COMPUTING OPTIMAL PUMPING STRATEGIES FOR GROUNDWATER CONTAMINANT PLUME REMEDIATION

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Abstract

Simulation/Optimization (S/O) models can greatly simplify the process of designing remediation systems for contaminated groundwater. We describe some technical aspects of using S/O models and possible S/O model formulations for groundwater remediation design. We: discuss some S/O model optimization algorithms; illustrate simple optimization problem solution; describe two real-world S/O model applications; and demonstrate S/O model application under uncertainty.

1. Introduction

Groundwater remediation using pumping has been widely applied during the last decade. Extracting contaminated water and injecting clean (treated) water to the groundwater aquifer (termed 'pump and treat') has been the selected remediation technology for many groundwater contaminant plumes. Generally, pump-and-treat systems are designed to achieve plume containment, plume cleanup, or a combination of the two. Plume containment is achieved by preventing further spreading of the plume into clean areas of the aquifer. Plume cleanup is achieved by reducing contaminant concentrations to below acceptable levels, such as the maximum contamination limit (MCL). Figures 1 and 2 clarify typical use of containment and cleanup. Figure 1 shows a finite difference grid for a groundwater flow model superimposed over an idealized plume. One sees the outer nondetect contour and the inner MCL contour. Figure 2 uses the same plume to represent how plume management might be mandated. To achieve plume containment, one will not want contaminant concentrations to reach any new cells at any time during the management period. To achieve plume cleanup, one wants concentrations at all cells to not exceed MCL at the end of the management period.

A pumping strategy refers to a spatially and possibly temporally distributed set of pumping rates. It can include both extraction and injection rates. Moving a well location, albeit slightly, or even changing a pumping rate at one well constitutes creating a different pumping strategy. S/O models greatly facilitate the process of finding pumping strategies that satisfy a number of management constraints while predicting the best (optimal) performance for prescribed management goals.

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 cleanup and/or containment.

The remainder of this chapter is organized as follows. Section 2 introduces S/O models. Section 3 describes how state and decision variables can be related inside S/O models and S/O model formulations for groundwater remediation design. Section 4 discusses different optimization algorithms used in S/O models. Section 5 describes and solves a simple optimization problem and Section 6 describes S/O model application to two field problems. Section 7 discusses S/O model application under uncertainty.

2. Simulation/Optimization Models

Suppose a manager wants to minimize the cost of containing a plume using existing wells. In that case, minimizing pumping can be a practical surrogate for minimizing cost. The objective function would be the sum of pumping rates from all existing wells. Assuming constant pumping, the objective function would include as many pumping rates as there are wells.

The pumping strategy that achieves the best value for the objective function from among all feasible strategies is termed the 'optimal' strategy. By definition, an optimal strategy satisfies all constraints imposed by management.

How does one go about creating an optimal strategy? To develop a pumping strategy for a specific goal using a typical simulation (S) model such as MODFLOW (McDonald and Harbaugh, 1988), you probably employ the following process (from Peralta and Aly, 1993).

1. You specify what you want the pumping strategy to achieve (i.e. 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 the optimal strategy decreases. Even assuming a feasible strategy might become difficult.

On the other hand, a groundwater simulation/optimization (S/O) model directly computes the pumping strategy that best satisfies your goals. It contains both simulation equations and an operations research optimization algorithm. The simulation equations permit the model to appropriately represent aquifer response to hydraulic stimuli and boundary conditions. The optimization algorithm permits the specified management objective to serve as the function driving the search for an optimal strategy.

Table 1 summarizes differences in inputs and outputs of groundwater flow S and S/O models. Both model types require data describing the physical system. However, model capabilities differ and other inputs and outputs differ.

The familiar 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 ensure that the computed strategy indeed satisfies all your management goals. For example, upper or lower bounds of pumping rates, heads or gradients reflect the ranges of values that management considers acceptable. The model automatically considers those bounds while calculating optimal pumping strategies. One 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.

Contaminant transport S and S/O models can both consider contaminant mass or concentration. Again, the most important difference between S and S/O models is that one must input a pumping strategy to an S model, while an S/O model finds an optimal pumping strategy.

Many researchers have developed S/O models for specific problems. Generally applicable S/O models for hydraulic (flow) optimization include MODMAN, REMAX and MODOFC. No generally applicable S/O model is commercially available at this moment for transport optimization, although a WINDOWS version of REMAX has that capability. Appendix B lists some unique features of REMAX.

3. State and Decision Variables

An S/O model is considered to contain two types of variables: decision and state variables. Decision variables represent variables that can be controlled by the decision maker in the field. State variables represent physical system responses to the decision variables. State variable values are controlled by adjusting the values of decision variables. Contaminant transport S/O models can include as decision variables: water injection rate, concentration and rate of injected nutrients, oxygen or carbon sources. State variables include groundwater gradients, contaminant concentrations, and plume mass.

S/O models must have a means of quantifying the relationship between decision and state variables. For example, an S/O model must be able to predict the concentration that will result at a monitoring (compliance) point from a particular set of pumping rates. These quantitative relationships are sometimes termed simulation constraints.

Several exact and approximation approaches are used to form simulation constraints. One exact approach (the embedding method) employs separate constraint equations to represent each flow and transport equation for each stress period (Aguado and Remson, 1980; Gharbi and Peralta, 1993). Although preferred for some situations, the embedding method can sometimes result in an impracticably huge optimization problem.

Another exact approach calls a full simulation model (such as MODFLOW or MT3D) during each iteration of an optimization algorithm (Gorelick, 1983; McKinney et al., 1995, Wang and Zheng,1998). If calling a full simulation model thousands of times within an optimization algorithm, this approach can require more computer time than is practicable.

A third method employs linear systems theory and superposition via a discretized convolution expression. This response matrix method is exactly applicable for linear (confined) aquifers and has been implemented in several software packages: MODMAN (Greenwald, 1998); MODOFC (Ahlfeld and Riefler,

1998); and REMAX (Peralta and Aly, 1993) and applied widely (Hegazy and Peralta, 1997; and many others). Sometimes this method can be reasonably applied to slightly nonlinear aquifers (those having saturated thickness which is large by comparison with the change in head with time). REMAX includes an adaptation of the superposition approach to accurately address nonlinear (unconfined) aquifers and piece-wise linear (e.g. river-aquifer seepage) flows.

Except for some cases of injecting contaminated water, transport optimization problems are usually nonlinear. S/O models addressing transport optimization problems sometimes apply surrogate expressions to describe physical system response to stimulti. Lefkoff and Gorelick (1990), Ejaz and Peralta (1995) Cooper et al (1997) and Aly and Peralta (1999a) used polynomial functions to simulate contaminant concentrations. A promising approximation function is an artificial neural network applied to simulate contaminant peak concentration as a function of pumping rates (Aly and Peralta, 1999b).

The previous discussion describes how linear and nonlinear equations can be used as simulation constraints in a S/O model. Depending on whether linear or nonlinear equations are used, different optimization algorithms can be used to solve the formulated optimization problem. The following section describes different kinds of optimization problems and the corresponding optimization algorithms.

4. Optimization Problems: Types and Algorithms

Figure 3 lists common terminology descriptive of optimization problem types. Linear optimization problems are usually solved using simplex or other techniques that check vertices of the feasible solution space. Historically, nonlinear problems were most commonly solved using gradient search methods. Branch and bound techniques were most commonly used for MIP problems, and outer approximation methods were applied to MINLP techniques. Currently, evolutionary optimization techniques are used increasingly for NLP, MIP and MINLP problems.

Several researchers applied nonlinear optimization to aquifer contamination problems (*Gorelick et al.*, 1984; *Ahlfeld*, 1990; *Gharbi and Peralta*, 1994; *Peralta et al.*, 1995, *Peralta and Aly*, 1996). Nonlinear programming techniques cannot guarantee global optimality when applied to large non-convex problems. For real problems, where the time required to simulate the groundwater system is significant, nonlinear programming methods may need prohibitive amounts of CPU time.

The limitations of mathematical programming have motivated researchers to use alternative optimization techniques such as simulated annealing (*Rizzo and Dougherty*, 1996; Shieh and Peralta, 1998b) and genetic algorithms (GAs) (*McKinney and Lin*, 1994; *Ritzel et al.*, 1994; *Rogers and Dowla*, 1994; Shieh and Peralta, 1998a). *Aly and Peralta* (1999a) found that a GA performed better than mathematical programming for nonlinear and mixed-integer nonlinear problems. *McKinney et al.* (1994) found that using a GA to compute the starting point for a nonlinear gradient-based optimization algorithm provided significant advantages and allowed them to locate solutions that are approximately globally optimal. *Aly and Peralta* (1999b) used neural networks and a genetic algorithm in designing of an aquifer cleanup system to reduce the concentrations of two contaminants simultaneously.

5.   A Simple Optimization Problem

For relatively simple problems, one can manually determine the optimal pumping strategy. Figure 4 and the following example, (after Peralta and Aly, 1993) illustrate a graphical approach for a simple containment problem in a confined aquifer patterned after a real problem from the northeastern United States.   Assume the potentiometric surface is initially horizontal and at equilibrium. The box in the upper right corner depicts a plan (map) view of the study area and management problem. There are two existing extraction wells, and four observation wells. The observation wells are paired to permit describing head difference between members of a pair.

The goal is to minimize the cost of from the two wells necessary to cause:

(a) the groundwater level at the head of arrow 1 to be at least 0.2 m lower than at the tail; and

(b) the groundwater level at the head of arrow 2 to be at least 0.15 m lower than at the tail.

The strategy is also constrained in that:

(c) the sum of pumping rates from wells 1 and 2 must be at least 15 units;

(d) and (e) pumping at wells 1 and 2 must be extraction.

The upper left insert box in Figure 4 describes the optimization problem mathematically.   It includes the objective function (top unnumbered equation) and five constraint equations. The goal is to minimize the value of the objective function, Z, which is a sum of pumping rates times pumping costs. The 1.5 value indicates that pumping at well 2 costs 150% of pumping at well 1.

Pumping rates are considered 'decision variables'.   These are variables that management can control directly. Groundwater heads or head differences are 'state variables'—variables defining the state of the physical system.

Equations (d) and (e) are sometimes termed 'bounds' in that they are simply limits on acceptable variable values. They can also be termed constraints. Equation (c) assures that total pumping is at least 15 units. Equations (a) and (b) constrain final head differences between observation well pairs. The linear superposition Equations (a) and (b) are applicable because confined aquifers are linear. Those expressions employ the additive and multiplicative properties of linear systems theory (Appendix A discusses formation of Equations (a) and (b)[1].

As described below, restrictions (a)-(e) represent constraints that define the set of feasible solutions (the feasible solution space). The feasible solution space is two dimensional because there are two pumping rates being optimized, (i.e. two degrees of freedom).

Figure 4 illustrates how the constraints restrict the two-dimensional solution space. Because Equation (a) is an $\geq$ constraint, all points in the graph to the right of Line (a) satisfy that equation.   All points to the right of Lines (b) and (c) satisfy

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[1]

Equations a and b are applications of Equation A-4.   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.

Equations b and c, respectively. Equation (b) is similar to Equation (a)--it describes the effect of pumping on head difference across control pair 2.

'Bound' Equations (d) and (e) 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.

Only points inside or on the boundaries of the region formed by all five 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. Because all involved equations are linear, 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. Note how the Z isocontour lines decrease as one moves toward the optimal solution.

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

6. S/O Models for Contaminant Plume Containment and Cleanup

6.1 Plume Containment

Norton Air Force Base (NAFB) lies in the San Bernardino Valley of California, a graben filled with deep unconsolidated alluvial material (Figure 5). Peralta and Aly (1995a) provides a more-detailed description for the site. In the NAFB vicinity are three groundwater-bearing zones--the upper two are semiconfining. The top layer is contaminated by dissolved trichloroethylene (TCE), which is migrating from NAFB toward water supply wells. A Record of Decision (ROD) mandates that NAFB is to 'maintain hydraulic control to the extent possible of the plume while extracting contaminated groundwater, and reinjecting treated groundwater into the contaminant plume or the clean portion of the aquifer". NAFB addressed this goal by installing two pump and treat systems--one in the central base area near the TCE plume source (for cleanup) and the other near the southwestern base boundary (for containment). Section 6.2 describes development of a cleanup pumping strategy (after Peralta and Aly, 1995b).

REMAX was used to compute optimal pumping strategies that would achieve plume containment by preventing any contaminated groundwater from migrating outside base boundaries. Figure 6 shows the candidate wells. Figure 7 shows the final pumping strategy and rates.

The well locations shown in Figure 7 are a subset of those in Figure 6. REMAX indicated that there should be no pumping at the other wells shown in Figure 6. The locations of subset well locations were checked to ensure physical feasibility of installation wells at the selected locations.

Figure 7 shows that total extraction equals total injection. All extracted water is treated and reinjected. Figure 7 shows how extraction and injection can be used together to prevent contaminated groundwater 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. The presented optimal pumping strategy required 2,250 gpm of extraction while satisfying all management criteria. This is 10% below the 2,500 gpm upper limit of the originally envisioned treatment equipment. The 10% reduction provided some capacity for future pumping strategy modification, should that be necessary, without requiring additional treatment capacity. Table 2 shows the savings.

6.2. Plume Cleanup

As mentioned in the previous section (6.1), a pump and treat system was needed to maximize contaminant removal from the central base area near the plume source. Peralta and Aly (1995b) provides a more-detailed description for the site. A consultant specified fixed injection well locations to be placed along existing pipelines. The consultant also proposed locations for extraction wells. Due to the time restrictions on accomplishing this optimization effort, REMAX was used to: (1) utilize the proposed well locations, (2) assume 100 gpm injection rate at each of proposed 4 injection locations, and (3) determine optimal extraction rates for 5 proposed extraction locations. A REMAX precursor determined the optimal (maximum mass of contaminant extraction) strategies needed to achieve cleanup. Figure 8 shows the potential pumping locations.

Results showed that about 31% of the original plume mass can be removed using a treatment facility size of 400 gpm. At 2,000 gpm, about 50% removal could be achieved.

Other sites at which optimization has been formally applied to plume remediation include March AFB (containment), Mather Air Force Base (cleanup), Travis Air Force Base (containment), Wurtsmith Air Force Base (cleanup and containment).

Optimization methods rely on the prediction accuracy of flow and transport simulators. Since accurate modeling of any aquifer can be very difficult, developed optimal strategies may not be optimal for the real aquifer system. There is a growing attention to considering the stochastic nature of aquifer parameters while designing remediation strategies. *Gorelick* (1990) discusses some techniques used to account for uncertainty in designing groundwater management systems. In the following section, we describe the most significant proposed approaches and discuss their applicability.

7. S/O Models for Planning under Uncertainty

Groundwater remediation system design is often complicated by the random nature of aquifer parameters. Three general techniques have been used for solving groundwater management problems under uncertainty. In the first, the sources of uncertainty are not defined but it is assumed that optimal pumping rates can be modified after a period of implementation and monitoring (*Jones et al.*, 1987, *Whiffen and Shoemaker*, 1993). In this technique, the differences between variable values predicted via optimization and the measured variable values (obtained from the field after the optimal strategy is implemented) are used to guide subsequent modification of the optimal strategy. The relation used to modify the computed optimal strategies is termed a feedback law. The process is continued as the modified optimal strategy is implemented.

In the second technique, a probability distribution is either derived or assumed for the variables of interest. Then, analytical relations are developed to relate the quantiles of this distribution to the decision variables. These analytical relations are used as constraints in the optimization problem. These constraints are termed chance constraints and the resulting optimization model is known as the chance-constrained model (*Cantiller and Peralta*, 1989; *Peralta and Ward*, 1991).

In the third stochastic groundwater management technique, a group of constraints is formulated — each for a different realization of the uncertain aquifer parameters (*Wagner and Gorelick*, 1987). A realization is a set of the uncertain parameter values. Typically, each realization is generated from the probabilistic model of the uncertain parameters. The resulting optimal strategy must satisfy all (or some) of the realizations simultaneously. The idea is to find optimal strategies that are robust (satisfy all management constraints) for a range of the uncertain parameters. Several studies tried to estimate the reliability of optimal strategies computed using the multiple-realization technique (*Morgan et al.*, 1993; *Chan*, 1993; *Chan*, 1994).

All cited studies concluded that in order to assure a design that has a high level of reliability, at least 50 to 100 realizations are needed (*Chan*, 1993; *Chan*, 1994; *Morgan et al.*, 1993). For large problems, where the time required to simulate the system is significant, the time required to generate all the constraint equations can be prohibitive. However, since the response surfaces for different realizations can be evaluated simultaneously, one can greatly speed the process by computing them in parallel. Another possible remedy is to determine whether some realizations can be dropped without having to carry out the optimization (*Gomez-Hernandez and Carrera*, 1994; *Ranjithan et al.*, 1993). Aly and Peralta (1999b) present and apply an approximation method that develops the tradeoff curve between the treatment facility size (total groundwater extraction) and estimated reliability.

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Appendix A (Derived from Peralta and Aly, 1993)

A particular type of S/O model, termed a response matrix (RM) model, utilizes the multiplicative and additive properties of linear systems. 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 ê.

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

where

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

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

$p(\hat{e})$ = pumping rate at location ê $[L^3/T]^2$;

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

$$\delta^{\Delta h}(\hat{u},\hat{e}) = \delta^h(\hat{o}_{\hat{u},1},\hat{e}) - \delta^h(\hat{o}_{\hat{u},2},\hat{e})$$

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[2] 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 REMAX those signs are reversed to be consistent with MODFLOW.

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

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

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

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

$$\Delta h(\hat{o}) = \sum_{\hat{e}=1}^{M^P} \delta^h(\hat{o},\hat{e}) \frac{p(\hat{e})}{p^{m}(\hat{e})}$$

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.

$$\Delta\Omega(\hat{u}) = \sum_{\hat{e}=1}^{M^P} \delta^{\Delta h}(\hat{u}, \hat{e}) \frac{p(\hat{e})}{p^{''}(\hat{e})}$$

where

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

Appendix B. Unique Features of REMAX
(From Peralta and Aly, 1993)

1. Well-proven, diverse simulation modules to address porous and fractured media. REMAX is appropriate for optimizing flow and transport management in heterogeneous multilayer porous or fractured aquifers. To develop influence coefficients describing hydraulic head or flow response to stimuli, REMAX uses MODFLOW and MT3D for porous media simulation or SWIFT for fractured media. Other simulation models are easily added as necessary.

2. Robust and proven optimization solvers. REMAX contains all software needed to solve the described optimization problems.

3. Easily maintained data sets. For any particular problem, REMAX reads all data files from a user-specified subdirectory (or folder in WIN95/NT). This allows REMAX users to save all problem-specific input and output in a distinct location.

4. User-friendly data files, error checking, and diagnostics. Innovative REMAX input file organization allows users to write comments, use blank lines, or use blank spaces as desired. This permits thorough data set documentation. REMAX also checks every input file entry and generates error messages with diagnostic explanations.

5. Compatibility with other software. REMAX can read standard MODFLOW, MT3D and SWIFT data sets. Users can prepare these files using their preferred pre-processor and use the generated input files within REMAX.

6. Ability to compute head at well casing or at cell center. This feature is useful for managing unconfined aquifers of small saturated thickness and for computing hydraulic lift costs.

7. Ability to address systems in which pumping cells or head control cells might initially be or might become fully dewatered. This nonlinear or piecewise linear problem is not addressed by normal response matrix models.

8. Automatic cycling and post-optimization simulation. This enables users to accurately address nonlinear systems (unconfined aquifers and stream/aquifer systems). Cycling proceeds until user-specified maximum number of cycles or convergence criteria for decision variables are achieved. Post-optimization simulation verifies that the results in the nonlinear physical system should be like those in the optimization model.

9. Almost infinite flexibility in addressable problem types. Any of the different types of objective functions can be combined into composite objective functions. Any type of the mentioned constraints can be used with any of the objective function types.

10. Optimization under uncertainty or for risk management. Optimization can satisfy constraints for an unrestricted number of sets of assumed boundary conditions and

aquifer parameters (realizations) simultaneously. Reliability of computed strategies is determined via Monte Carlo post optimization simulation. This feature can be used with any combination of objective function(s) and constraints.

11. Ability to develop cost-reliability tradeoff curves. This ability is provided by employing the following REMAX features:
- optional use of head at well casing instead of average cell heads.
- use of quadratic objective function including pumping rate, volume, and cost.
- use of binary and mixed integer variables to include cost of well installation or water treatment plant sizing within the optimization.
- coupled use of cost optimization with the multiple realization option.

12. Adaptability for special situations (available within a special REMAX version). Additional constraints can be added as needed, such as those for: (1) managing reservoir releases and conjunctive water delivery to a system of irrigation unit command areas (Belaineh et al, 1998); or (2) assuring that legal water right priorities are satisfied (Assume two adjacent surface water users. User 1 has a higher legal water right than User 2. Special constraints can assure that User 2 will not receive any water unless all of User 1 water right is satisfied).

TABLE 1.   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.

Figure 1. A typical finite-difference grid and idealized plume (Peralta, 1999).
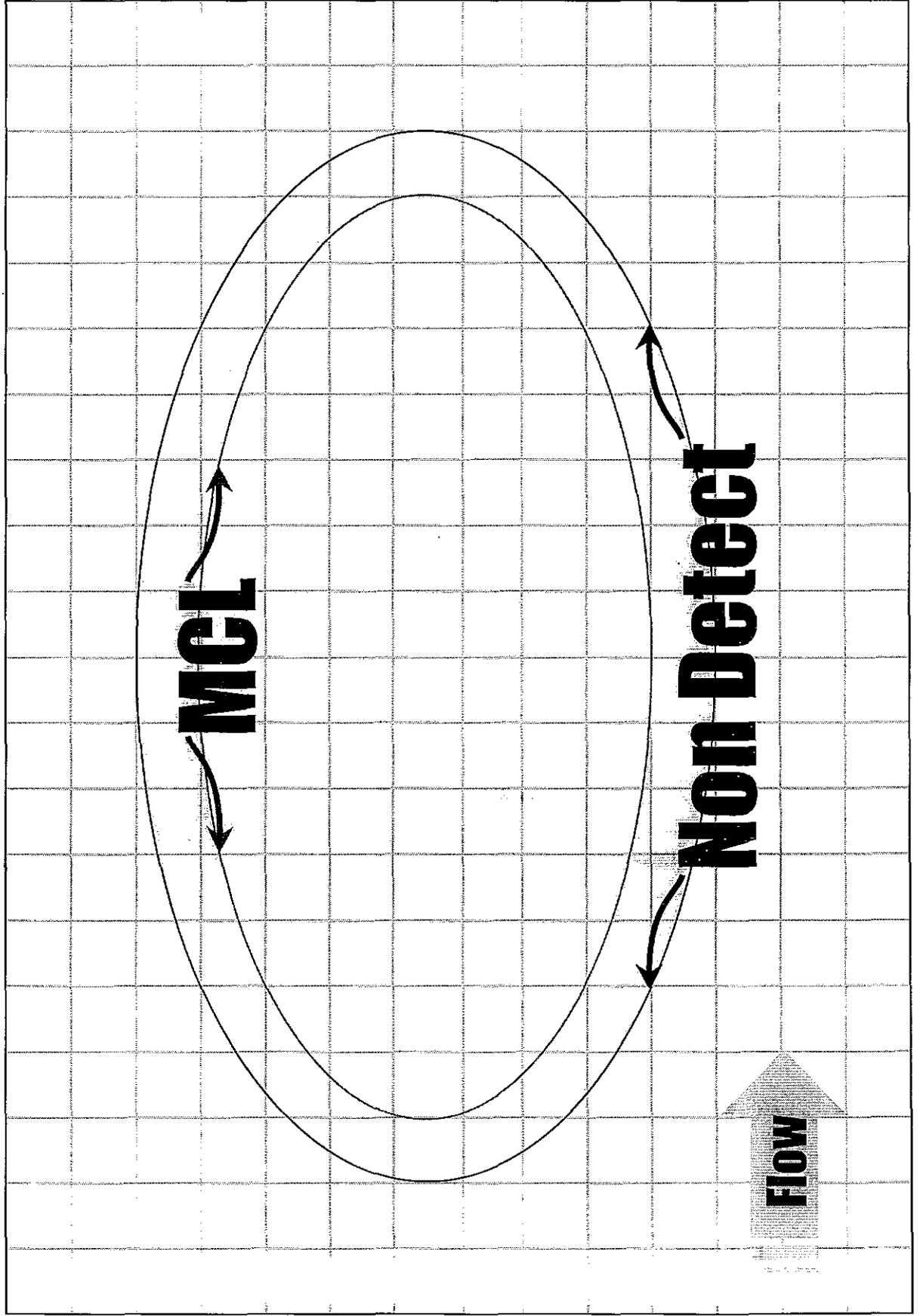
Figure 2. Contaminant plume management: containment and cleanup (Peralta, 1999).

$$C_{\text{end-of-period}} \leq MCL$$

Flow

$$C_{\text{all times}} = \text{NonDetect}$$
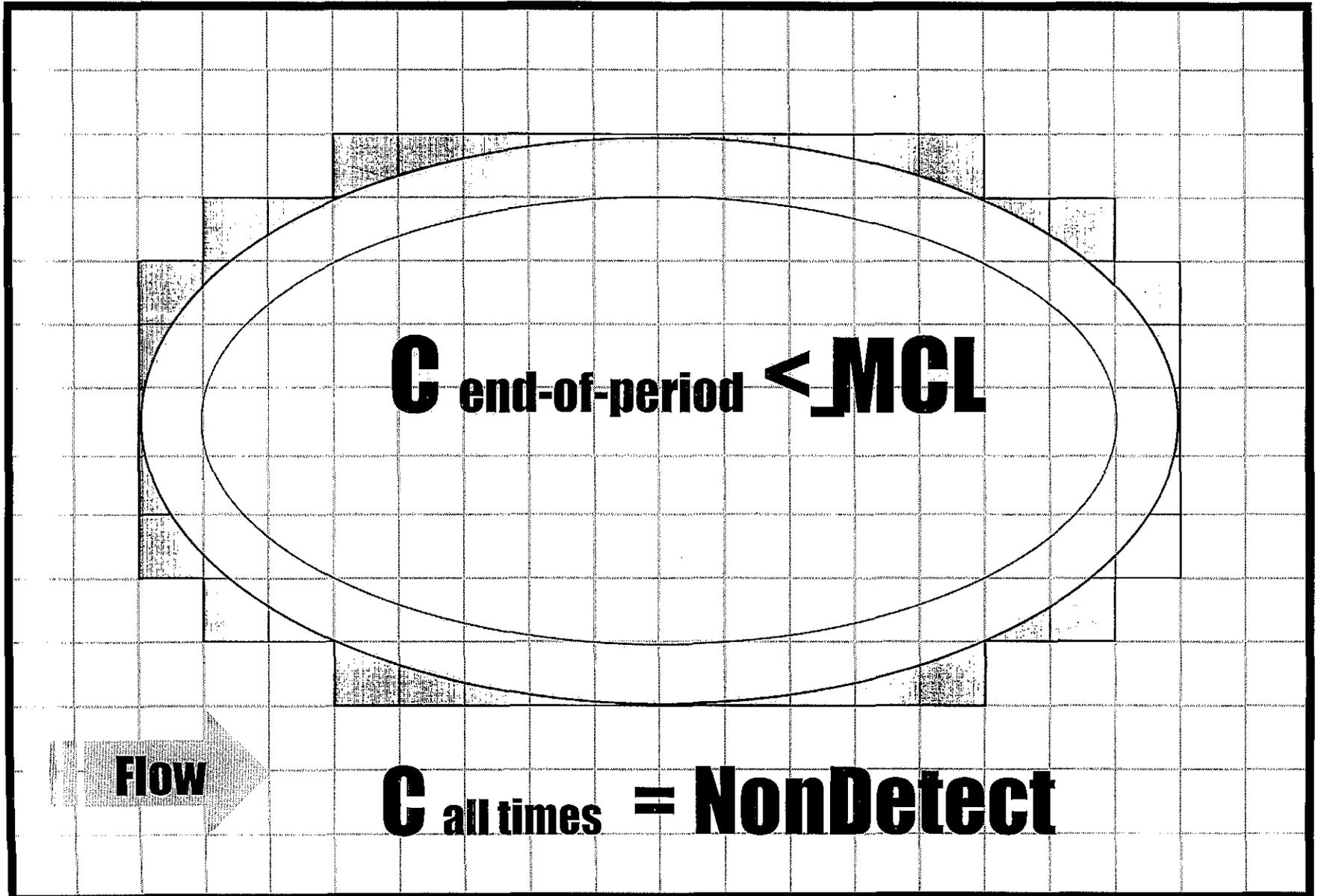
Figure 3. Optimization problem types (modified from Peralta, 1999).

Obj. Fnctn	Constraints	Optimiz Pblm	Optimality
Linear	Linear	Linear (LP)	Global
Some quadratic	Linear	Quadratic (QP)	Global
Linear & integer	Linear & integer	Mixed integer (MIP)	Generally local
Linear or nonlinear	Nonlinear	Nonlinear (NLP)	Local
Linear, integer & nonlinear	Linear, integer or nonlinear	Mixed integer nonlinear (MINLP)	Local

Figure 4. Graphical solution to linear two-well containment optimization problem (modified from Peralta and Aly, 1993).
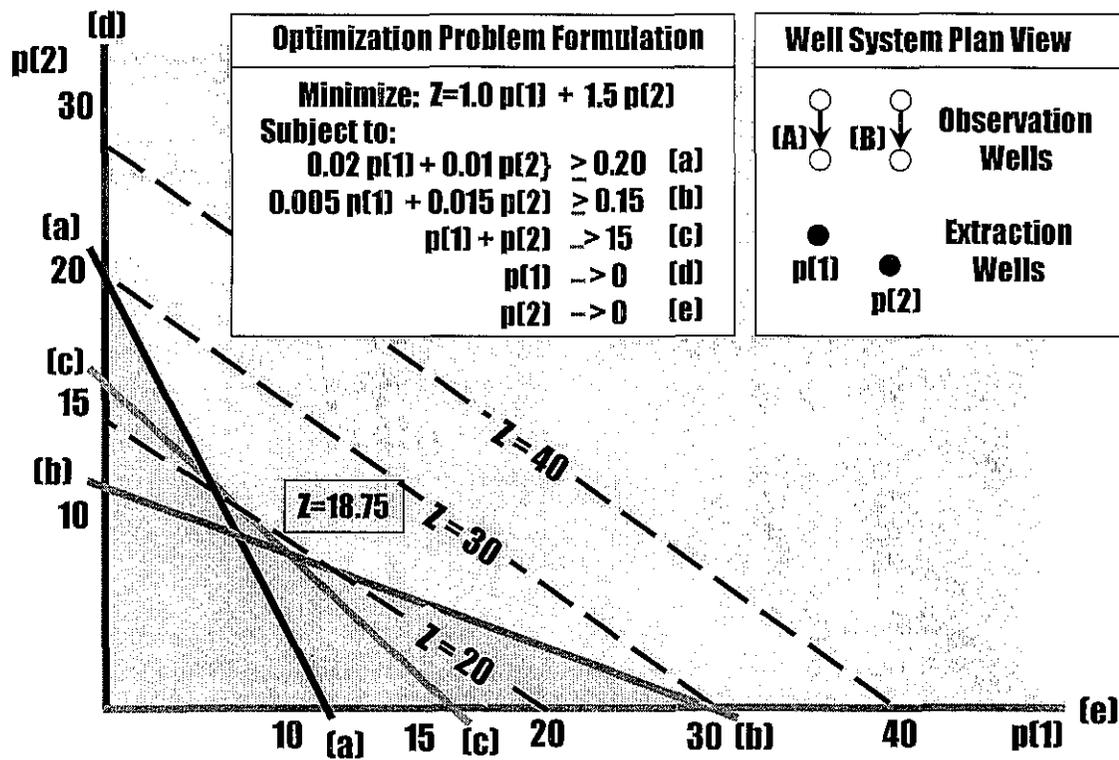
Figure 5. Regional aquifer: Norton Air Force Base, Southwest Boundary Area (from Peralta and Aly, 1995a).
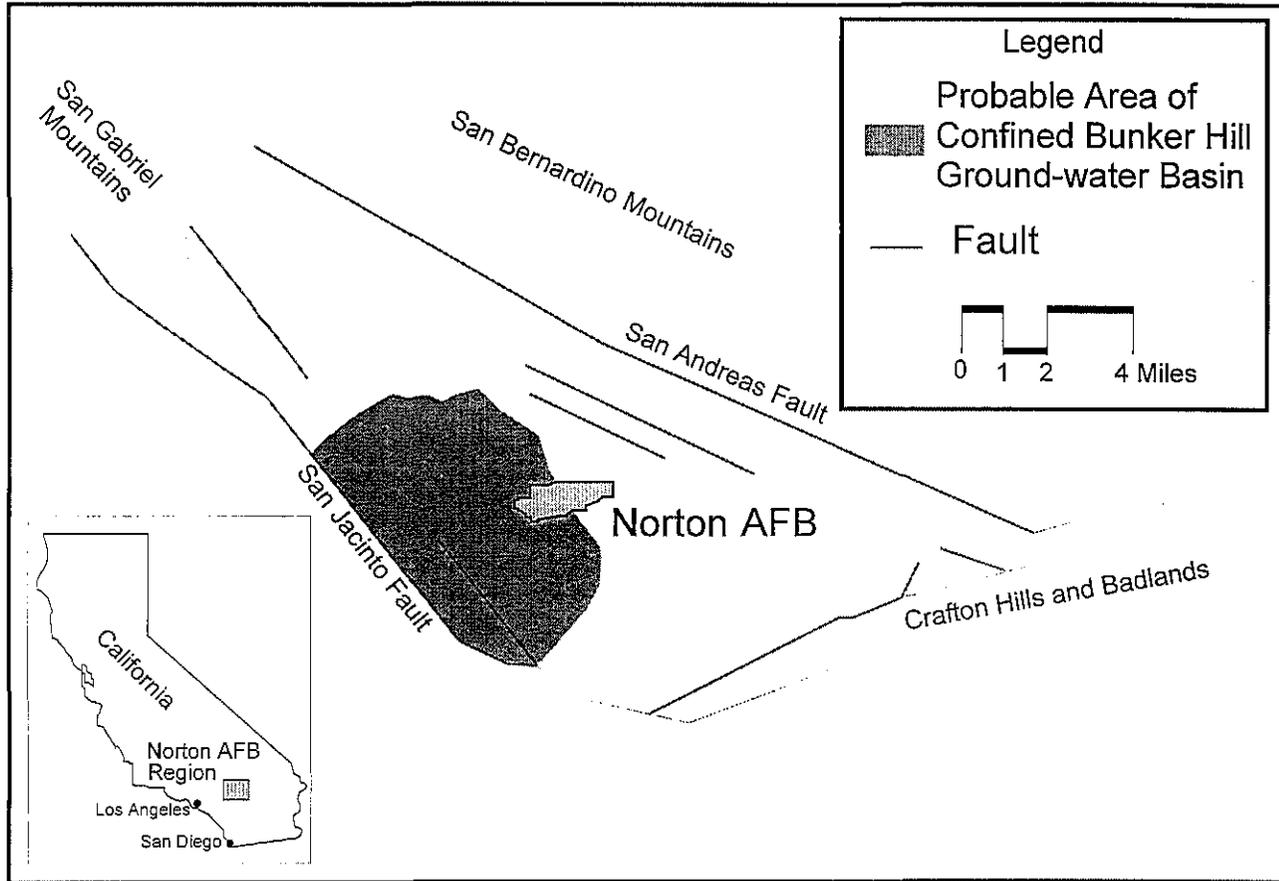
Figure 6. Candidate wells, gradient control locations, and finite difference grid: Norton Air Force Base, Southwest Boundary Area (Peralta and Aly, 1995a).
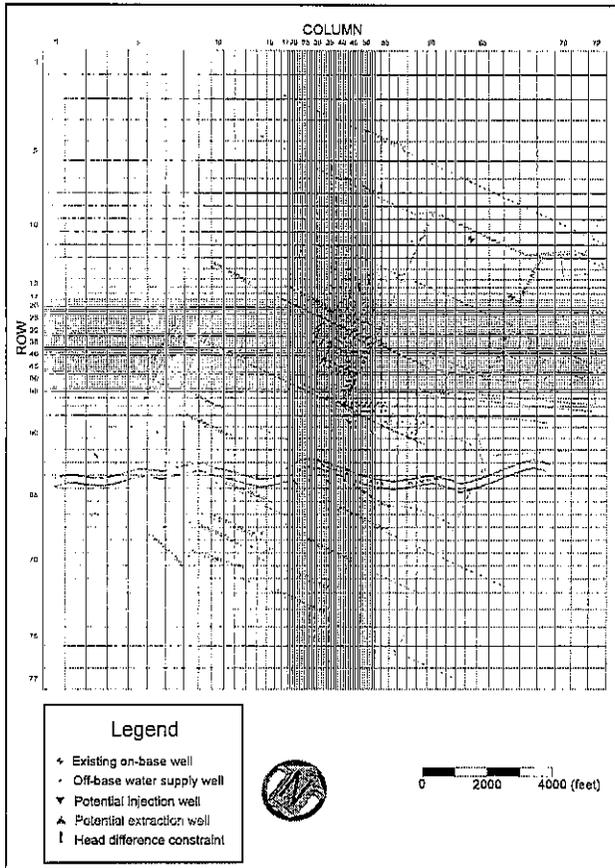
Figure 7. Pathlines for optimal pumping strategy: Norton Air Force Base, Southwest Boundary Area (Peralta and Aly, 1995a).

NORTON AFB

Legend

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

Pathlines of uncontaminated water

Public supply well

Base Boundary

BACKGROUND PUMPING

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
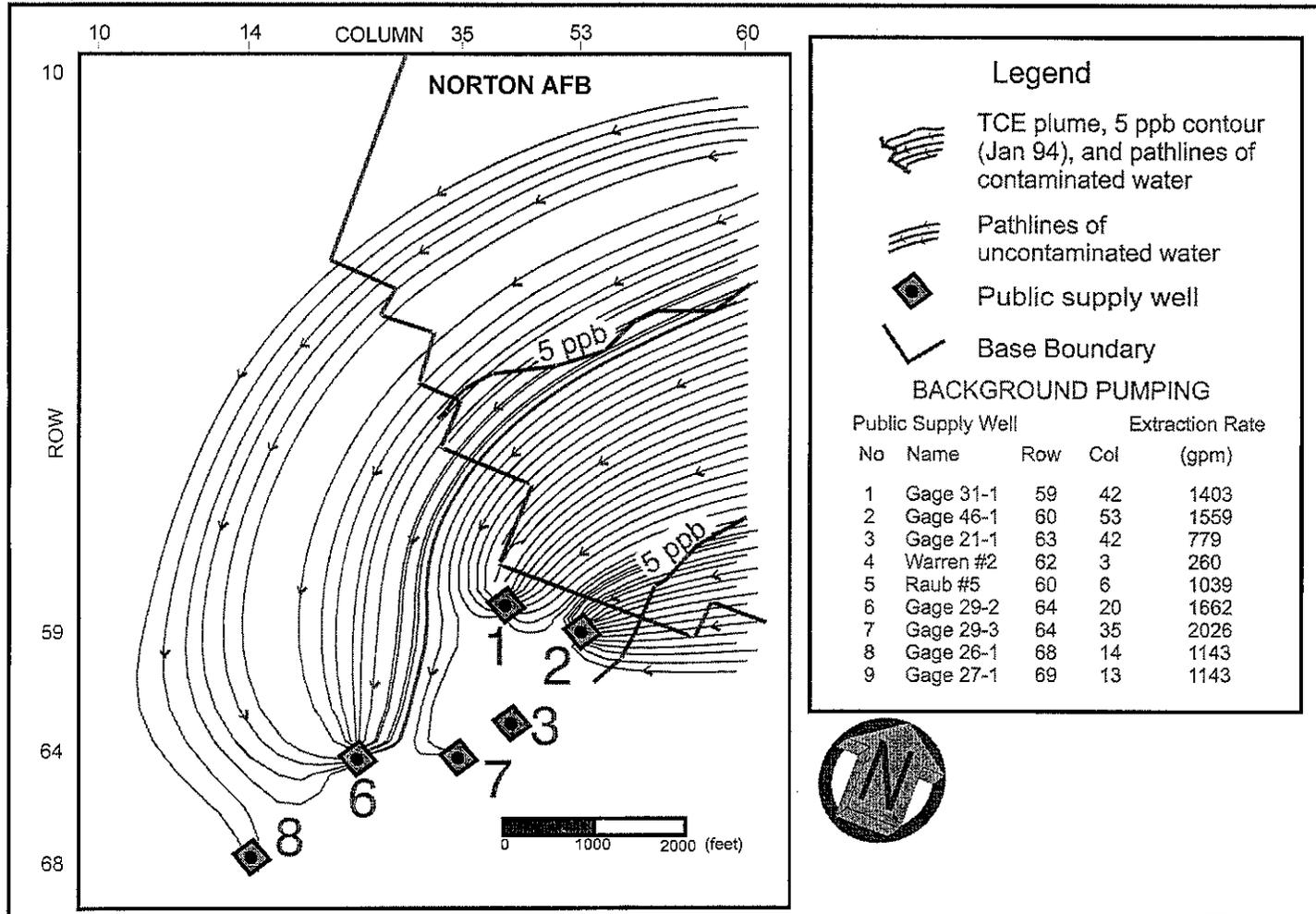
Figure 8. Potential pumping locations and initial TCE concentration: Norton Air Force Base, Central Base Area (Peralta and Aly, 1995b).
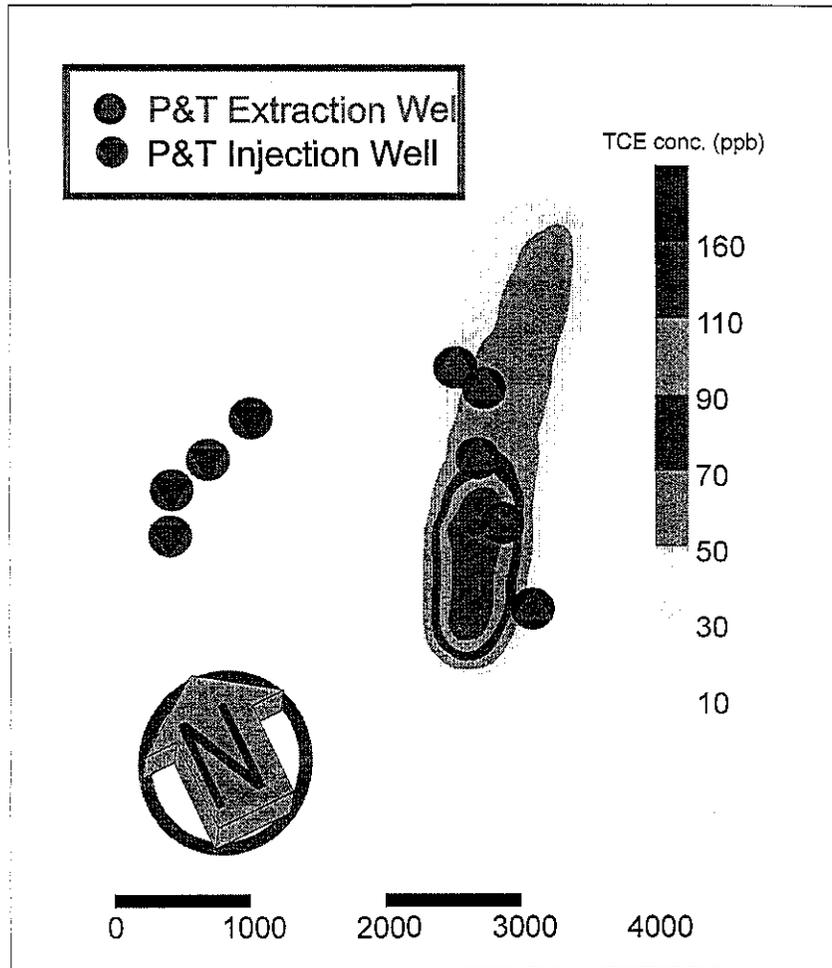
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