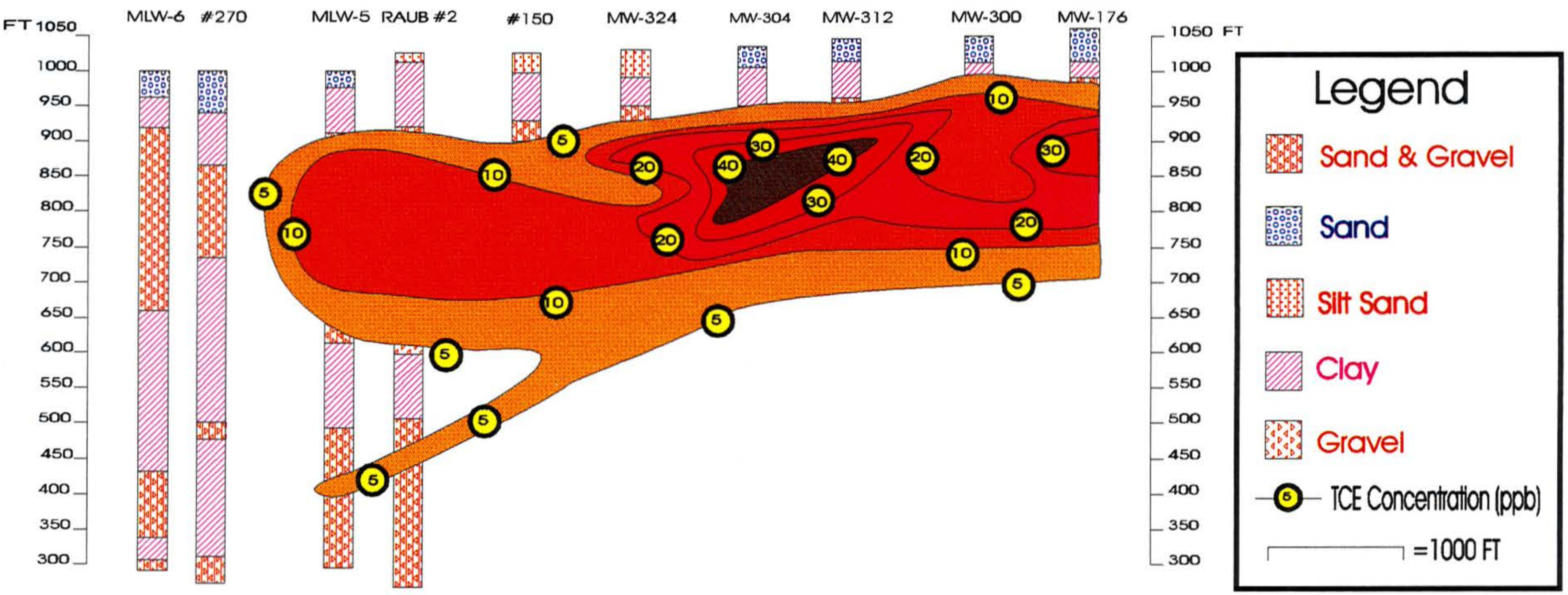


FIGURE 6. Borehole logs and TCE plume along cross section A-A', Aug 1993

Norton AFB, CA
SW Boundary Area

Modified from Earth Technology, 1994

USU used US/REMAX (Peralta and Aly, 1993) to compute an optimal pumping strategy. US/REMAX is a simulation / optimization (S/O) model which incorporates both simulation ability and operations research optimization algorithms. It directly calculates the best extraction and injection rates for a defined management problem.

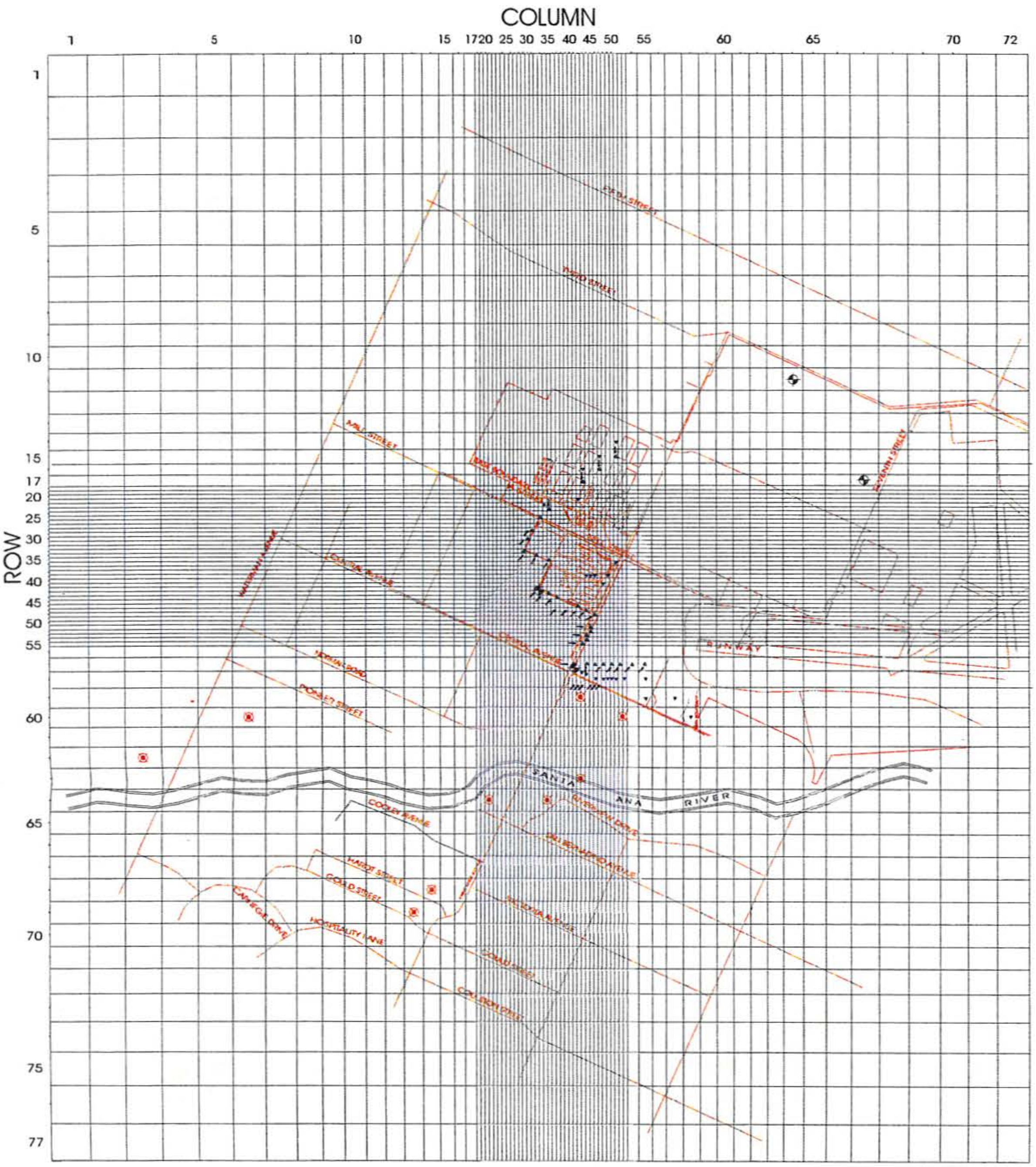
Appendix A illustrates how an optimal solution can be derived from an infinite number of acceptable solutions for a very simple problem. It also clarifies differences between simulation and S/O models. For example, in one optimization, the US/REMAX S/O model determines the least total pumping needed at all potential injection and extraction wells (Figures 7a & 7b) to capture the plume. The model indicates that NAFB should only extract at three and inject at seven of the approximately 50 wells considered.

USU used MODPATH (Pollock, 1989) to compute flowpaths (pathlines) that would result under steady-state conditions from different management scenarios. MODPATH utilizes output from MODFLOW, and considers the heterogeneous nature of the aquifer system. MODPATH reads heads and flows from MODFLOW output. It computes velocities at the centers of grid cells, and interpolates to estimate velocities for each particle that is tracked. The user specifies the cells and layers in which particles are placed. Particles will move and remain in their source layer, unless computed flow causes them to move to another layer.

Figure 8 shows the Layer 1 steady-state water table elevations computed to result from current municipal pumping plus the minor pumping at the upgradient CBA P&T system. The dissolved TCE plume is moving toward the municipal wells.

Figure 9 shows computed steady-state pathlines that water would follow in the area, with no water extracted along the NAFB southwestern boundary to halt plume movement. Given these conditions, pathlines originating within the 5 ppb contours will reach municipal wells. In Figure 9, all pathlines begin in column 60, rows 10-61 of Layer 1.

The next section describes criteria that a developed P&T system must satisfy. Then we describe development of an optimal pumping strategy that captures the plume using the pump and treat system.

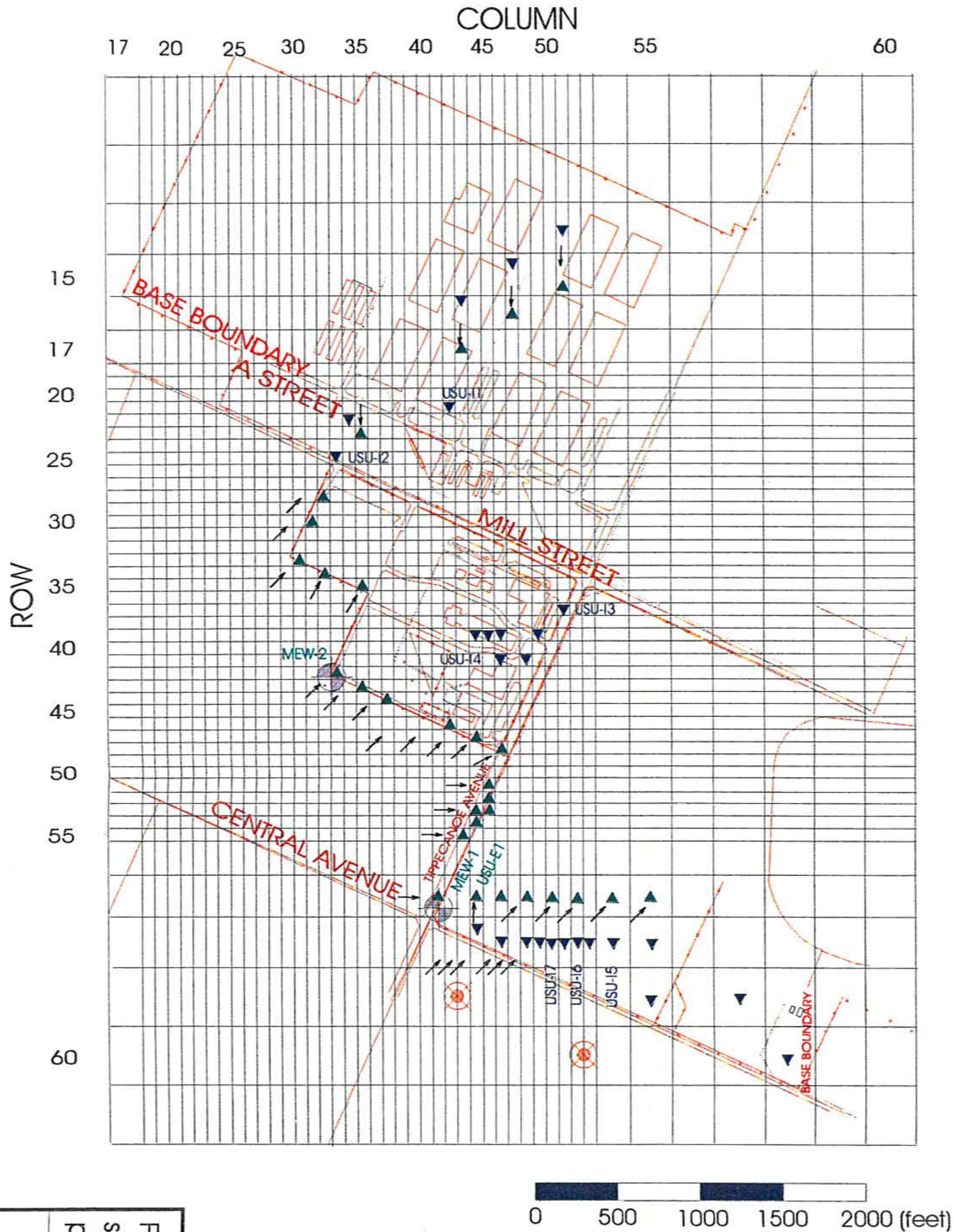


Legend

- Existing on-base well
- Off-base water supply well
- Potential injection well
- Potential extraction well
- Head difference constraint

FIGURE 7a. Finite difference grid and potential P&T wells

Norton AFB, CA
SW Boundary Area



Legend

- Existing on-base well
- Off-base water supply well
- Potential injection well
- Potential extraction well
- Head difference constraint

FIGURE 7b. Study area close-up showing head-difference and potential well locations

Norton AFB, CA
SW Boundary Area

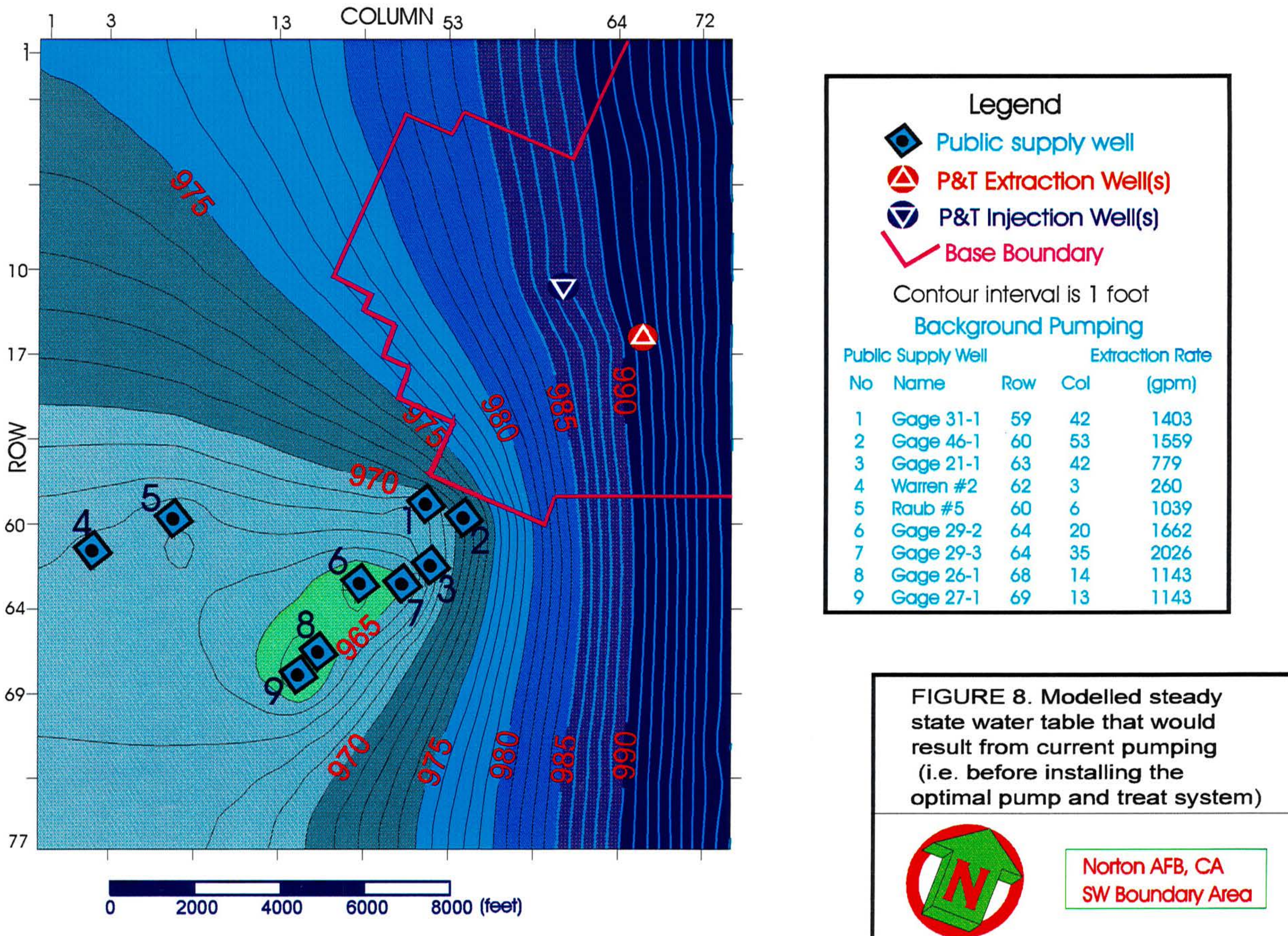
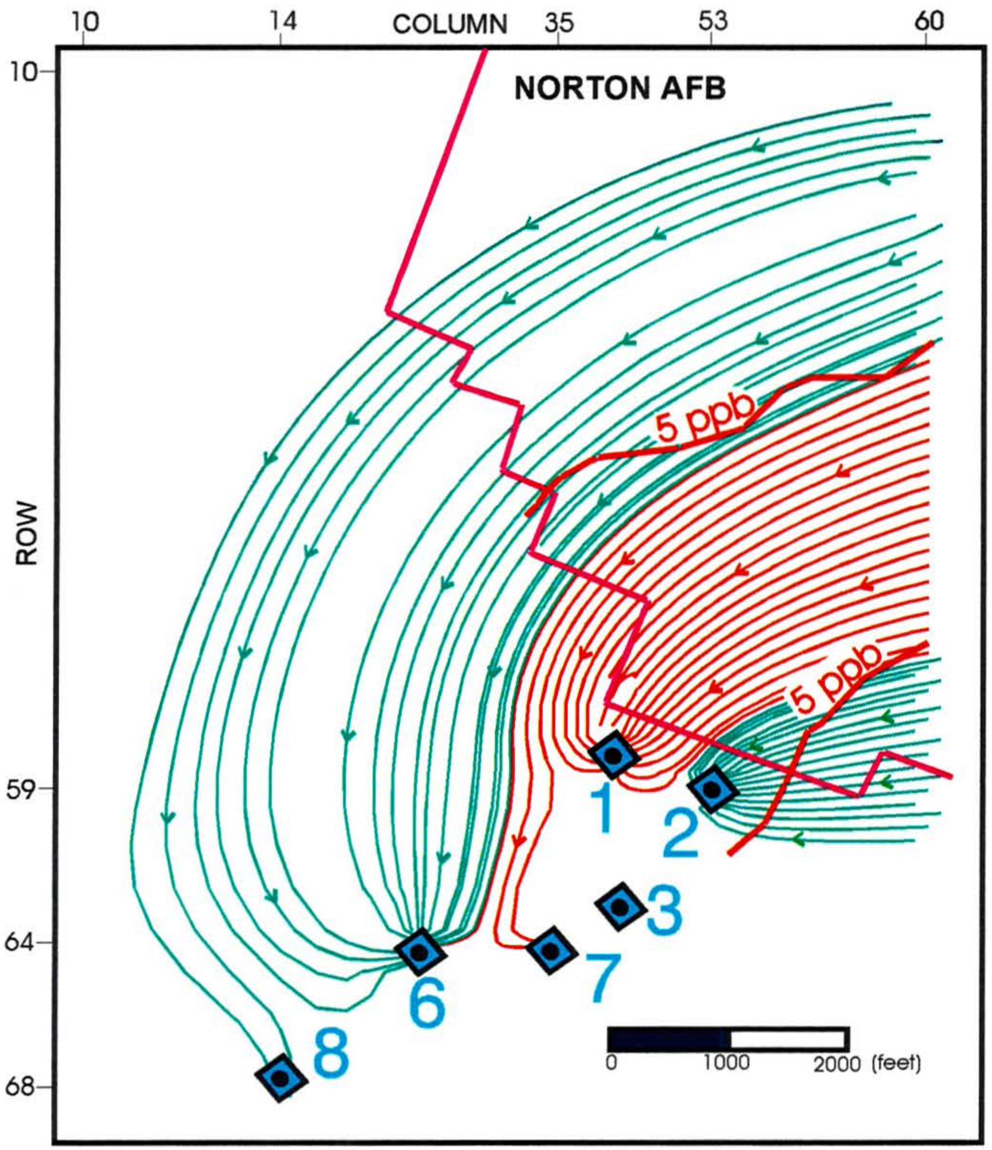


FIGURE 8. Modelled steady state water table that would result from current pumping (i.e. before installing the optimal pump and treat system)



Legend

TCE plume, 5 ppb contour (Jan 94), and pathlines of contaminated water

Pathlines of uncontaminated water

Public supply well

Base Boundary

BACKGROUND PUMPING

Public Supply Well No	Name	Row	Col	Extraction Rate (gpm)
1	Gage 31-1	59	42	1403
2	Gage 46-1	60	53	1559
3	Gage 21-1	63	42	779
4	Warren #2	62	3	260
5	Raub #5	60	6	1039
6	Gage 29-2	64	20	1662
7	Gage 29-3	64	35	2026
8	Gage 26-1	68	14	1143
9	Gage 27-1	69	13	1143

FIGURE 9. Computed ground-water pathlines originating from the northeast before the pump and treat system is implemented

Norton AFB, CA
SW Boundary Area

Pumping Strategy Criteria

The following characteristics are considered as being essential for developing a pumping strategy.

1. prevent TCE (beginning in column 60 and lying within Jan 1994 5ppb TCE contours) from reaching public supply wells.
2. prevent TCE-contaminated ground water from reaching lower water-bearing strata.
3. perform steady-state evaluation.
4. total extraction must equal total injection.
5. place all extraction and injection wells within NAFB boundaries.
6. utilize 750 gpm as the upper limit on discharge from currently existing base extraction wells MEW1 and MEW2.
7. use 500 gpm as the upper limit on injection at all injection wells, and 1000 gpm as the upper limit on discharge at all extraction wells other than MEW1 and MEW2.
8. utilize currently existing base extraction wells MEW1 and MEW2, if practical.
9. use 2500 gpm as the upper bound on total extraction.

Further analysis includes: evaluating the time needed for steady state conditions to prevail after implementing the optimal pumping strategy, and evaluating the sensitivity of the computed optimal pumping strategy to the assumed aquifer parameters.

Developed Pumping Strategy and Satisfaction of Criteria

USU uses the procedure discussed in Appendix B to develop optimal pumping strategies. A steady pumping strategy consists of a spatially distributed set of extraction and injection rates. The strategy computed by US/REMAX for this study is optimal in that it minimizes the total pumping rate that is needed to achieve the management goals (including plume capture) for its posed management situation (scenario). A scenario consists of a set of assumptions (management preferences, potential well locations, imposed gradient controls) 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.

Changing potential pumping or control locations changes a posed management scenario. More than one scenario was examined. Only the final recommended scenario and pumping strategy are discussed here.

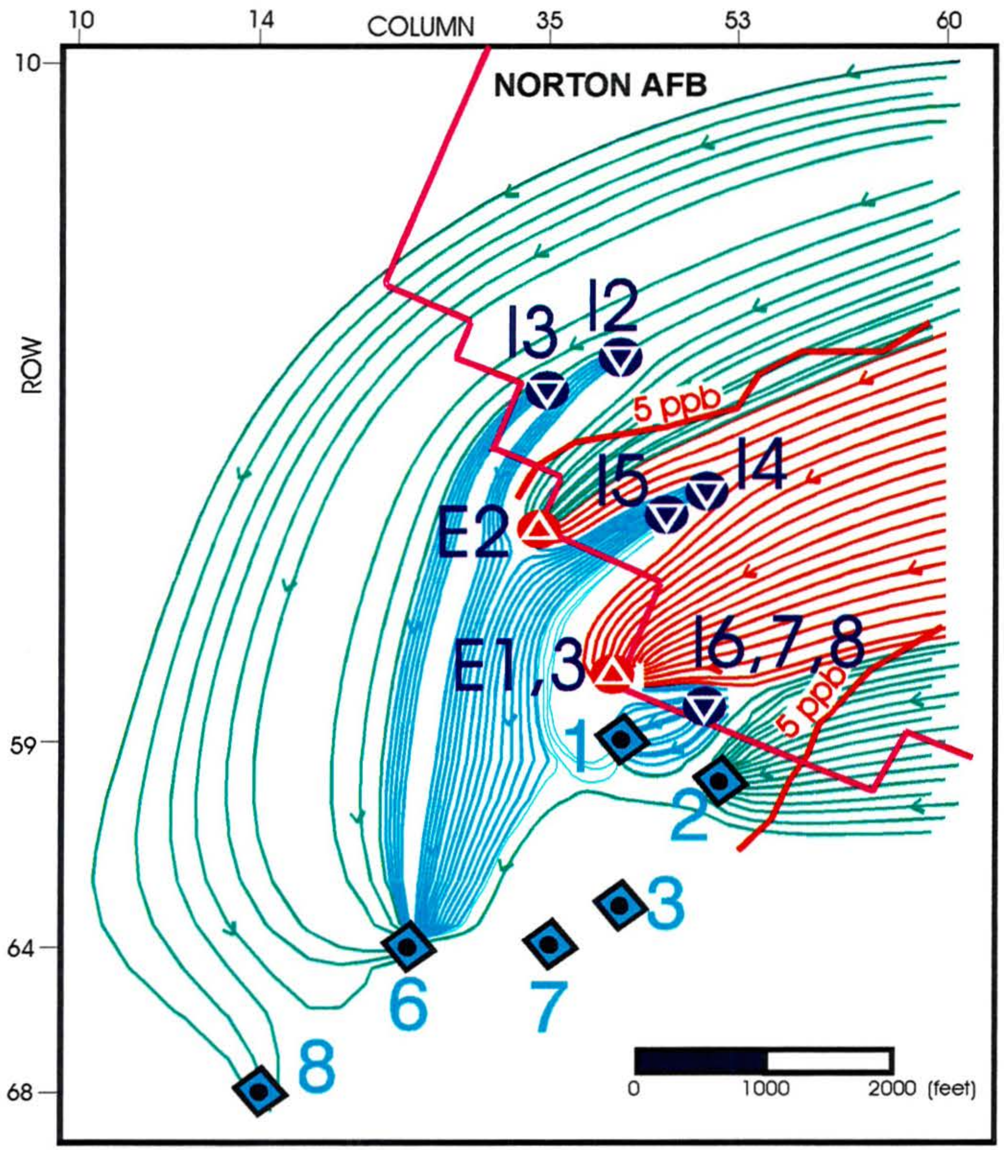
Appendix C summarizes the optimization model formulation and scenario for which the recommended strategy is computed. Figures 7a & 7b show the potential pumping locations considered by US/REMAX for layer 1 when developing that strategy. These potential well locations were input by the modeler.

US/REMAX determined that it is not necessary to pump at all the potential well locations in order to capture the pathlines originating within the 5 ppb TCE contours. US/REMAX computed an optimal pumping strategy consisting of the locations and pumping rates shown in Figure 10.

Figure 10 shows the pathlines that particles (originating in column 60) would follow in reaching extraction wells after the optimal strategy is implemented. All pathlines originating within the 5 ppb TCE contaminant plume contour lines are captured by the plume extraction wells--MEW-1, MEW-2, and USU-E1. In other words, each pathline beginning within the 5 ppb contours in column 60 ends in a P&T extraction well. None of those pathlines reach any of the public supply wells.

The shape of the plume contours will change after the optimal pumping strategy is implemented. The plume will change shape--elongating and orienting itself in the direction of the new pathlines. Capture will still be achieved.

The well locations shown in Figure 10 are a subset of those in Figures 7a & 7b. US/REMAX indicated that there should be no pumping at the other potential well locations shown in Figures 7a & 7b. The locations of the proposed wells (Fig. 10) were further checked in the field to verify that their locations do not conflict with utility or facility easements.



Legend

TCE plume, 5 ppb contour (Jan 94), and pathlines of contaminated water

Pathlines of uncontaminated water

Pathlines of Injected treated water

P&T Extraction Well(s)

Public supply well

P&T Injection Well(s)

Base Boundary

BACKGROUND PUMPING

Public Supply Well				Extraction Rate
No	Name	Row	Col	(gpm)
1	Gage 31-1	59	42	1403
2	Gage 46-1	60	53	1559
3	Gage 21-1	63	42	779
4	Warren #2	62	3	260
5	Raub #5	60	6	1039
6	Gage 29-2	64	20	1662
7	Gage 29-3	64	35	2026
8	Gage 26-1	68	14	1143
9	Gage 27-1	69	13	1143

OPTIMAL PUMPING STRATEGY

Total Extraction = Total Injection = 2250 gpm

Extraction Well				Extraction Rate
No	Name	Row	Col	(gpm)
E1	MEW-1	57	41	507
E2	MEW-2	42	33	750
E3	USU-E1	57	44	993

Injection Well				Injection Rate
No	Name	Row	Col	(gpm)
I2	USU-I2	21	42	208
I3	USU-I3	25	34	156
I4	USU-I4	37	51	261
I5	USU-I5	41	46	273
I6	USU-I6	58	54	446
I7	USU-I7	58	52	446
I8	USU-I8	58	50	460

FIGURE 10. Ground-water pathlines computed to result from implementing the optimal pump and treat pumping strategy.

Norton AFB, CA
SW Boundary Area

Table 1 shows all pumping rates assumed or computed in the US/REMAX run that produced Figure 10. These include public supply wells and the CBA P&T wells (which are known input values, and are not computed). Pumping rates assumed for public supply wells are the maximum rates expected to occur during the year (providing a worst case evaluation). Subsequent figures show only a portion of the entire study area, and only show the wells tapping the upper layer. Thus, not all wells listed in Table 1 are shown in subsequent figures.

Note in Figure 10 that total P&T extraction equals total injection. All extracted water is treated and reinjected. Figure 10 shows how extraction and injection can be used together to prevent contaminated ground water from reaching off-base supply wells. Injection is used to split the plume and direct contaminated water toward extraction wells. Without this coordinated application of injection and extraction, much more extraction would be required.

Aquifer response to implementing the optimal pumping strategy is simulated using MODFLOW. Vertical gradients were evaluated (to satisfy criterion number 2). In the plume vicinity, hydraulic gradients are slightly upward, from layer 3 to layer 1; therefore, contaminated ground water is not expected to move from layer 1 downward.

In summary, according to post-optimization simulation using MODFLOW and MODPATH, the proposed pumping strategy satisfies all specified criteria. It captures all of the contaminant plume within the 5 ppb TCE contours (Fig. 10) without causing contaminant to move from the top layer down to layer 3. To accomplish the management and regulatory goals, the model selected 10 of 50 potential well locations.

Well Name	Layer	Row	Column	Pumping Rate[1] (gpm)
Gage 21-1	3	63	42	-520
Gage 29-3	3	64	34	-1559
Gage 29-2	3	64	20	-1039
Gage 26-1	3	68	14	-1143
Gage 27-1	3	69	13	-1143
Raub #5	3	60	6	-1766
Warren #2	3	62	3	-675
Gage 21-1	1	63	42	-779
Gage 29-3	1	64	35	-2026
Gage 29-2	1	64	20	-1662
Gage 26-1	1	68	14	-1143
Gage 27-1	1	69	13	-1143
Raub #5	1	60	6	-1039
Warren #2	1	62	3	-260
Gage 51-1	3	66	16	-1351
CBA P&T[2]	1	16	67	-400
CBA P&T[2]	1	12	62	400
Gage 31-1	1	59	42	-1403
Gage 46-1	1	60	53	-1559
Gage 31-1	3	59	42	-1039
Gage 30-1	3	60	44	-1402
Gage 92-3	3	60	48	-3000
Gage 56-1	3	61	48	-2598
Gage 92-2	3	60	43	-3000
Gage 92-1	3	64	34	-3000
MEW-1	1	57	41	-507
MEW-2	1	42	33	-750
USU-E1	1	57	44	-993
USU-I2	1	21	42	208
USU-I3	1	25	34	156
USU-I4	1	37	51	261
USU-I5	1	41	46	273
USU-I6	1	58	54	446
USU-I7	1	58	52	446
USU-I8	1	58	50	460

Notes: [1] Extraction is negative and injection is positive.
[2] In sensitivity analysis the distribution of this extraction and injection was changed.

Table 1 List of all water supply and plume control wells pumping in accordance with the proposed optimal pumping strategy.

Sensitivity and Other Physical System Analyses

Physical system response to implementing the optimal strategy was analyzed, if the physical system actually differs somewhat from model assumptions, i.e. if the calibration is imperfect. To do this, several MODFLOW and subsequent MODPATH simulations were made. Each of these MODFLOW sensitivity runs used the optimal pumping strategy presented previously, but assumed a different set of Layer 1 hydraulic conductivity values. After each MODFLOW run, MODPATH was used to determine whether the pumping strategy still captured the contaminated pathlines.

The optimal pumping strategy captured all contaminated pathlines if the assumed Layer 1 hydraulic conductivity values ranged from 60% to 180% of the values used in computing the optimal strategy (ie.., of the best calibrated values). The optimal pumping strategy is considered robust within this range of variation of conductivity. That means that the strategy is considered insensitive to error in assumptions within this range.

The robustness of a variation of the optimal pumping strategy was also tested. This variant assumed that base boundary P&T extraction totalled 2500 gpm (the maximum flowrate of the treatment facility). The variant differs only in using pumping rates of 750, 1000, 570, and 570 gpm at wells MEW-1, USU-E1, USU-I7, and USU-I8, respectively. The variant strategy captured all contaminated pathlines for conductivity values ranging from 50-220% of the best calculated values. Because it uses the same well locations, but more pumping, the variant is more robust than the proposed strategy.

In summary, the proposed optimal pumping rates and well locations should capture the plume, or it can be easily modified to ensure complete capture, if monitoring shows that modification is necessary. Because the summer (maximum) pumping rates for the public supply wells were assumed, the pumping strategy captures the plume against the maximum gradients toward the supply wells that are expected to occur. The optimal pumping strategy will improve in performance during the fall, winter, and spring.

The optimal pumping strategy assumes steady state conditions. It is important to evaluate the time required for the ground-water system to reach steady state after the optimal pumping strategy is implemented. To do this, several transient MODFLOW simulations were concluded, all of which employed the optimal pumping strategy. All runs used a storativity of 0.0006 for layers 2 and 3. The runs differed in the storativity assumed for Layer 1. For Layer 1 storativities ranging from 0.0006 to 0.06, the ground-water system reached steady state in 1 to 2 months, respectively. In essence, it will probably require no more than 1-2 months for the optimal pumping strategy to establish the gradients necessary to capture the plume. This supports the use of a steady state optimization evaluation.

An evaluation was also performed of the effect of changes in the central base area P&T operation on contaminant capture at the base boundary. Results show that capture will still be achieved by the SW boundary P&T system, despite anticipated changes to the CBA P&T strategy.

To reach this conclusion, two additional pairs of MODFLOW and MODPATH simulations were carried out. The spatial distribution of the extraction and injection rates assumed for the CBA P&T were changed from those listed in Table 1. Optimal extraction rates computed for the CBA in a concurrent project were used (Peralta and Aly, 1995). For both new test situations, injection locations are (ETC well name, row, column; ETC well name, row, column; etc): IW-1, 12,61; IW-2, 13,62; IW-3, 13,63; IW-4, 12,60). The ETC well names listed here are referenced by Peralta and Aly (1995).

It is assumed that each of the four wells injects at 100 gpm and injection and extraction both total 400 gpm. However, as described below, the spatial distribution of the CBA extraction rates differed.

In the first pair of MODFLOW and MODPATH simulations, it is assumed that there is no continuing source of TCE contamination. The CBA pumping strategy that maximizes the mass of dissolved TCE contaminant removal during a three-year period includes extraction at ETC wells (name, row, column, rate: MEW-9, 27,63, 200 gpm; and MEW-10, 33,61, 200 gpm).

In the second case, it is assumed that there is a continued source of TCE contamination for two years. The CBA pumping strategy that maximizes the mass of dissolved TCE contaminant removal during a three-year period includes extraction at wells: (MEW-7, 21,65, 150; MEW-9, 27,63, 150; MEW-10, 33,61, 100).

Results of MODFLOW and subsequent MODPATH simulations showed that all contaminated pathlines are still captured. The southwestern boundary P&T effectiveness is not adversely affected by the change in the pumping at the CBA.

Economic Consequences of Optimized Strategy

The proposed pumping strategy requires less total pumping and fewer wells than the strategy originally expected to be implemented. The result is a present value savings of about $5.8 M over a 15 year project life, assuming a 5% discount factor.

This savings is achieved by reducing the number of extraction wells by one and the number of injection wells by one (Table 2), reductions of 25% and 12.5% respectively. Also reduced is the expense of auxiliary construction and operation and maintenance costs.

	Original	Optimized	Reduction in cost after optimization
Injection Wells	8	7	$100K
Extraction Wells	4	3	$150K
Auxiliary, Construction (Pipelines, etc.)	$8M	$6M	$2,000K
Extraction Rates (gpm)	3500	2250	
O & M Costs (per year)	$1.6M	$1.25M	$350K
O & M Costs (project life)	$24M	$18.75M	$5.25M
Operation Time	15 years	15 years	

Table 2 Estimated economic benefit of optimized pumping strategy (AFCEE/ERC).

Conclusions and Recommendations

The optimal pumping strategy for the NAFB southwestern boundary satisfies all the stated management criteria. It requires only 2250 gpm of extraction. This is 10% below the 2500 gpm upper limit of the treatment equipment originally envisioned. The 10% provides some capacity for future pumping strategy modification, should that be necessary, without requiring additional treatment capacity.

NAFB should implement the proposed optimal pumping strategy to achieve their stated goals. The strategy requires only 3 extraction wells (two of which are already in place) and 7 injection wells. The coupled use of simulation / optimization and pathline modeling has proven effective for this study.

Pumping strategies developed in this study 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 analyses allow us to expect that implementing the optimal pumping strategy will capture the contaminant plume.

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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 ground-water management

Simulation/optimization (S/O) models can be used to greatly speed the process of computing desirable ground-water 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 ground-water 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 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 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 ground-water head computation. Here we assume that the initial water table is horizontal and at equilibrium. Ground water 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 $\hat{o}$ [L];

$\delta^h(\hat{o},\hat{a})$ = influence coefficient describing effect of steady ground-water 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.

Assume that a 'unit' steady pumping extraction rate of 1 m^3/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 $p^{ut}(\hat{a})$ = 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 $\hat{a}$ on the final difference in potentiometric surface elevation between locations 1 and 2, of a pair of locations, $\grave{o}$, can be expressed as:

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

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

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

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

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.

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

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.

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

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 ground-water 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, ($\delta = 1$), 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 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]

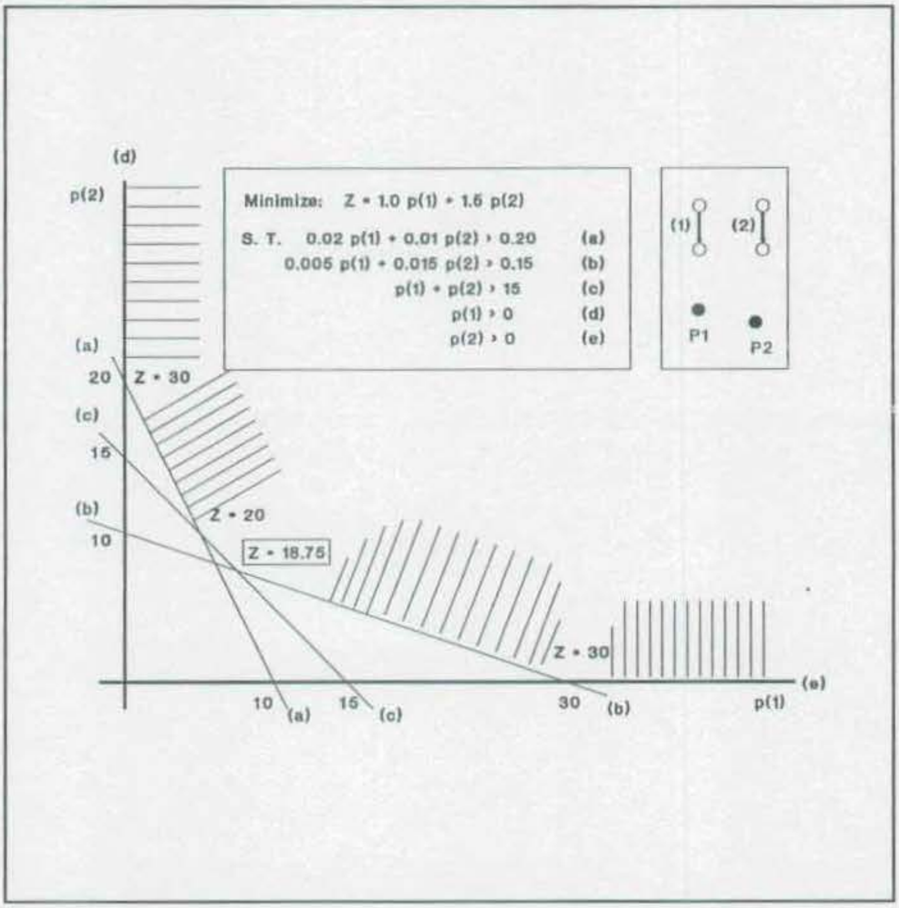

FIGURE A1.Graphical representation of simple pumping optimization problem.

[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 ground-water management. US/REMAX contains such algorithms and makes formulation and solution of ground-water 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.

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[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 ground-water 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 ground-water 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	Some boundary flows	Some boundary flows
(S)	Some boundary heads	Heads at 'variable' head cells
	Pumping	
Simulation/	Some boundary flows	Optimal boundary flows
Optimizatio n	Some boundary heads	Optimal heads at 'variable' head cells
(S/O)	Bounds on pumping, heads, flows	Optimal Pumping

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

Appendix B
Optimizing Hydraulic Capture of Contaminated Ground Water with US/REMAX:

Purpose:

The purpose of this document is to describe how to use US/REMAX to optimize capture of a ground-water contaminated plume in a complicated situation. Such situations might arise when the capture zones must be geometrically complex. 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 MODPATH are used to simulate the consequences of implementing pumping strategies.
- MODPATH/PLOT (or other graphics program) is used to display the resulting capture zone after each optimal pumping strategy is implemented.

Procedure:

1.Develop a pumping strategy to be used as the starting point for US/REMAX optimization.

a) Identify a pumping strategy which achieves complete capture of the plume. One way to accomplish this is to do the following. Assume a large number of wells in the downgradient portion of the plume. Pump all these wells at their greatest capacity. Injection (recharge) wells can be used, to help control contaminant movement. If desired, total extraction can be forced to equal total injection.

b) Simulate aquifer response to implementing this strategy (MODFLOW, MODFLOW + MT3D, or SWIFT are preferred simulators). Use MODPATH (or alternative particle tracking model) to compute pathlines. Check the resulting pathlines to ensure that the implemented pumping strategy does capture the entire contaminated plume and no contaminant reaches prohibited locations (such as public supply wells).

If MODPATH is used to simulate the pathlines, best results are obtained using the forward tracking option with particles placed upstream from any prohibited locations. Place particles only in one strip (e.g., one column, row, diagonal; continuous or broken) roughly perpendicular to the direction of flow. This ensures that flowpaths will remain distinguishable. If more particles are used than necessary, MODPATH will generate a huge output file (called PATHLINE) and will waste much time in processing.

2. Begin preparing to apply US/REMAX to the problem, using the pumping strategy of step (1) as a starting point.

a) Select locations for head difference constraints to be used to control advective contaminant movement. Locations of these constraints are most easily identified by placing arrows of head-difference (gradient direction) control around the perimeter of the plume or around the area that must be captured.

b) Prepare US/REMAX data. Include in data file REMAX.DAT data identifying all wells simulated in step (1). Designate head difference constraints in data file CONTROL.DAT.

3. Use US/REMAX to simulate system response to the pumping strategy of step (1). To accomplish this, do not give it any freedom to select a pumping strategy. In other words, in data file BOF.DAT, for a pumping well, use the pumping rates of step (1) as both upper and lower bounds. Assure a feasible solution by using very low lower bounds on heads and head differences and very high upper bounds on heads and head differences. The purpose of this step is to calculate the resulting heads and head differences that will result if the simulated pumping strategy is implemented.

4. Develop marginal (sensitivity) values to guide subsequent modification of the pumping strategy of step (1). This requires using US/REMAX to compute an optimal pumping strategy which will achieve head differences at least as great as those determined in step (3). This requires editing file BOF.DAT.

a) Use the head differences resulting from step 3 as lower bounds on head differences.

b) Use more reasonable lower and upper bounds on pumping rates (give US/REMAX the freedom to change pumping rates as necessary.)

c) Use the appropriate objective function and other constraints (e.g., total extraction = total injection, bounds on hydraulic heads, etc.).

5. Use the marginals computed in step (4 or 6) to prepare to refine the optimal strategy computed in that step.

a) Examine the marginals in REMAX.OUT and select several head difference constraints to be relaxed in the next US/REMAX optimization (those with the greatest marginals). The greater the marginal, the greater the effect of relaxing the tight bound or constraint on the value of the objective function. Relaxing constraints with the greatest marginals improves the next computed pumping strategy the most.

b) Edit file BOF.DAT to reflect the new lower bounds on head differences.

6. Compute a new optimal pumping strategy using US/REMAX.

7. Evaluate the optimal pumping strategy computed in step (6).

a) Simulate system response to the optimal pumping strategy.

b) Examine the resulting pathlines and capture zone.

- If capture is not achieved, restore to their previous values those head difference values closest to the escaping pathline(s). Return to step (6).
- If capture is achieved, and the new pumping strategy is better than the previous strategy, return to step (5).
- If capture is achieved, but the new pumping strategy is not better than the previous strategy, stop the procedure. The iterative procedure terminates when no further relaxation of head difference constraints results in an optimal pumping strategy which achieves complete capture of the contaminated plume.

Appendix C

Optimization Problem Formulation

A mathematical representation of the Norton AFB base boundary pumping minimization problem is shown below. This considers 28 possible extraction cells, 23 possible injection cells, and 32 locations at which head differences are constrained. (All are in layer 1.) The model will compute a pumping strategy that minimizes the value of the objective function, Eq. C1, while simultaneously satisfying Equations C2-C8.

$$\text{MINIMIZE:} \quad \sum_{\hat{a}=1}^{28} \left((-1)\, p(\hat{a},1) \right) + \sum_{\hat{a}=29}^{51} \left((1)\, I \right. \qquad \text{(C1)}$$

$$-750 \text{ gpm} \le p(\hat{a},1) \le 0 \quad \text{for } \hat{a} = 1 \ldots \qquad \text{(C2)}$$

subject to:

$$-1000 \text{ gpm} \le p(\hat{a},1) \le 0 \quad \text{for } \hat{a} = 3 \ldots 28 \qquad \text{(C3)}$$

$$0 \le p(\hat{a},1) \le 500 \text{ gpm} \quad \text{for } \hat{a} = 29 \ldots 51 \qquad \text{(C4)}$$

$$\Omega^{L}(\grave{o},1) \le \Omega(\grave{o},1) \le \Omega^{H}(\grave{o},1) \quad \text{for } \grave{o} = 1 \qquad \text{(C5)}$$

$$\Omega(\grave{o},1) = 1\,[\, h(\hat{o}_{\grave{o},1},1) - h(\hat{o}_{\grave{o},2},1) \,] \qquad \text{(C6)}$$

$$\sum_{\hat{a}=1}^{51} p(\hat{a},1) = 0 \qquad \text{(C7)}$$

$$\sum_{\hat{a}=1}^{28} p(\hat{a},1) \ge -2500 \text{ gpm} \qquad \text{(C8)}$$

where:

â =Index designating location of potential ground-water extraction or injection;

p(â,1) =Steady-state ground-water pumping rate [L^3T^{-1}]. This is extraction (-) at pumping locations 1-28, and injection (+) in locations 29-51;

L, U =Superscripts designating lower and upper limits, respectively;

ô =Index designating head observation location;

h(ô,1) =Potentiometric surface elevation at location ô;

$h(\hat{o}_{\grave{o},1}, 1)$ = steady-state potentiometric surface elevation at point 1 (a location ô) of HGV pair ò at end of period 1 (where period 1 represents steady-state conditions), [L];

$h(\hat{o}_{\grave{o},2}, 1)$ = steady-state potentiometric surface elevation at point 2 (a second location ô) of HGV pair ò, [L];

ò =Index designating location of HGV (head difference, gradient or ground-water velocity) constraint.

There is no correlation between the above â index value and the order in which wells are listed in Table 1 or Figure 4 of the report body. Assume existing wells MEW-1 and MEW-2 have â indices of 1 and 2. Through Equation C2 the model has the freedom to select any extraction rate between 0 and 750 gpm for the cells containing those two wells. By Equation C3, the model can select any rate between 0 and 1000 gpm for all other potential extraction cells shown in Figure 3 of the report body. These potential extraction cells do not include any wells whose pumping rates are known, and used in computing the pathlines of the no-change-in-management scenario (Figure 2). For example, these 28 potential extraction wells do not include any of the public water supply wells, or ETC's pump and treat wells listed in Table 1.

Via Equation C4 we permit the model to inject up to 500 gpm at the 23 potential injection locations seen in Figure 3. ETech's injection wells are not included in these 23 wells, since ETC flow rates are assumed known.

In the objective function (Eq. C1), extraction is multiplied by a weight of -1 and injection is multiplied by +1. The resulting sum of two positive sums is minimized.

Equation C6 defines the difference in final steady-state heads that will result between two cells considered together as a control location. 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 great and the model is seeking to minimize, rather than maximize, pumping).

Equation C5 is used to impose limits on the difference in head that must occur between the pair of cells constituting a control location. These limints are determined using the procedure of Appendix B.

Equation C7 forces total extraction to equal total injection (recall that extraction and injection have opposite signs). Equation C8 prevents total extraction from exceeding 2500 gpm.

For simplicity, constraint equations describing aquifer response to extraction and injection are not shown above. For each location at which head must be computed to constrain head differences, the model contains one superposition expression (discretized convolution integral). Such an expression describes the steady state head that will result at that location due to all unmanaged (assumed) pumping rates plus all computed optimal extraction and injection rates.