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Hydraulic Optimization Demonstration for Groundwater Pump-and-Treat Systems

Volume II: Application of Hydraulic Optimization

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Hydraulic Optimization Demonstration For Groundwater Pump-and-Treat Systems

Volume 2: Application of Hydraulic Optimization

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NOTICE

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PREFACE

This work was performed for the U.S. Environmental Protection Agency (U.S. EPA) under EPA Contract No. 68-C4-0031with Dynamac Corporation. The technical work was performed by HSI GeoTrans under Subcontract No. S-0K00-001. The final report is presented in two volumes:

- Volume 1: Pre-Optimization Screening (Method and Demonstration)
- Volume 2: Application of Hydraulic Optimization

Volume 1 provides a spreadsheet screening approach for comparing costs of alternative pump-and-treat designs. The purpose of the screening analysis is to quickly determine if significant cost savings might be achieved by modifying an existing or planned pump-and-treat system, and to prioritize subsequent design efforts. The method is demonstrated for three sites. Volume 1 is intended for a very broad audience.

Volume 2 describes the application of hydraulic optimization for improving pump-and-treat designs. Hydraulic optimization combines groundwater flow simulation with linear and/or mixed-integer programming, to determine the best well locations and well rates subject to site-specific constraints. The same three sites presented in Volume 1 are used to demonstrate the hydraulic optimization technology in Volume 2. Volume 2 is intended for a more technical audience than Volume 1.

The author extends thanks to stakeholders associated with the following three sites, for providing information used in this study:

- Chemical Facility, Kentucky
- Tooele Army Depot, Tooele, Utah
- Offutt Air Force Base, Bellevue, Nebraska

At the request of the facility, the name of the Kentucky site is not specified in this report.

Information was provided for each site at a specific point in time, with the understanding that new information, if subsequently gathered, would not be incorporated into this study. Updated information might include, for instance, revisions to plume definition, remediation cost estimates, or groundwater models.

The author also extends thanks to Kathy Yager of the U.S. EPA Technology Innovation Office (TIO) and Dr. David Burden of the U.S. EPA Subsurface Protection and Remediation Division (SPRD), for their support. Finally, the author extends thanks to the participants of the three Stakeholder Workshops for providing constructive comments during the course of the project.

FOREWORD

The U.S. Environmental Protection Agency is charged by Congress with protecting the Nation's land, air, and water resources. Under a mandate of national environmental laws, the Agency strives to formulate and implement actions leading to a compatible balance between human activities and the ability of natural systems to support and nurture life. To meet these mandates, EPA's research program is providing data and technical support for solving environmental problems today and building a science knowledge base necessary to manage our ecological resources wisely, understanding how pollutants affect our health, and preventing or reducing environmental risks in the future.

The National Risk Management Research Laboratory is the Agency's center for investigation of technological and management approaches for reducing risks from threats to human health and the environment. The focus of the Laboratory's research program is on methods for the prevention and control of pollution to air, land, water, and subsurface resources; protection of water quality in public water systems; remediation of contaminated sites and ground water; and prevention and control of indoor air pollution. The goal of this research effort is to catalyze development and implementation of innovative, cost-effective environmental technologies; develop scientific and engineering information needed by EPA to support regulatory and policy decisions; and provide technical support and information transfer to ensure effective implementation of environmental regulations and strategies.

These case studies demonstrate ways in which hydraulic optimization techniques can be applied to evaluate pump-and-treat designs. The types of analyses performed for these three sites can be applied to a wide variety of sites where pump-and-treat systems currently exist or are being considered. However, the results of any particular hydraulic optimization analysis are highly site-specific, and are difficult to generalize. For instance, a hydraulic optimization analysis at one site may indicate that the installation of new wells yields little benefit. That result cannot be generally applied to all sites. Rather, a site-specific analysis for each site is required. A spreadsheet-based screening analysis (presented in Volume 1 of this report) can be used to quickly determine if significant cost savings are likely to be achieved at a site by reducing total pumping rate. Those sites are good candidates for a hydraulic optimization analysis.

Clinton W. Hall

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EXECUTIVE SUMMARY

Hydraulic optimization couples simulations of groundwater flow with optimization techniques such as linear and mixed-integer programming. Hydraulic optimization allows all potential combinations of well rates at specific locations to be mathematically evaluated with respect to an objective function (e.g., minimize total pumping) and series of constraints (e.g., the plume must be contained). The hydraulic optimization code quickly determines the best set of well rates, such that the objective function is minimized and all constraints are satisfied.

For this document, the term "optimization" for pump-and-treat design was refined as follows:

> *Mathematical Optimal Solution.* The best solution, determined with a mathematical optimization technique, for a specific mathematical formulation (defined by a specific objective function and set of constraints); and
>
> *Preferred Management Solution.* A preferred management strategy based on a discrete set of mathematical optimal solutions, as well as on factors (e.g., costs, risks, uncertainties, impediments to change) not explicitly considered in those mathematical solutions.

For this demonstration project, hydraulic optimization was applied at three sites with existing pump-and-treat systems. For each case study, many mathematical formulations were developed, and many mathematical optimal solutions were determined. For each site, a preferred management solution was then suggested. The three sites can be summarized as follows:

Site	Existing Pumping Rate	Cost Per gpm	Potential Savings from System Modification
Kentucky	Moderate	High	$Millions
Tooele	High	Low	$Millions
Offutt	Low	Low	Little or None

At two of the sites (Kentucky and Tooele), pumping solutions were obtained that have the potential to yield millions of dollars of savings, relative to costs associated with the current pumping rates.

In cases where only a few well locations are considered, the benefits of hydraulic optimization are diminished. In those cases, a good modeler may achieve near-optimal (or optimal) solutions by performing trial-and-error simulations. This was demonstrated by the Offutt case study. However, as the number of potential well locations increases, it becomes more likely that hydraulic optimization will yield improved pumping solutions, relative to a trial-and-error approach. This was demonstrated by potential pumping rate reductions suggested by the hydraulic optimization results for the Kentucky and Tooele case studies.

These case studies illustrate a variety of strategies for evaluating pump-and-treat designs with hydraulic optimization. Components of mathematical formulations demonstrated with these case studies include:

Item Demonstrated	Kentucky	Tooele	Offutt
objective function minimizes total pumping	X	X	X
objective function minimizes cost		X	
multi-aquifer wells		X	X
plume containment with head limits	X		
plume containment with head difference limits		X	X
plume containment with relative gradient limits		X	X
integer constraints (limiting # of wells selected)	X	X	X
sensitivity of solutions to # of wells selected	X	X	X
scenario for "containment only"	X	X	X
scenarios with core zone extraction	X	X	X
"containment efficiency" of core zone wells evaluated	X		X
multiple target containment zones		X	
reinjection of treated water		X	
sensitivity of solutions to conservatism of constraints	X		
sensitivity of solution to non-managed stresses			X

For each of the three case studies, an analysis was performed to illustrate the sensitivity of mathematical optimal solutions to limits placed on the number of wells. For each of the three case studies, an analysis was also performed to evaluate changes in the mathematical optimal solution when new well locations were considered. For the Kentucky site, an analysis was performed to illustrate the sensitivity of the mathematical optimal solution to conservatism in the constraints representing plume containment. All of these types of analyses can be efficiently conducted with hydraulic optimization techniques. In most cases, these types of analyses are difficult (if not impossible) to comprehensively perform with a trial-and-error approach. It is important to note that the case studies presented in this report are for facilities with existing pump-and-treat systems. Mathematical optimization techniques can also be applied during initial system design, to generate improved solutions versus a trial-and-error approach.

Hydraulic optimization cannot incorporate simulations of contaminant concentrations or cleanup time. For that reason, hydraulic optimization is generally most applicable to problems where plume containment is the prominent goal. However, two of the case studies (Kentucky and Offutt) illustrate that hydraulic optimization can be used to determine the "containment efficiency" of wells placed in the core zone of a plume. This type of analysis can be performed to compare a "containment only" strategy to a strategy with additional core zone wells (to accelerate mass removal). The "containment efficiency" of the core zone wells, determined with hydraulic optimization, quantifies potential pumping

reductions at containment wells when the core zone pumping is added, such that containment is maintained. These pumping reductions (also difficult or impossible to determine with a trial-and-error approach) can potentially yield considerable savings, as demonstrated for the Kentucky site.

It is very important to distinguish the benefits of applying hydraulic optimization technology from other benefits that may be achieved simply by "re-visiting" an existing pump-and-treat design. In some cases, the underlying benefits associated with a system modification may be primarily due to a modified conceptual strategy. For instance, the Tooele case study includes analyses for different target containment zones. The potential pumping reductions and cost savings that result from a change to a smaller target containment zone primarily result from the change in conceptual strategy. The benefit provided by hydraulic optimization is that it allows mathematical optimal solutions for each conceptual strategy to be efficiently calculated and compared (whereas good solutions for each conceptual strategy may be difficult or impossible to achieve with trial-and-error).

The case studies demonstrate that there are a large variety of objective functions, constraints, and application strategies potentially available within the context of hydraulic optimization. Therefore, the development of a "preferred management solution" for a specific site depends not only on the availability of hydraulic optimization technology, but also on the ability to formulate meaningful mathematical formulations. That ability is a function of the skill and experience of the individuals performing the work, as well as the quality of site-specific information available to them.

These case studies demonstrate ways in which hydraulic optimization techniques can be applied to evaluate pump-and-treat designs. The types of analyses performed for these three sites can be applied to a wide variety of sites where pump-and-treat systems currently exist or are being considered. However, the results of any particular hydraulic optimization analysis are highly site-specific, and are difficult to generalize. For instance, a hydraulic optimization analysis at one site may indicate that the installation of new wells yields little benefit. That result cannot be generally applied to all sites. Rather, a site-specific analysis for each site is required. A spreadsheet-based screening analysis (presented in Volume 1 of this report) can be used to quickly determine if significant cost savings are likely to be achieved at a site by reducing total pumping rate. Those sites are good candidates for a hydraulic optimization analysis.

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1.0 INTRODUCTION

This report (Volume 2 of 2) demonstrates the application of hydraulic optimization for improving the design of pump-and-treat systems. "Hydraulic Optimization" refers to the use of mathematical optimization techniques (linear or mixed-integer programming), linked with a groundwater flow model, to determine the best set of well locations and well rates for a pump-and-treat design. The goal of this demonstration is to highlight strategies for applying hydraulic optimization techniques. The work presented herein was commissioned by the U.S. EPA Subsurface Protection and Remediation Division (SPRD) and the U.S. EPA Technology Innovation Office (TIO).

1.1 PURPOSE OF PERFORMING HYDRAULIC OPTIMIZATION

Numerical simulation models for groundwater flow, such as MODFLOW-96 (Harbaugh and McDonald, 1996a,b), are often used to evaluate potential pump-and-treat system designs. The groundwater model is executed repeatedly to simulate different pumping scenarios. Specific scenarios (i.e., the well locations and well rates) are usually defined with a "trial-and-error" approach, guided by professional insight. The simulation results for each scenario are evaluated with respect to objectives and constraints of the specific problem (e.g., Does the design contain the plume? Are drawdowns acceptable? What is the total pumping rate? How many new wells are required?).

One disadvantage of the "trial-and-error" flow modeling approach is that problem-specific objectives and constraints are often not clearly stated. This makes selection of the "best" strategy somewhat nebulous. Perhaps more significantly, the "trial-and-error" approach does not ensure that optimal management alternatives are even considered. This is because the potential combinations of well locations and well rates is infinite, whereas only a small number of numerical simulations is practical.

Hydraulic optimization is an attractive alternative to the "trial-and-error" flow modeling approach. Hydraulic optimization yields answers to the following groundwater management questions: (1) where should pumping and injection wells be located, and (2) at what rate should water be extracted or injected at each well? The optimal solution maximizes or minimizes a formally-stated objective function, and satisfies a formally-stated set of constraints. For example, the objective function may be to minimize the total pumping rate from all wells, and constraints might consist of limits on heads, drawdowns, gradients, and pumping rates at individual wells.

Unlike the "trial-and-error" approach, the use of hydraulic optimization requires a formal statement of a site-specific objective function, and a site-specific set of constraints. This clarifies the evaluation of different scenarios, to determine which is "best". More significantly, hydraulic optimization allows all potential combinations of well rates and all potential well locations to be rigorously evaluated, rather than the small number of scenarios that can be considered with "trial-and-error".

1.2 CASE STUDY EXAMPLES

Three sites with existing pump-and-treat systems were evaluated in this study:

- Chemical Facility, Kentucky (hereafter called "Kentucky");
- Tooele Army Depot, Tooele, Utah (hereafter called "Tooele"); and
- Offutt Air Force Base, Bellevue, Nebraska (hereafter called "Offutt").

A brief comparison of the three sites is provided below:

	Kentucky	Tooele	Offutt
Pumping rate, current system (gpm)	600	7500	200
Annual Operations & Maintenance (O&M)	$1,800,000(1)	$1,800,000	$122,000
Type of treatment	Steam Stripping	Air Stripping	POTW(2)
Discharge of treated water	River	Reinjection	N/A
Most significant annual cost	Steam	Electricity	Discharge Fee
Year system started	1992	1993	1996(3)
Cost of a new well	$20,000	$300,000	$40,000
Flow model exists?	Yes	Yes	Yes
Transport model exists?	No	Being Developed	Yes

(1) Does not include analytical costs.
(2) Water is treated at a Publicly Owned Treatment Works.
(3) An interim system has operated since 1996, and a long-term system has been designed.

Three sites were included in this study to demonstrate different strategies for applying hydraulic optimization that result from site-specific factors.

1.3 STRUCTURE OF THIS REPORT

This report is structured as follows:

- Section 2: Defining "Optimization"
- Section 3: Application Strategies For Hydraulic Optimization
- Section 4: Case #1: Kentucky
- Section 5: Case #2: Tooele
- Section 6: Case #3: Offutt
- Section 7: Discussion and Conclusions
- Section 8: References

The MODMAN code (Greenwald, 1998a), in conjunction with the LINDO software (Lindo Systems, 1996), was utilized for the hydraulic optimization simulations. MODMAN incorporates MODFLOW-96 (Harbaugh and McDonald, 1996a,b) as the groundwater flow simulator. LINDO solves mathematical optimization problems that are created by MODMAN, in the form of linear and mixed-integer programs. The linear and mixed-integer programs are written by MODMAN in Mathematical Programming System (MPS) format. A description of the MODMAN code is provided in Appendix A.

2.0 DEFINING "OPTIMIZATION"

2.1 TERMINOLOGY (LINEAR AND MIXED-INTEGER PROGRAMMING)

The word "optimal", according to Webster's New World Dictionary, means "*most favorable or desirable; best*". Mathematical techniques have been developed to determine optimal solutions for a wide variety of mathematical problems. For instance, consider the following mathematical problem, which is in the form of a **linear program**:

$$\text{Maximize} \quad 3x + 5y \qquad \{\text{Objective Function}\}$$

Subject to:

$$\begin{aligned} x \quad & \leq 4 \\ 2y \quad & \leq 12 \\ 3x + 2y \quad & \leq 18 \\ x \quad & \geq 0 \\ y \quad & \geq 0 \end{aligned} \qquad \{\text{Constraints}\}$$

The **decision variables** are the variables for which optimal values are desired. A **feasible solution** is a combination of values for the decision variables that satisfies all constraints. If there are no feasible solutions, the problem is called **infeasible**. A feasible solution that maximizes the objective function is called an **optimal solution**. The optimal solution for this problem is "x = 2, y = 6", which yields an optimal value of 36 for the objective function. It can be mathematically demonstrated that this is the most favorable (i.e., optimal) solution.

A **mixed-integer program** is similar to a linear program, but some variables may only take integer values (integer variables). Integer variables that are restricted to values of 0 or 1 are called **binary variables**. Binary variables are often used for logical or yes/no decisions.

A **quadratic program** is similar to a linear program, except that the objective function may be a nonlinear combination of the decision variables. Examples of nonlinear combinations of decision variables are:

$$2X + Y^2$$
$$X^4 - 6Y^3$$
$$X + 4XY$$

A **nonlinear program** exists when one or more constraints is a nonlinear combination of decision variables. In a nonlinear program, the objective function may be a linear or nonlinear combination of decision variables.

In general, linear programs are relatively easy to solve, quadratic programs are harder to solve, and nonlinear programs are difficult and sometimes impossible to solve. Mixed-integer programs can be

relatively simple to solve, but can also be extremely difficult to solve. As a rule, mixed-integer programs become increasingly difficult to solve as the number of integer variables increases.

2.2 SIMULATION-MANAGEMENT MODELING FOR GROUNDWATER SYSTEMS

There is a significant body of literature devoted to the coupling of groundwater simulation models with the mathematical optimization techniques described above, for the purpose of designing groundwater pump-and-treat systems. These coupled models are referred to as "simulation-management models". The goal is to determine a set of well locations and well rates that minimizes or maximizes an objective function (e.g., "minimize total pumping rate"), while satisfying all pertinent constraints (e.g., "the plume may not grow in size"). To utilize these simulation-management models, the user must formulate a mathematical problem to solve. The mathematical formulation includes a specific objective function and a specific set of constraints. The objective function and/or constraints are related to the well rates through the groundwater simulation model.

Different "optimal solutions" will result if the mathematical formulation is modified (Gorelick et. al., 1993, page 136). Modifications might include alterations to the objective function, the constraint set, or the underlying simulation model. For example, one formulation may include only existing wells, another formulation may include existing wells plus new wells, and a third formulation may include existing wells plus a barrier wall. Those authors suggest that "*the best use of [simulation-management modeling] is to develop a family of so-called 'optimal solutions' under a broad and varied menu of design considerations*".

2.3 "MATHEMATICAL OPTIMAL SOLUTION" VERSUS "PREFERRED MANAGEMENT SOLUTION"

The term "optimization" can be vague when applied to pump-and-treat designs. In one sense, "optimization" refers to the use of mathematical solution techniques to determine the best solution for a specific mathematical formulation. In another sense, "optimization" refers to the process of arriving at a preferred or improved management strategy, which may be based on multiple "optimal solutions" for different mathematical formulations, as well as on factors that may not have been explicitly incorporated in mathematical solutions due to mathematical complexity (e.g., cleanup timeframe, discount rate).

For this document, the term "optimization" for pump-and-treat design was refined as follows:

> *Mathematical Optimal Solution.* The best solution, determined with a mathematical optimization technique, for a specific mathematical formulation (defined by a specific objective function and set of constraints).
>
> *Preferred Management Solution.* A preferred management strategy based on a discrete set of mathematical optimal solutions, as well as on factors (e.g., costs, risks, uncertainties, impediments to change) not explicitly considered in those mathematical solutions.

For each case study in this report, many mathematical formulations were developed, and many mathematical optimal solutions were determined. For each site, a preferred management solution was then suggested.

2.4 DETERMINISTIC HYDRAULIC OPTIMIZATION VERSUS MORE ADVANCED ALTERNATIVES

This demonstration project utilizes deterministic hydraulic optimization, which is a relatively simple and easy-to-apply simulation-management method for the following reasons:

- **Flow-Based Constraints**. Limits on management alternatives are based on groundwater flow conditions (e.g., heads, drawdowns, gradients), such that a transport simulation model is not required, and linear or mixed-integer programming algorithms can be employed (techniques incorporating contaminant concentrations and/or cleanup times as constraints require nonlinear programming techniques, as discussed in Appendix B); and

- **Deterministic Simulations**. Simulations of groundwater flow are based on one discrete set of initial conditions, boundary conditions, and parameter values (techniques incorporating uncertainty and/or risk are discussed in Appendix C).

The use of deterministic hydraulic optimization has advantages and limitations. These are discussed below.

2.4.1 Advantages of Deterministic Hydraulic Optimization

Advantages of deterministic hydraulic optimization include the following:

- for most sites with groundwater contamination, a deterministic flow model exists or can be easily created at relatively low cost;

- many practitioners of groundwater modeling understand the application of groundwater flow modeling, but have limited understanding or ability to apply transport modeling or uncertainty (e.g., stochastic) modeling;

- the construction of a groundwater transport model requires significantly more input than a groundwater flow model (e.g., initial concentrations, dispersivity, retardation/sorption, decay, porosity);

- predictions of groundwater flow are subject to less uncertainty than predictions of contaminant concentrations and/or cleanup time (which form the basis of transport optimization);

- computational effort for transport models and/or stochastic simulations can be significantly greater than for groundwater flow models;

- tools for performing deterministic hydraulic optimization (e.g., MODMAN) are available as "off-the-shelf" technology;

- solution of linear and/or mixed-integer programs associated with hydraulic optimization is straightforward and easily achieved with inexpensive "off-the-shelf" technology;

- computational effort for solutions of nonlinear programs (e.g., transport optimization) is significantly greater than for linear or mixed-integer programs.

For these reasons, real-world applications of hydraulic optimization have been performed for many years. Appendix D provides a partial listing of MODMAN applications. Appendix I includes discussion and/or references for real-world applications with other simulation-management codes, some of which pertain to hydraulic optimization.

2.4.2 Limitations of Deterministic Hydraulic Optimization

The limitations of deterministic hydraulic optimization must be considered when evaluating the potential application of simulation-management modeling for a specific site. Major limitations include:

- contaminant concentrations cannot be included in the mathematical formulation;
- cleanup time cannot be rigorously included in the mathematical formulation;
- for thin unconfined aquifers (and several other circumstances), linear superposition (which allows the use of linear programming techniques) may be violated; and
- since a deterministic modeling approach is used, uncertainty in model parameters cannot be directly incorporated into the mathematical formulation (e.g., one cannot specify that "the constraint must be met with 95% certainty, given anticipated variation in hydraulic conductivity").

Because contaminant concentrations and cleanup times cannot be included in the mathematical formulation, hydraulic optimization is generally most applicable to problems where hydraulic containment of a groundwater plume is the primary goal. However, hydraulic optimization can be utilized to evaluate some tradeoffs between containment strategies and more aggressive pumping strategies (discussed later).

For sites where cleanup is the main objective, and predictions of contaminant concentrations or cleanup time are central to evaluation of the objective function and/or key constraints, the limitations of hydraulic optimization may be prohibitive. Transport modeling and transport optimization may be applied in such cases (see Appendix B). However, developing a transport simulation model and performing a transport-based optimization analysis may require significantly effort and cost, and transport model predictions are subject to additional uncertainties (relative to flow model predictions).

It is important to note that any simulation-management technique is limited by the predictive ability of the underlying simulation model, which is not only affected by uncertainty in parameter values, but also by available data, the conceptual hydrogeological model of the site, the experience of the modeler, input errors, and many other factors.

3.0 APPLICATION STRATEGIES FOR HYDRAULIC OPTIMIZATION

The use of hydraulic optimization for plume management requires the specification of a mathematical formulation, consisting of an objective function and a series of constraints. Various constraint types are presented in Section 3.1, and various objective functions are presented in Section 3.2.

Alternative pump-and-treat strategies for a specific site can be evaluated with hydraulic optimization by defining and solving multiple mathematical formulations (e.g., considering only existing wells in one formulation, and then considering additional well locations in another formulation). Section 3.3 presents typical variations that are considered by varying the mathematical formulation at a specific site.

3.1 CONSTRAINTS

3.1.1 Constraints Representing Plume Containment

One technique utilized in plume management problems uses a line of head difference, gradient, or velocity constraints to represent a flow divide. Such a strategy might be used in a case where a plume flows towards a river. The constraints would mandate that any feasible solution include a hydraulic divide between the plume and the river. A similar scenario might involve a plume and one or more water supply wells, where a flow divide between the plume and the water supply wells prevents contamination of the water supply. An approach of this type, that uses velocity constraints to impose a groundwater flow divide, is described by Colarullo et al. (1984). Vertical flow can also be restricted with head difference constraints, to prevent fouling of aquifers above and/or below a contaminated aquifer.

A second useful technique is to apply head difference, gradient, or velocity constraints to create inward flow perpendicular to a plume boundary. If desired, lower limits other than zero can be imposed, to increase assurance that the plume will in fact be contained. This type of technique is described by Gorelick and Wagner (1986). A variation of this technique, utilizing velocity constraints, was described by Lefkoff and Gorelick (1986). In that project, target boundaries of a shrinking plume were set for four 1-year periods. The velocity constraints insured that these target boundaries were met.

Another technique allows flow directions to be constrained, using relative gradient constraints. This approach is illustrated by Greenwald (1998a), and is also described by Gorelick (1987). These constraints limit the direction of flow according to the resultant of two gradients, oriented 90° apart, that share the same initial location. The concept is illustrated in the schematic presented below. There are two gradient constraints, A and B. The shared point is the initial point in each gradient constraint.

The user typically desires the actual flow direction, defined by Θ, to be greater than some limiting flow direction (defined by angle ß in the schematic). The constraint is derived as follows:

$$\Theta \geq \beta$$

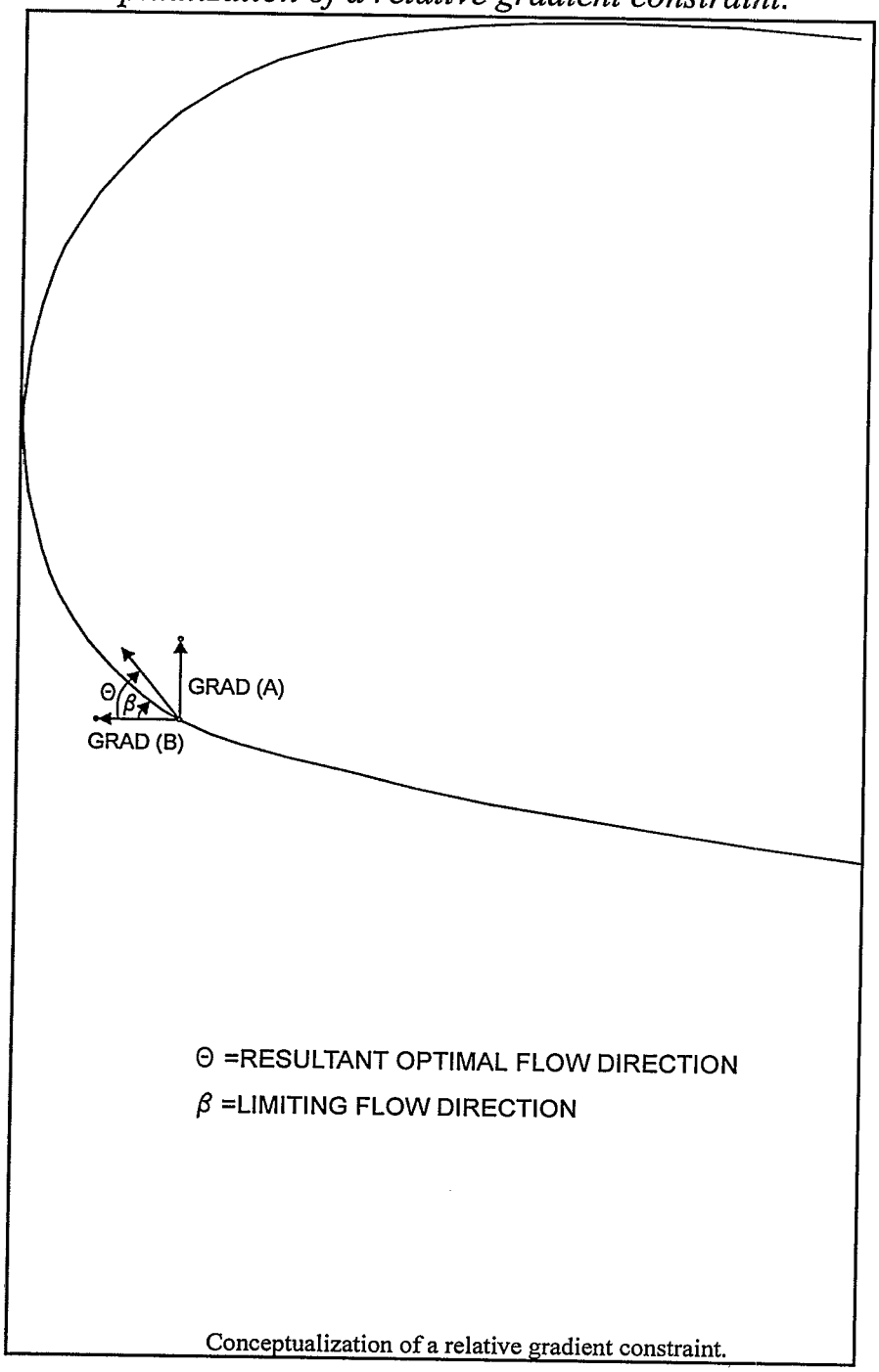
$$\tan\Theta \geq \tan\beta$$

$$\text{GRAD(A)} / \text{GRAD(B)} = \tan\Theta \qquad \text{[by trigonometry]}$$

$$\text{GRAD(A)} / \text{GRAD(B)} \geq \tan\beta \qquad \text{[substitute for } \tan\Theta\text{]}$$

$$\text{GRAD(A)} - \tan\beta * \text{GRAD(B)} \geq 0 \qquad \text{[rearrange terms as a linear constraint]}$$

Conceptualization of a relative gradient constraint.



Conceptualization of a relative gradient constraint.

3.1.2 Constraints Representing Multi-Aquifer Wells

Multi-aquifer wells in MODFLOW are wells that are screened in more than one model layer. Specification of these wells in MODFLOW presents a problem, because MODFLOW allows a well to be specified only in one layer. The technique most widely used is to represent a multi-aquifer well with multiple wells in MODFLOW, with the rate at each MODFLOW well weighted by transmissivity in each model layer.

Example: well pumps 100 gpm, and is screened in model layers 1 and 2

transmissivity of layer 1:	2500 ft^2/d
transmissivity of layer 2:	7500 ft^2/d
apportionment layer 1:	2500 / (2500 + 7500) = 25%
apportionment layer 2:	7500 / (2500 + 7500) = 75%
well rate layer 1 (Q1):	100 gpm * 25% = 25 gpm
well rate layer 2 (Q2):	100 gpm * 75% = 75 gpm

When performing hydraulic optimization, the ratio of well rates between layers can be preserved with properly constructed constraints. For the example above, the following constraint is derived:

$$Q2 / Q1 = 3.00$$
$$Q2 - 3.00Q1 = 0.00$$

This constraint is a linear function of the decision variables. If pumping occurs at one of the wells, it must also occur at the other well, at the proper ratio. The total rate at the well can be limited by placing a bound on either of the component wells, or on the sum of the component wells. For instance, assume the maximum rate to be allowed at the well is 200 gpm. Any of the following constraints will enforce this limit:

$$Q1 \leq 50 \text{ gpm}$$
- or -
$$Q2 \leq 150 \text{ gpm}$$
- or -
$$Q1 + Q2 \leq 200 \text{ gpm}$$

This approach is easily extended to multi-aquifer wells screened across more than two layers.

3.1.3 Constraints Limiting Number of Wells Selected

This type of constraint is sometimes desirable when considering a large number of potential well locations for siting a small number of wells. For instance, assume the objective is to minimize the total extraction rate, subject to plume containment constraints. Suppose that only 2 wells are desired due to installation costs and piping construction required, but 9 sites are being considered. If an "x out of y" constraint is not included, the optimal solution may be to pump at a small rate at all 9 wells, which is not a desirable solution.

Constraints limiting the number of wells selected can be implemented with two types of constraints:

- well on/off constraints; and
- integer variable summation constraints.

The on/off constraints are constructed with binary variables, which are integer variables that can only have a value of 0 or 1. The on/off constraint for a well forces the binary variable to a value of 1 if the well is on. The form of the on/off constraint is :

EXTRACTION	INJECTION
(Negative Well Rate)	(Positive Well Rate)
$Q_j + M^*I_j \geq 0$	$Q_j - M^*I_j \leq 0$

where:

Q_j = rate at well j (negative for pumping);
M = a large number with an absolute value greater than that of the largest well rate; and
I_j = a binary variable acting as on/off switch for well j.

If Q has a non-zero value, the on/off constraint will only be satisfied if the binary variable is 1.

The integer variable summation constraint, based on the binary variables, enforces the limit on the number of active wells allowed. For example, if there are nine potential well locations, but only two may be selected, the integer summation constraint would be:

$$I_1 + I_2 + I_3 + I_4 + I_5 + I_6 \; I_7 + I_8 + I_9 \quad \leq \quad 2$$

This technique is describe in more detail in Greenwald (1998a).

3.1.4 Constraints Limiting Head at the Well

Groundwater flow models based on finite differences (e.g., MODFLOW) typically calculate head for a representative volume (i.e., an entire grid block). In some cases, it is important to constrain head at the actual location of the well, as opposed to a representative head for larger grid block. For instance, there may be a legal restriction on allowable drawdown, or there may be a physical constraint associated with too much drawdown such as drawing water below a pump. Some hydraulic optimization codes (e.g., MODMAN) allow head limits to be imposed at a well and/or an entire grid block. The calculations to approximate head at the well are based on the Thiem equation, and are explained in detail on pages 9 to 10 of the USGS Finite-Difference Model for Aquifer Simulation in Two Dimensions (Trescott et al., 1976). It is important to recognize that the calculation of head in a well is based on many assumptions, such as:

- the grid block is square;
- all pumping is at one fully penetrating well, located in the center of the grid block;
- flow can be described by a steady-state equation with no source term except for the well discharge;

- the aquifer is homogeneous and isotropic within the grid block containing the well; and
- well losses are negligible.

Many of these assumptions are typically not met. As a result, heads calculated at wells should be viewed as a more accurate approximation of head at the well, but still an estimate nevertheless.

3.1.5 Other Common Constraints

Many other types of constraints can be represented within a hydraulic optimization formulation. These include:

- limits on head in specific grid cells;
- limits on drawdown at specific grid cells;
- limits on well rate at specific wells;
- limits on total well rates at combinations of wells; and
- limits on the difference between total pumping and total injection.

A description of constraint types that can be formed as linear functions of the well rates is presented in the MODMAN documentation (Greenwald, 1998a).

3.2 OBJECTIVE FUNCTIONS

Optimization implies that different solutions are compared to each other, and that a determination can be made as to which solution is best. This comparison can be made by computing the value of an objective function based on values of the decision variables for each solution (pumping/injection rates). The optimal solution is one that minimizes (or maximizes) the objective function.

A general linear objective function for a steady-state plume management problem is:

$$\text{Min} \quad \sum_{i=1,n} c_i Q_i + d_i I_i$$

where:

n = total number of pumping and/or injection wells
Q_i = pumping or injection rate at well i
I_i = 1 if well i is active, 0 if well i is not active
c_i = coefficient for well i multiplied by pumping/injection rate at well i
d_i = addition to objective function if well i is active (pumping or injection)

The values for coefficients (c_i and d_i) will depend on site-specifics factors related to the cost of pumping water, treating water, discharging water, installing new wells, and other factors. The general form of the objective function is easily extended to transient cases (i.e., multiple stress periods, where pumping rates are potentially altered each stress period).

In many cases the objective function can be simplified, with many of the coefficients assigned values of 0 or 1. An example of a simplified objective functions is:

$$\text{Min} \sum_{i=1,n} Q_i \qquad \text{(e.g., minimize the total pumping rate)}$$

The applicability of different forms of the objective function for specific types of sites is discussed below. Examples are provided to illustrate how different types of objective functions can be applied.

3.2.1 Objective Functions Based Indirectly on Costs (e.g., Minimize Pumping Rate)

The true objective of plume management is generally to minimize costs, subject to all constraints associated with maintaining containment and/or providing satisfactory cleanup. However, developing cost functions that rigorously account for all costs associated with pumping, treatment, and discharge can be difficult. Fortunately, many problems can be evaluated with simple objective functions that are only indirectly based on cost. Examples include:

$$\text{Min} \sum_{i=1,n} Q_i \qquad \text{(e.g., minimize the total pumping rate)}$$

$$\text{Min} \sum_{i=1,n} I_i \qquad \text{(e.g., minimize the number of active wells or new wells)}$$

In these cases, the units of the objective function are not units of cost, although it is assumed that the optimal solution will in fact minimize the total cost.

Minimizing the total pumping rate is appropriate when the cost of pumping, treating, or discharging the water is rate-sensitive and is the dominant cost factor. Minimizing the number of active wells is appropriate if the number of pumps (e.g., electrical demand from pumping water) is the dominant cost factor. Minimizing the number of new wells is appropriate if the capital cost of installing a new well is the dominant cost factor.

Despite the fact that these objectives do not rigorously consider cost, they can also be used, in conjunction with appropriate constraints, to evaluate problems where some wells are qualitatively preferred to others. For example, assume an existing system has four extraction wells, and the treatment cost is sensitive to total rate (i.e., minimizing total rate is the simplified objective). At the same time, it may be qualitatively preferable to pump from wells 1 and 2 (located near the source) than from wells 3 and 4 (located near the toe of the plume). This may occur because wells 1 and 2 remove more mass, or because it costs less to pump at wells 1 and 2 due to depth to water and/or topographic lift back to the treatment plant.. Assume this problem is initially evaluated with the following objective function:

$$\text{Min } Q_1 + Q_2 + Q_3 + Q_4 \quad \text{[minimize total pumping]}$$

and that the following optimal solution is determined (total pumping rate = 700 gpm) :

$Q_1 = 50$ gpm $\quad$ $Q_3 = 250$ gpm
$Q_2 = 30$ gpm $\quad$ $Q_4 = 370$ gpm

The tradeoff between increased total pumping rate versus additional pumping at the preferred wells can then be evaluated with the same objective function, by adding a constraint:

$$Q_1 + Q_2 \geq 100 \text{ gpm}$$

The resulting optimal solution can then be compared to the original optimal solution. This process can be repeated with different limits assigned in the new constraint:

Constraint	Optimal Solution (Total Rate)	Comments
$Q_1 + Q_2 = 80$ gpm	700 gpm	Original problem
$Q_1 + Q_2 \geq 100$ gpm	705 gpm	Shift 20 gpm to preferred wells, total rate increases 5 gpm
$Q_1 + Q_2 \geq 200$ gpm	720 gpm	Shift 120 gpm to preferred wells, total rate increases 20 gpm
$Q_1 + Q_2 \geq 300$ gpm	850 gpm	Shift 220 gpm to preferred wells, total rate increases 150 gpm
$Q_1 + Q_2 \geq 400$ gpm	980 gpm	Shift 320 gpm to preferred wells, total rate increases 280 gpm

Although the objective function for all of these problems ("minimize total pumping rate") does not directly account for cost, the tradeoff between increased total pumping rate versus the benefits of increased pumping at the preferred wells can now be analyzed qualitatively. In the example above, 120 gpm can be shifted to the preferred wells with only a small increase (20 gpm) in total pumping rate, which qualitatively appears favorable. The increased costs of treating an additional 20 gpm can presumably then be estimated (external to the optimization problem that is actually solved) if a more detailed cost/benefit analysis is desired.

3.2.2 Objective Functions Based Directly on Costs

Direct consideration of costs in the objective function allows costs to be more quantitatively evaluated in the determination of the optimal solution. The objective function can be specified directly in units of cost as follows:

$$\text{Min} \sum_{i=1,n} c_i Q_i + d_i I_i$$

where:

$c_i =$ approximate cost per unit pumping rate at well i
$d_i =$ additional cost incurred if well i is active (e.g., well installation cost)

Because actual cost functions are quite complex, simplifications are typically required to assign the coefficients (c_i and d_i). An example is provided below.

Assume a system has 4 existing extraction wells (wells 1 through 4), and that treatment consists of metals precipitation, Ultraviolet (UV) oxidation, and GAC in series, followed by discharge to POTW (reinjection is not an option). Current total rate is 400 gpm. The current cost of treating water and discharging water is $200K/yr. Electrical cost is $10K/yr and monitoring cost is $100K/yr, but neither of these costs is sensitive to pumping rate. The goal is to contain the plume within the property boundary. Up to three new wells are to be considered (wells 5 through 7), but installation of a new well and associated piping will cost approximately $50K per well.

The development of a simple cost function in terms of pumping rates is complicated for this problem, because the cost of treating and discharging water is an annual cost, while the cost of installing a new well is a one-time cost. This can be resolved several different ways:

(1) annualize the one-time cost of installing a well over a specific planning horizon (e.g., if a new well costs $50K to install, approximate it's cost as $10K/yr over a 5 year planning horizon), so the units of the objective function are "costs per year over a 5 year planning horizon";

-or-

(2) multiply the annual costs of pumping and treating water by a specified time horizon (e.g., 5 years) so the units of the objective function are "total cost over 5 year period".

Using the first approach as an example, a simplified objective function (based on cost) for the stated problem is:

$$\text{Min} \quad 500Q_1 + 500Q_2 + 500Q_3 + 500Q_4 + 500Q_5 + 500Q_6 + 500Q_7 + 10000I_5 + 10000I_6 + 10000I_7$$

where:

500	=	approximate cost (in dollars/yr) to treat/discharge 1 gpm of water
10000	=	approximate cost (in dollars/yr) to install a new well (annualized for 5 yrs)
Q_i	=	pumping rate at well i (in gpm)
I_i	=	1 if new well i is installed (i.e., active)

This objective function *minimizes annual cost,* over a 5-year period. Up-front and annual costs are simultaneously considered and rigorously evaluated within the optimization process. Of course, this cost function includes simplifications, such as the simple annualization of the one-time costs over a five-year period. However, it still provides a reasonable cost-based framework for comparing alternate strategies (in this case, the tradeoff between potential pumpage reductions from a new well versus the costs of installing that well).

Using the second approach, a simplified objective function (based on cost) for the stated problem is:

$$\text{Min} \quad 2500Q_1 + 2500Q_2 + 2500Q_3 + 2500Q_4 + 2500Q_5 + 2500Q_6 + \\ + 2500Q_7 + 50000I_5 + 50000I_6 + 50000I_7$$

where:

2500	=	approximate cost (in dollars) to treat/discharge 1 gpm of water for 5 yrs
50000	=	approximate cost (in dollars) to install a new well
Q_i	=	pumping rate at well i (in gpm)
I_i	=	1 if new well i is installed (i.e., active)

This objective function *minimizes total cost* over a 5-year period. Up-front and annual costs are simultaneously considered and rigorously evaluated within the optimization process.

3.3 TYPICAL SCENARIOS CONSIDERED WITH HYDRAULIC OPTIMIZATION

3.3.1 Existing Wells or Additional Wells

First, an optimal solution can be obtained with existing wells only. Then optimization can be performed with one or more new well locations considered. With some optimization packages (e.g., MODMAN), it is possible to consider many different potential locations for new wells, but to only select a specified number of those locations in the optimal solution. The costs and benefits of adding the new wells can then be evaluated.

3.3.2 Extraction or Extraction Plus Reinjection

Pumpage optimization can be performed for cases with and without reinjection of treated water. The costs and benefits of reinjecting water can then be evaluated.

3.3.3 "Containment Only" versus Accelerated Mass Removal (Containment Efficiency)

For sites where containment is the remediation objective, application of hydraulic optimization is straightforward. At some sites, however, strategies that incorporate accelerated mass removal are also considered. As previously discussed, hydraulic optimization is based on groundwater flow, and does not rigorously account for contaminant concentrations, mass removal, or cleanup time. However, hydraulic optimization can be used to quantify the "containment efficiency" of wells intended for accelerated mass removal. This allows the costs and benefits of additional wells intended for accelerated mass removal to be more rigorously evaluated.

For example, assume hydraulic optimization indicates that three wells located near the toe of a plume, pumping a total of 500 gpm, will provide containment. However, site managers want to consider several additional wells near the core of the plume (where concentrations are higher), pumping at 200 gpm, to accelerate mass removal. Should the resulting strategy consist of 700 gpm? The answer is usually "no". because pumping in the core of the plume may also contribute to overall plume containment, such that the addition of core-zone pumping may permit total pumping near the toe of the plume to be reduced without compromising plume containment.

Hydraulic optimization can be used to quantify that relationship. This can be expressed as "containment efficiency" of the core zone pumping, as follows:

containment efficiency = (Potential reduction in toe pumping) / (increase in core pumping)

Assume in the previous example that hydraulic optimization is used to determine that, after 200 gpm is implemented in the core zone, total pumping at the toe wells can be reduced from 500 gpm to 380 gpm without compromising containment. Adding 200 gpm in the core zone permits pumping at the toe wells to potentially be reduced by 120 gpm (500 gpm - 380 gpm). The "containment efficiency" of the core zone pumping is:

containment efficiency = 120/200 = 60%

Therefore, if this analysis is performed, increased costs associated with the core zone pumping (well installation and/or treatment costs) can be partially offset by implementing a corresponding pumping rate reduction at the toe wells.

3.3.4 Modifications to the Target Containment Zone

Hydraulic optimization can be performed for alternate definitions of the target containment zone. This can provide information regarding the potential reduction in total pumping and/or cost that can result if a smaller region of water must be contained.

3.4 ROLE OF THE HYDRAULIC OPTIMIZATION CODE

The role of the hydraulic optimization code is to provide mathematical optimal solutions for specific mathematical formulations. Given the large variety of objective functions, constraints, and application strategies potentially available, it is clear that the development of a "preferred management solution" for a specific site depends not only on the availability of hydraulic optimization technology, but also on the ability of individuals to formulate meaningful mathematical formulations. That ability is a function of the skill and experience of the individuals performing the work, as well as the quality of site-specific information available to them.

4.0 CASE #1: KENTUCKY

4.1 SITE BACKGROUND

4.1.1 Site Location and Hydrogeology

The facility is located in Kentucky, along the southern bank of a river (see Figure 4-1). There are in excess of 200 monitoring points and/or piezometers at the site. The aquifer of concern is the uppermost aquifer, called the Alluvial Aquifer. It is comprised of unconsolidated sand, gravel, and clay. The Alluvial Aquifer has a saturated thickness of nearly 100 feet in the southern portion of the site, and a saturated thickness of approximately 30 to 50 feet on the floodplain adjacent to the river. The decrease in saturated thickness is due to a general rise in bedrock elevation (the base of the aquifer) and a decrease in surface elevation near the floodplain. The hydraulic conductivity of the Alluvial Aquifer ranges from approximately 4 to 75 ft/d.

Groundwater generally flows towards the river, where it is discharged (see Figure 4-2). However, a groundwater divide has historically been observed between the site and other nearby wellfields (locations of wellfields are illustrated on Figure 4-1). The groundwater divide is presumably caused by pumping at the nearby wellfields.

4.1.2 Plume Definition

Groundwater monitoring indicates site-wide groundwater contamination. Two of the most common contaminants, 1,2-dichloroethane (EDC) and benzene, are used as indicator parameters because they are found at high concentrations relative to other parameters, and are associated with identifiable site operations. Shallow plumes of EDC and benzene are presented in Figures 4-3 and 4-4, respectively. Concentrations are very high, and the presence of residual NAPL contamination in the soil column is likely (SVE systems have recently been installed to help remediate suspected source areas in the soil column).

4.1.3 Existing Remediation System

A pump-and-treat system has been operating since 1992. Pumping well locations are illustrated on Figures 4-3 and 4-4. There are three groups of wells:

- BW wells: River Barrier Wells
- SW wells: Source Wells
- OW wells: Off-site Wells

The primary goal is containment at the BW wells, to prevent discharge of contaminated groundwater to the river. The purpose of the SW wells is to accelerate mass removal. The purpose of the OW wells is to prevent off-site migration of contaminants towards other wellfields. A summary of pumping rates is as follows:

	Number of Wells	Design Rate (gpm)	Typical Rate (gpm)
BW wells:			
Original Design	18	549	N/A
Current System	23	N/A	420-580
SW wells	8	171	80-160
OW wells	8	132	25-100
Total System:			
Original Design	34	852	N/A
Current System	39	N/A	500-800

Five BW wells were added after the initial system was implemented, to enhance capture where monitored water levels indicated the potential for gaps. The operating extraction rates are modified as the river level rises and falls (when the river level falls, aquifer water levels also fall, and transmissivity at some wells is significantly reduced). The eight OW wells controlling off-site plume migration have largely remediated that problem, and will likely be phased out in the near future.

Contaminants are removed by steam stripping. The steam is purchased from operations at the site. Treated water is discharged to the river. Approximate costs of the current system are presented in Table 4-1 (see Volume 1 for a more detailed discussion of costs).

Site managers have indicated their desire for accelerated mass removal, if it is not too costly. They do not favor significant reductions in pumping (and associated annual costs) if that will result in longer cleanup times.

4.1.4 Groundwater Flow Model

An existing 2-dimensional, steady-state MODFLOW (McDonald and Harbaugh, 1988) model is a simple representation of the system. There are 48 rows and 82 columns. Grid spacing near the river is 100 ft. The model has historically been used as a design tool, to simulate drawdowns and capture zones (via particle tracking) resulting from specified pumping rates.

4.1.5 Goals of a Hydraulic Optimization Analysis

A screening analysis performed for this site (see Volume 1) suggests that significant savings (millions of dollars over 20 years) might be achieved by reducing the pumping rate associated with the present system, even if five new wells (at $20K/well) were added. In that screening analysis, a pumping rate reduction of 33 percent was assumed. This could potentially be accomplished by:

- a reduction in rates at the BW wells required to maintain containment (via optimization);
- a reduction in pumping at the OW wells; and/or
- a reduction in pumping at the SW wells.

The goals of the optimization analysis are:

(1) quantify potential pumping rate reductions at the BW wells, without compromising containment at the river (with the SW and OW wells operating as designed);

(2) quantify the tradeoff between the number of BW wells operating and the total pumping rate required for containment;

(3) quantify the total pumping required for containment if only the BW wells are operated (i.e., no pumping at the existing SW or OW wells);

(4) quantify the increase (or decrease) in pumping required for containment if more (or less) conservative constraints for containment are imposed at the river;

(5) quantify the degree to which pumping at additional core zone wells might be offset by pumping reductions at barrier wells, while maintaining containment.

Mathematical formulations for achieving these goals are presented below. Then "mathematical optimal solutions" for these formulations are presented. and discussed within the context of a "preferred management solution".

4.2 COMPONENTS OF MATHEMATICAL FORMULATION

4.2.1 Representation of Plume Containment

Head constraints were used to represent plume containment at model grid cells adjacent to the river (i.e., to prevent discharge of contaminated water to the river). In the groundwater flow model, the river is simulated with specified head cells, which are assigned a water elevation of 302 ft MSL. In MODMAN, an upper limit of 301.99 ft MSL is specified at 54 cells adjacent to the river (Figure 4.5). These head limits prevent discharge of groundwater to the river in each of those cells. Note that head difference limits and gradient limits are also available in MODMAN, and either could have been used instead of the head limits to represent plume containment.

The locations of the cells where head limits were assigned correspond to the capture zone of the designed pump-and-treat system, as determined by the groundwater flow model (with particle tracking). Use of the containment zone associated with the original system design allows for a fair comparison between total pumping rates in the original design versus pumping solutions obtained with hydraulic optimization.

The specific head value of 301.99 was selected because a head difference of 0.01 ft (between the river and a cell adjacent to the river) is measurable in the field. Sensitivity analyses for some optimization scenarios were performed, to assess the change in mathematical optimal solutions resulting from a smaller head difference limit (e.g., 0.00 ft) and a larger head difference limit (e.g., 0.10 ft).

4.2.2 Representation of Wells

Existing Well Locations:

Locations of existing wells are illustrated on Figures 4-3 and 4-4, and are summarized on Table 4-2. As previously discussed, five of the BW wells were installed subsequent to the original design (indicated on Table 4-2).

New Well Locations Considered:

Four additional well locations, in areas of high contaminant concentrations, were considered in some scenarios. These locations are illustrated on Figure 4-5. The purpose of considering new wells in these scenarios was to quantify the "containment efficiency" of wells located in key areas of high concentration (see Section 3.3.3 for a discussion of "containment efficiency").

Well Rate Limits:

For existing wells, daily well rates were available for June 1997 through November 1997. For managed wells (i.e., wells in a specific scenario for which an optimal rate was being determined), the maximum rate observed at each well over this time period (see Table 4-2) was assigned as an upper limit on well rate. This is conservative, because some wells may be actually be capable of producing more water. For some wells, the assigned upper limit is less than the original design rate, which was determined on the basis of groundwater modeling.

Limiting the Number of New Wells Selected:

For some hydraulic optimization scenarios, integer constraints (see section 3.1.3) were specified, to allow the number of selected wells to be limited.

4.2.3 Objective Function

The objective function is "minimize total pumping in gpm". To achieve this, each pumping rate variable was multiplied by an objective function coefficient of -0.005194. The value of the coefficient converts from MODFLOW units (ft^3/d) into gpm, and the negative value of the coefficient accounts for the fact that pumping rates in MODFLOW are negative. By multiplying the negative MODFLOW rates by a negative objective function coefficient, the use of the term "minimize" becomes straightforward for the objective function.

For this site, the objective function is not based directly on cost. However, impacts on annual O&M costs resulting from pumping rate modifications are easily evaluated, external to the hydraulic optimization algorithm. As discussed in Volume 1, the most significant annual cost of this system is steam (approximately $2000/yr/gpm). Up-front costs associated with new wells are estimated at $20K/well.

4.3 CONTAINMENT SOLUTIONS, ORIGINAL WELLS

4.3.1 Scenario 1: Minimize Pumping at Original 18 BW Wells, Design Rates at SW and OW Wells

The first hydraulic optimization formulation considers all of the well locations associated with the original design. Rates at the SW wells and OW wells are fixed at the original design rates (see Table 4-2). The goal is to determine if hydraulic optimization suggests improved rates at the BW wells, relative

to the original design (i.e., had hydraulic optimization been applied during the design, would a better solution have been determined, using the same well locations?).

As previously discussed, a head difference of 0.01 feet is imposed between the river and adjacent cells in the aquifer. The target containment zone is identical to the containment zone associated with the original design (as determined with the model), and the upper limit on well rate at each BW well is based on the maximum rate observed between June 1997 and November 1997.

The mathematical optimal solution for this scenario is summarized below:

	Design Rate (gpm)	Mathematical Optimal Solution (gpm)
BW wells	549	273
SW wells	171	171 (fixed)
OW wells	132	132 (fixed)
Total System:	852	576

The mathematical optimal solution includes 17 of the 18 original BW well locations, and represents a reduction of 276 gpm at the BW wells (over 50%). Using the simple relationship between pumping rate and total annual cost based on steam ($2000/yr/gpm), a reduction of 276 gpm corresponds to a reduction in annual O&M of $552K/yr.

The same hydraulic optimization scenario was then solved with additional constraints limiting the number of well locations that may be selected. Results are summarized below:

# of BW Wells Allowed	Mathematical Optimal Solution, Total Pumping at BW Wells (gpm)
17+	273
16	274
15	274
14	275
13	279
12	283
11	288
10	297
9	infeasible

Hydraulic optimization makes this type of analysis easy to perform, and the results suggest that some of the 18 BW wells in the original design were not necessary. For instance, reducing the number of wells selected from 17 to 14 only increases the pumping rate required for containment by 1 gpm ($2000/yr in steam costs).

The results presented above are significant. Had hydraulic optimization been applied when the pump-and-treat system was originally designed, the design pumping rates at the BW wells might have been cut in half (potential savings in steam costs of over $500K/yr), and the number of BW wells would likely have been reduced from 18 wells to 14 wells, and perhaps to as little as 10 or 11 wells. This might have saved $100K or more in Up-Front costs associated with the installation of those wells.

4.3.2 Scenario 2: Minimize Pumping at Original 18 BW Wells, No Pumping at SW and OW Wells

This optimization formulation is similar to the previous formulation, except that rates at the SW wells and OW wells are fixed at zero. This represents a scenario where containment at the river is the only priority. The goal is to use hydraulic optimization to quantify the "containment efficiency" of the SW and OW wells in the original design, which allows a more meaningful evaluation of the additional costs associated with the SW and OW wells.

The mathematical optimal solution for this scenario is summarized below:

	Mathematical Optimal Solution, Scenario 2 (gpm)	Mathematical Optimal Solution, Scenario 1 (gpm)
BW wells	409	273
SW wells	0 (fixed)	171 (fixed)
OW wells	0 (fixed)	132 (fixed)
Total System:	409	576

When 303 gpm of pumping is added at the SW and OW wells, a corresponding decrease of 136 gpm can potentially be implemented at the BW wells. As discussed in Section 3.3.3, this can be expressed as "containment efficiency" of the combined pumping at the SW and OW wells:

$$\text{containment efficiency} = 136/303 = 45\%$$

This type of analysis, which is straightforward with hydraulic optimization, is very significant. When pumping is added upgradient of the containment wells, significant cost savings can be realized by implementing a corresponding rate reduction at the containment wells. In this case, the addition of 303 gpm at the SW and OW wells, at $2000/yr/gpm, would translate into $606K/yr in added steam costs. However, by implementing a corresponding reduction of 136 gpm at the BW wells, the net increase in pumping rate would only be 167 gpm, which would translate into $334K in added steam costs. Therefore, evaluating the "containment efficiency" could yield savings of $272K/yr for this particular example.

4.4 CONTAINMENT SOLUTIONS, CURRENT WELLS

4.4.1 Scenario 3: Minimize Pumping at Current 23 BW Wells, No Pumping at SW or OW Wells

This optimization formulation is similar to Scenario 2 (rates at the SW wells and OW wells are fixed at zero), but this scenario includes the five BW wells installed after the original system was installed. The locations of the five additional wells are indicated on Figure 4-5. The goal is to use hydraulic optimization to quickly determine if the five additional well locations significantly reduce the amount of pumping required for containment at the river.

The mathematical optimal solution for this scenario is summarized below:

	Mathematical Optimal Solution, Scenario 2 (gpm)	Mathematical Optimal Solution, Scenario 3 (gpm)
BW wells	409	399
SW wells	0 (fixed)	0 (fixed)
OW wells	0 (fixed)	0 (fixed)
Total System:	409	399

In this case, addition of the five additional wells has only a small impact. Of course, it is quite possible that the addition of wells in other locations might have a greater impact on the amount of pumping required for containment, and hydraulic optimization could provide an efficient evaluation of many other locations (that analysis was not performed as part of this demonstration).

4.4.2 Scenario 4: Same as Scenario 3, But Varying Limit on Head Adjacent to the River

This optimization formulation is similar to Scenario 3, but the head limits imposed adjacent to the river are varied. In Scenario 3, an inward head difference of 0.01 ft from the river to the aquifer is mandated, by assigning a head limit of 301.99 ft MSL at cells adjacent to the river (the river is represented with specified head of 302.00 ft MSL). In this scenario, the following alternative head limits are imposed in cells adjacent to the river:

302.00 ft MSL (0.00 ft head difference)
302.95 ft MSL (0.05 ft head difference)
392.90 ft MSL (0.10 ft head difference)

The mathematical optimal solutions for this scenario are summarized below:

Head Difference Limit Imposed (ft)	Mathematical Optimal Solution (gpm)	Annual Steam Cost ($/yr)
0.00	396	$792K
0.01	399	$798K
0.05	421	$842K
0.10	458	$916K

*Note: annual steam cost approximated as $2000/*yr/gpm

The results illustrate that, as limits representing containment are made more conservative, the amount of pumping required for containment increases. In this particular formulation, imposing a head difference limit of 0.10 ft rather than 0.0 ft leads to a more conservative pumping design, with an additional steam cost of more than $100K/yr. Hydraulic optimization allows an efficient evaluation of such tradeoffs (this analysis would be difficult or impossible by trial-and-error).

4.5 SCENARIO 5: SOLUTIONS WITH ADDITIONAL CORE ZONE WELLS

This optimization formulation considers the existing 23 BW wells (i.e., as in Scenario 3), plus five existing SW wells (SW-1920, SW-1921, SW-1926, SW-1942, SW-1943), and four additional wells in areas of high contaminant concentrations. These locations are indicated on Figure 4-5. All other SW and OW wells are not pumped. The goal is to determine if the "containment efficiency" of these nine core zone wells (the five SW wells and the four new wells) is greater than the "containment efficiency" of the original SW and OW wells (previously determined to be 45% in Section 4.3.2). The reason for improved containment efficiency would be that some of the OW wells in the original design are not directly upgradient of the containment wells near the river.

Two variations were evaluated:

(1) add 5 gpm at each of the nine core zone wells, for a total of 45 gpm; and

(2) add 10 gpm at each of nine core zone wells, for a total of 90 gpm.

The hydraulic optimization results are intended to quantify potential reductions in rates that can be implemented at the BW wells, while maintaining containment.

The mathematical optimal solutions are summarized below:

	Mathematical Optimal Solution, Scenario 3 (gpm)	Mathematical Optimal Solution, 45 gpm added in Core Zone (gpm)	Mathematical Optimal Solution, 90 gpm added in Core Zone (gpm)
BW wells	399	374	349
Core Zone Wells	0 (fixed)	45	90
Total System:	399	419	439

When 45 gpm of pumping is added in the core zone, a corresponding decrease of 25 gpm can potentially be implemented at the BW wells:

containment efficiency = 25/45 = 56%

When 90 gpm of pumping is added in the core zone, a corresponding decrease of 50 gpm can potentially be implemented at the BW wells:

containment efficiency = 50/90 = 56%

As expected, the containment efficiency of 56 percent is higher than the containment efficiency of 45 percent determined for the SW and OW wells in the original design. This is presumably due to the fact that combined locations of these wells are more favorable for containment than the combined locations of the original SW and OW wells.

As previously discussed, this type of analysis is important when additional pumping is considered upgradient of the containment wells, because implementing a corresponding rate reduction at the containment wells can result in considerable savings. Without hydraulic optimization, quantifying the potential rate reduction at the containment wells would be difficult, if not impossible. In this case, the addition of 90 gpm at the core zone wells, at $2000/yr/gpm, would translate into $180K/yr in added steam costs. However, by implementing a corresponding reduction of 50 gpm at the BW wells, the net increase in pumping rate would only be 40 gpm, which would translate into $80K in added steam costs. Therefore, evaluating the "containment efficiency" could yield savings of $100K/yr for this particular scenario.

4.6 DISCUSSION & PREFERRED MANAGEMENT SOLUTION

Interesting results from the hydraulic optimization evaluations for this site include the following:

- had hydraulic optimization been applied when the pump-and-treat system was originally designed, the design pumping rates at the BW wells might have been cut in half (potential savings in steam costs of over $500K/yr), and the number of BW wells would likely have been reduced from 18 wells to 14 wells, and perhaps to as few as 10 or 11 wells (potential savings of $100K or more in Up-Front costs associated with the installation of those wells);

- as limits representing containment at the river are made more conservative, the amount of pumping required for containment increases (in this particular formulation, imposing a head difference limit of 0.10 ft rather than 0.0 ft leads to a more conservative pumping design, with an additional steam cost of more than $100K/yr);

- core zone wells at this site have a "containment efficiency" of 45% to 55%, such that each increase of 10 gpm in the core zone can be partially offset with approximately a 5 gpm reduction at containment wells (the containment efficiency improves with better placement of wells);

- for cases where core zone pumping is considered, implementing corresponding rate reductions at containment wells (based on the "containment efficiency") will potentially yield significant savings (as much as $100K/yr or more);

All of these analyses were efficiently conducted with hydraulic optimization techniques. In most cases, these types of analyses are difficult (if not impossible) to comprehensively perform with a trial-and-error approach. This is because of the large number of well locations being considered. With a trial-and-error approach, only a small number of well rate combinations can be evaluated with the simulation model, whereas hydraulic optimization allows all potential combinations of well rates to be rigorously evaluated for each scenario.

According to the hydraulic optimization results, a preferred management strategy might include pumping rate reductions at the BW wells. However, the groundwater flow model at this site is quite simplified, and additional effort in refining the groundwater flow model (and subsequent re-analysis with hydraulic optimization) may be worthwhile. If pumping at the SW and OW wells is reduced (or terminated), corresponding pumping rate increases will be required at the BW wells to maintain containment (for every 10 gpm reduced, approximately 5 gpm will need to be added at the BW wells.

A significant management issue at this site relates to the net benefits provided by core zone wells (e.g., the SW wells). Contaminant levels at this site are high, and residual NAPL in the soil column is likely. Therefore, cleanup at this site may never be achieved via pump-and-treat (i.e., accelerated mass removal from groundwater may not provide any tangible benefits). Although hydraulic optimization does not incorporate predictions of future contaminant concentrations, it does allow the costs of core zone pumping to be quantified, in conjunction with the "containment efficiency". Assuming steam costs of $2000/yr/gpm, the increased annual cost for each 50 gpm in the core zone is approximately $50K/yr (assuming the corresponding pumping rate reduction of 25 gpm at the containment wells indicated by the "containment efficiency"). These costs can be assessed with respect to the perceived benefits associated with these core zone wells.

For this site, the hydraulic optimization results potentially lead to large cost savings ($millions over a 20 to 30 year planning horizon). This is partly due to the fact that the remediation technology at this site (steam stripping) is expensive. A management strategy at this site might also include an evaluation of potential alternatives to the steam-stripping technology currently utilized.

5.0 CASE #2: TOOELE

5.1 SITE BACKGROUND

5.1.1 Site Location and Hydrogeology

The facility is located in Tooele Valley in Utah, several miles south of the Great Salt Lake. (see Figure 5-1). The aquifer of concern generally consists of alluvial deposits. However, there is an uplifted bedrock block at the site where groundwater is forced to flow from the alluvial deposits into fractured and weathered rock (bedrock), and then back into alluvial deposits.

The unconsolidated alluvial deposits are coarse grained, consisting of poorly sorted clayey and silty sand, gravel, and cobbles eroded from surrounding mountain ranges. There are several fine-grained layers assumed to be areally extensive but discontinuous, and these fine-grained layers cause vertical head differences between adjacent water-bearing zones. Bedrock that underlies these alluvial deposits is as deep as 400 to 700 feet. However, in the vicinity of the uplifted bedrock block, depth to bedrock is shallower, and in some locations the bedrock is exposed at the surface.

Depth to groundwater ranges from 150 to 300 ft. The hydraulic conductivity of the alluvium varies from approximately 0.13 to 700 ft/day, with a representative value of approximately 200 ft/day. In the bedrock, hydraulic conductivity ranges from approximately 0.25 ft/day in quartzite with clay-filled fractures to approximately 270 ft/day in orthoquartzite with open, interconnected fractures.

Groundwater generally flows to the north or northwest, towards the Great Salt Lake (see Figure 5-2). Recharge is mostly derived from upgradient areas (south of the facility), with little recharge from precipitation. Gradients are very shallow where the water table is within in the alluvial deposits. There are steep gradients where groundwater enters and exits the bedrock block, and modest gradients within the bedrock block. There is more than 100 ft of head difference across the uplifted bedrock block. This suggests that the uplifted bedrock area provides significant resistance to groundwater flow. North (i.e., downgradient) of the uplifted bedrock block, the vertical gradient is generally upward.

5.1.2 Plume Definition

The specific plume evaluated in this study originates from an industrial area in the southeastern corner of the facility, where former operations (since 1942) included handling, use, and storage of TCE and other organic chemicals. Groundwater monitoring indicates that the primary contaminant is TCE, although other organic contaminants have been detected. TCE concentrations in the shallow (model layer 1) and deep (model layer 2) portions of the aquifer are presented on Figure 5-2. Concentrations are significantly lower in the deeper portions of the aquifer than in shallow portions of the aquifer. Also, the extents of the shallow and deep plumes do not directly align, indicating a complex pattern of contaminant sources and groundwater flow. Continuing sources of dissolved contamination are believed to exist.

5.1.3 Existing Remediation System

A pump-and-treat system has been operating since 1993. The system consists of 16 extraction wells and 13 injection wells (see Figure 5-3 for well locations). An air-stripping plant, located in the center of the plume, is capable of treating 8000 gpm of water. It consists of two blowers operated in parallel, each capable of treating 4000 gpm. Sodium hexametaphosphate is added to the water prior to treatment, to prevent fouling of the air stripping equipment and the injection wells. Treated water is discharged via gravity to the injection wells. Approximate costs of the current system are presented in Table 5-1 (see Volume 1 for a more detailed discussion of costs).

Based on the well locations and previous plume delineations, the original design was for cleanup. At the time the system was installed, the source area was assumed to be north of the industrial area (near a former industrial waste lagoon). Subsequently, it was determined that the source area extended far to the south (in the industrial area). As a result, the current system essentially functions as a containment system (there are no extraction wells in the area of greatest contaminant concentration).

Historically, the target containment zone has been defined by the 5-ppb TCE contour. Given the current well locations, anticipated cleanup time is "a very long time". However, a revised (i.e., smaller) target containment zone is now being considered, based on risks to potential receptors. A revised target containment zone might correspond to the 20-ppb or 500ppb TCE contour.

5.1.4 Groundwater Flow Model

A three-dimensional, steady-state MODFLOW model was originally constructed in 1993 (subsequent to the design of the original system), and has been recalibrated on several occasions (to both non-pumping and pumping conditions). The current model has 3 layers, 165 rows, and 99 columns. Cell size is 200 ft by 200 ft. Model layers were developed to account for different well screen intervals, and are assigned as follows:

Layer 1:	0 to 150 ft below water table
Layer 2:	150 to 300 ft below water table
Layer 3:	300 to 600 ft below water table

Boundaries include general head conditions up- and down-gradient, no flow at the sides and the bottom. The model has historically been used as a design tool, to simulate drawdowns and capture zones (via particle tracking) that result from specified pumping and injection rates.

The current groundwater model is a useful tool for approximating drawdowns and capture zones. However, the following are noted: (1) near the source area, simulated flow directions are not consistent with the shape of the observed plume; and (2) the bedrock block is a very complex feature, and accurate simulation of that feature is very difficult.

5.1.5 Goals of a Hydraulic Optimization Analysis

A screening analysis performed for this site (see Volume 1) suggests that significant savings (millions of dollars over 20 years) might be achieved by reducing the pumping rate associated with the present system, even if five new wells (at $300K/well) were added. In that screening analysis, a pumping rate reduction of 33 percent was assumed. This could potentially be accomplished by:

- optimizing rates to achieve more efficient containment of the 5-ppb plume; and/or
- reducing the size of the target containment zone (if independently demonstrated to maintain protection of human health and the environment).

Therefore, the goals of the optimization analysis are:

(1) determine the extent to which pumping rates can actually be reduced at this site, with and without the addition of new wells, given the current target containment zone (5-ppb plume);

(2) quantify cost reductions associated with these achievable pumping rates;

(3) quantify the tradeoff between the number of wells operating and the total pumping rate (and/or cost) required for containment;

(4) quantify potential pumping rate and cost reductions associated with a modified target containment zone (i.e., the 20-ppb plume or the 50–ppb plume).

Mathematical formulations for achieving these goals are presented below. Then "mathematical optimal solutions" for these formulations are presented, and discussed within the context of a "preferred management solution".

5.2 COMPONENTS OF MATHEMATICAL FORMULATION

5.2.1 Representation of Plume Containment

A combination of head difference constraints, gradient constraints, and relative gradient constraints were used to represent plume containment (see section 3.1.1 for an overview of the approach). For this site, constraints representing containment were developed for four different plume boundaries:

- shallow 5-ppb plume (Figure 5-4);
- deep 5-ppb plume (Figure 5-5);
- shallow 20-ppb plume (Figure 5-6); and
- shallow 50-ppb plume (Figure 5-7).

Along the northeast boundary of the shallow 5-ppb plume, constraints were applied along a "smoothed" approximation of the plume boundary, rather than the actual plume boundary (which has an irregular shape). Also, constraints representing plume containment were only applied north of the bedrock block (for the 5-ppb and 20-ppb plume), near the toe of each plume. This was done because containment at the toe of each plume was the focus of these efforts. Assigning plume containment constraints in the vicinity of the bedrock block may have caused infeasible solutions to result, simply because the simulation model is imperfect in that highly complex region.

Constraints representing plume containment were not applied to the deep 20-ppb plume. Preliminary simulations indicated that wells containing the shallow 20-ppb plume would also contain the deep 20-ppb plume. For optimization simulations based on containment of the 20-ppb plume, this simplifying assumption was verified with particle tracking simulations.

A summary of the number of constraints used to represent containment for each plume is provided below:

Plume	Number of Head Difference Limits	Number of Gradient Limits	Number of Relative Gradient Limits
5 ppb, shallow	3	38	19
5 ppb, deep	9	22	11
20 ppb, shallow	1	16	8
50 ppb, shallow	9	14	7

5.2.2 Representation of Wells

Multi-aquifer wells:

Presently, 16 extraction wells and 13 injections wells are in operation (see Section 5.1.3). Some of these wells are multi-aquifer wells. In MODFLOW, the amount of water discharged from a multi-aquifer well in each model layer is weighted by the relative transmissivity of each layer at the specific grid block. Balance constraints were specified in MODMAN (see section 3.1.2) to preserve the ratio of pumping between model layers for multi-aquifer wells, as follows:

Well	MODMAN Well Numbers	Relationship	
E-6	Q8 (Layer 1), Q9 (Layer 2)	Q8 - 4.88Q9 = 0	(i.e., Q8/Q9 = 4.88)
E-8	Q10 (Layer 1), Q11 (Layer 2)	Q10 - 1.50Q11 = 0	(i.e., Q10/Q11 = 1.50)
E-9	Q12 (Layer 1), Q13 (Layer 2), Q14 (Layer 3)	Q12 - 0.20Q13 = 0 Q12 - 0.56Q14 = 0	(i.e., Q12/Q13 = 0.20) (i.e., Q12/Q14 = 0.56)
E-10	Q15 (Layer 1), Q16 (Layer 2)	Q15 - 0.15Q16 = 0	(i.e., Q15/Q16 = 0.15)
E-14	Q20 (Layer 1), Q21 (Layer 2)	Q20 - 0.33Q21 = 0	(i.e., Q20/Q21 = 0.33)
E-15	Q22 (Layer 1), Q23 (Layer 2)	Q22 - 4.00Q23 = 0	(i.e., Q22/Q23 = 4.00)
I-2	Q25 (Layer 1), Q26 (Layer 2)	Q25 - 3.54Q26 = 0	(i.e., Q25/Q26 = 3.54)
I-6	Q30 (Layer 1), Q31 (Layer 2)	Q30 - 1.22Q31 = 0	(i.e., Q30/Q31 = 1.22)
I-7	Q32 (Layer 1), Q33 (Layer 2)	Q32 - 1.22Q33 = 0	(i.e., Q32/Q33 = 1.22)
I-9	Q35 (Layer 1), Q36 (Layer 2)	Q35 - 1.50Q36 = 0	(i.e., Q35/Q36 = 1.50)
I-10	Q37 (Layer 1), Q38 (Layer 2)	Q37 - 3.00Q38 = 0	(i.e., Q37/Q38 = 3.00)
I-13	Q41 (Layer 1), Q42 (Layer 2)	Q41 - 4.00Q42 = 0	(i.e., Q41/Q42 = 4.00)

New Well Locations Considered:

Depending on the scenario, additional potential well locations were considered as follows:

Plume to Contain	Additional Well Locations Considered
5-ppb shallow	20 wells in layer 1 (see Figure 5-4)
5-ppb deep	18 wells in layer 2 (see Figure 5-5)
20-ppb shallow	6 wells in layer 1, and 1 well in layer 2 (see Figure 5-6)
50-ppb shallow	20 wells in layer 1 (see Figure 5-7)

The additional well in layer 2 for scenarios based on containment of the shallow 20-ppb plume is located near the toe of the deep 20-ppb plume. This allows consideration of solutions with a fixed pumping rate at that well, to increase efficiency of containing and/or remediating that portion of the plume.

Well Rate Limits:

Maximum pumping rates for all new wells was specified as 500 gpm. For existing wells extraction and injection wells, operational history was considered in specifying maximum rates. If operation rate on April 6, 1998 (provided earlier) was less than 500 gpm, then 500 gpm was specified as the maximum rate. If operation rate on April 6, 1998 (provided earlier) was greater than 500 gpm, then the rate observed on that date was set as the maximum rate. For multi-aquifer wells, an additional calculation was made to determine the maximum rate allowed in one specific model layer, based on the maximum rate allowed for the total well.

Example: *Well E-10, max rate = 714 gpm*

Well names in MODMAN:	Q15 (Layer 1), Q16 (layer 2)
Well rate relationship:	$Q15/Q16 = 0.15$ (i.e., $Q15 = 0.15Q16$)
Max rate for total well:	$Q15 + Q16 \leq 714$ gpm
Substitute for Q15:	$0.15Q16 + Q16 \leq 714$ gpm
Determine limit for Q16	$Q16 \leq 621$ gpm

Limiting the Number of New Wells Selected:

In simulations where additional wells were considered, integer constraints (see section 3.1.3) were specified, to allow the number of new wells to be limited.

Balance Between Total Pumping and Total Injection

The remediation system at Tooele includes reinjection of treated groundwater. Constraints were included so that total injection rate cannot exceed total pumping rate (which is not feasible for this system).

5.2.3 Objective Function Based on Minimizing Total Pumping

For most of the optimization simulations performed for this site, the objective function is "minimize total pumping in gpm". To achieve this, each pumping rate variable was multiplied by an objective function coefficient of -0.005194. The value of the coefficient converts from MODFLOW units (ft^3/d) into gpm, and the negative value of the coefficient accounts for the fact that pumping rates in MODFLOW are negative. By multiplying the negative MODFLOW rates by a negative objective function coefficient, the use of the term "minimize" becomes straightforward for the objective function.

For solutions with this objective function, associated "Total Managed Cost" was calculated external to the optimization algorithm. Managed costs refers to those aspects of total cost that are related to the variables being optimized (i.e., the well rates). Simple cost functions were established as follows:

managed Up-front Cost ($) = number of new wells * $300K/well
managed Annual Cost ($) = total pumping rate (gal/min) * $150/yr/gpm

The relationship for "managed annual cost" is a simplified and approximate relationship, based on the costs of electricity and sodium hexametaphosphate in the current system (which are related to total pumping rate), and an approximate rate of 8000 gpm for the present system:

$1,000,000/yr: electric
$ 200,000/yr: sodium hexametaphosphate

$1.2M/yr for 8000 gpm = $150/yr/gpm

"Total Managed Cost", combines the "Up-Front Costs" with the "Total of Annual Costs" over a specific time horizon (20 yrs), assuming a specific discount rate (5%). These calculations are performed in a spreadsheet. An example is provided in Table 5-2.

5.2.4 Objective Function Based on Minimizing Total Cost

For some optimization simulations, the cost functions described above were incorporated directly into the objective function. The goal was to minimize "Total Managed Cost" (Net Present Value, or NPV) over a 20-year time horizon, assuming a discount rate of 5%. The objective function takes the following form:

$$\text{Min} \sum_{i=1,n} c_i Q_i + \sum_{j=1,m} d_j I_j$$

where:

n = number of wells
c_i = coefficient for annual costs due to pumping rate at well i
Q_i = pumping rate at well i
m = number of potential new wells
d_j = additional cost incurred if new well j is selected (e.g., well installation cost)
I_j = 0 if new well j is not selected, 1 if new well j is selected

The coefficient c_i is \$1963/gpm, which represents "Managed Annual Cost" of \$150/yr/gpm summed over a 20 year time horizon, assuming a 5% discount rate (in MODMAN, the coefficient c_i is further multiplied by -0.005194, to convert from MODFLOW (ft^3/d) into gpm, and to account for the fact that pumping rates are negative in MODFLOW). The coefficient d_j is \$300K, which is the anticipated up-front cost of each new well.

Note that the MODMAN input file does not currently permit coefficients d_j to be entered into the objective function. To solve these problems, appropriate coefficients were manually added to the MPS file generated by MODMAN, prior to solution with LINDO (see Appendix H for an overview of modifying linear or mixed-integer programs generated by MODMAN).

5.3 CONTAINING THE 5-PPB TCE PLUME, MINIMIZE TOTAL PUMPING

5.3.1 Existing Wells (Shallow and Deep Plumes)

The first hydraulic optimization simulation considers containment of both the shallow 5-ppb plume and the deep 5-ppb plume (i.e., neither is allowed to expand beyond the present extent). Only existing well locations are considered. The objective function is to minimize total pumping.

The hydraulic optimization results indicate that the problem is infeasible. The constraints representing plume containment for both the shallow and deep 20-ppb plumes cannot all be satisfied, given the locations of the existing wells and the limits placed on rate at each well. This is consistent with particle tracking results for a simulation of the existing system, which shows some water within the shallow 5-ppb plume is not captured (see Figure 5-8). According to site managers, however, adequate remediation is believed to be occurring in areas near the toe of the plume where capture is not indicated by the model.

Another hydraulic optimization simulation was performed, with the limit on each existing well raised to 2000 gpm. Again, the result indicated that the problem as formulated is mathematically infeasible, given the groundwater flow model and the constraint set imposed.

5.3.2 Additional Wells (Shallow and Deep Plumes)

This hydraulic optimization formulation considers the same containment zone (i.e., both the shallow 5-ppb plume and deep 5-ppb plume). However, 20 additional well locations are considered in the shallow zone (see Figure 5-4), and 18 additional well locations are considered in the deep zone (see Figure 5-5). Again, the objective is to minimize total pumping. Mathematical optimal solutions (i.e., for minimum total pumping rate) were determined for different limits on the number of new wells. For each of these mathematical optimal solutions, Total Managed Cost (see section 5.2.3) was calculated, external to the optimization algorithm. The results are as follows:

# New Wells Allowed	Minimum Pumping Rate (gpm)	# Existing Wells Selected	Total Managed Cost, ($ NPV) (20 yrs, 5% discount)	Best Cost Solution
14	4163	3	$12.4M	
13	4178	3	$12.1M	
12	**4200**	**4**	**$11.8M**	*** BEST ***
11	4742	4	$12.6M	
10	4907	6	$12.6M	
9	5236	7	$13.0M	
8	5553	9	$13.3M	
7	5941	9	$13.7M	
Current System	*7500*	*15*	*$14.7M*	

Adding more than fourteen new wells does not yield a further reduction in total pumping. As the number of new wells is decreased, total pumping rate required for containment increases.

With the addition of fourteen new wells, containment of both the shallow 5-ppb plume and deep 5-ppb plume can be achieved with total pumping of 4163 gpm (a reduction of nearly 45% from the current pumping rate of 7500 gpm). Interestingly, the solution that minimizes total pumping does not minimize Total Managed Cost. This is because the benefits of reduced pumping rate afforded by two additional wells (the thirteenth and fourteenth) are not great enough to offset the high up-front costs of those additional wells ($300K/well). Particle tracking results depicting capture in the shallow and deep zones for the solution with 4163 gpm are presented in Figures 5-10 and 5-11).

5.3.3 Quantifying The Benefits of Reinjecting Treated Water

This formulation is the same as described in the previous section, but reinjection is not permitted (conceptually, all water is discharged further downgradient, such that plume capture is not impacted by the reinjection. The mathematical optimal solution (i.e., minimum pumping rate) for this formulation is:

Without Reinjection: 5237 gpm
With Reinjection: 4163 gpm

With respect to containment of the 5-ppb plumes, these results indicate that reinjection of treated water at existing locations, if optimally distributed, reduces pumping required for containment by 20 percent. Presumably, the benefits of reinjection at existing injection wells will decrease if the size of the target containment zone is reduced (reinjection would be further downgradient from the edge of the target containment zone).

5.3.4 Additional Wells (Shallow Plume Only)

This formulation is the same as described in section 5.3.2, but only the shallow 5-ppb plume is considered. The constraints representing containment of the deep 5-ppb plume are removed, and the 18 additional well locations in the deep zone are not included (particle tracking can be used to assess the fate of the deep plume for specific solutions determined with this formulation). Mathematical optimal solutions (i.e., for minimum total pumping rate) were determined for different limits on the number of new wells. For each of these mathematical optimal solutions, Total Managed Cost (see section 5.2.3) was calculated, external to the optimization algorithm. The results are as follows:

# New Wells Allowed	Minimum Pumping Rate (gpm)	# Existing Wells Selected	Total Managed Cost, ($ NPV) (20 yrs, 5% discount)	Best Cost Solution
7	**2622**	**2**	**$7.2M**	*** BEST ***
6	2852	3	$7.4M	
5	3127	4	$7.6M	
4	3766	7	$8.6M	
3	4051	6	$8.9M	
2	5873	10	$11.5M	
Current System	*7500*	*15*	*$14.7M*	

Adding more than seven new wells does not yield a further reduction in total pumping. As the number of new wells is decreased, total pumping rate required for containment increases.

With the addition of seven new wells, containment of the shallow 5-ppb plume can be achieved with total pumping of 2622 gpm. This is a reduction of approximately 65% from the current pumping rate of 7500 gpm. For this formulation, the solution that minimizes total pumping also minimizes Total Managed Cost. Particle tracking results depicting capture in the shallow and deep zones for the solution with 2622 gpm are presented in Figures 5-12 and 5-13. There are two major differences between this strategy and the strategy where both the shallow and deep 5-ppb plumes are contained:

- with this strategy, the western portion of the deep 5-ppb plume is not captured by any extraction wells; and
- with this strategy, many particles starting within the deep 5-ppb plume are captured by wells located outside the boundary of that plume.

Total Managed Cost is much lower (i.e., as much as $5M over 20 years, NPV) for this scenario than for the case where both the shallow 5-ppb and deep 5-ppb plumes are contained. This is because the total pumping rate is reduced, and the number of new wells is also reduced. Whether or not this represents an acceptable strategy is ultimately a regulatory issue.

5.4 OBJECTIVE FUNCTION BASED DIRECTLY ON COSTS

This formulation is the same as described in Section 5.2.3 (containment of the shallow 5-ppb plume), but the objective function is based directly on Total Managed Cost (see Section 5.2.4). The optimal solution is:

# New Wells Allowed	Minimum Pumping Rate (gpm)	# Existing Wells Selected	Total Managed Cost, ($ NPV) (20 yrs, 5% discount)
7	2622	2	$7.2M

This is the same solution that was determined with objective function of "Minimized Total Pumping".

5.5 CONTAINING THE 20-PPB AND/OR 50-PPB TCE PLUME

A variety of additional hydraulic optimization formulations were constructed for additional scenarios, to determine solutions that minimize pumping. The formulations included the following:

- contain only the shallow 50-ppb plume;
- contain only the shallow 20-ppb plume;
- contain the shallow 20-ppb plume, plus 500 gpm at a new well near the toe of the deep 20-ppb plume;
- contain the shallow 20-ppb plume, plus add a well pumping 500 gpm at a new well near the toe of the deep 20-ppb plume, plus contain the shallow 50-ppb plume.

For each of these mathematical optimal solutions, Total Managed Cost (see section 5.2.3) was calculated, external to the optimization algorithm. Results for select solutions are as follows:

Scenario	# New Wells	Minimum Pumping Rate (gpm)	# Existing Wells Selected	Total Managed Cost, ($ NPV) (20 yrs, 5% discount)	Capture Zone Figures
contain shallow 50-ppb plume	3	1124	0	$3.1M	5-14 & 5-15
contain shallow 20-ppb plume	2	1377	1	$3.3M	5-16 & 5-17
contain shallow 20-ppb plume, plus 500 gpm at toe of the deep 20-ppb plume	3	1573	1	$4.0M	5-18 & 5-19
contain shallow 20-ppb and 50-ppb plume, plus 500 gpm at toe of the deep 20-ppb plume	6	2620	0	$6.9M	5-20 & 5-21
Current System		*7500*	*15*	*$14.7M*	

Note that existing wells are not generally selected in these solutions, indicating that existing wells are not optimally located for containing the 20-ppb and/or 50-ppb plumes. The only existing well selected for any of these solutions is well E-2-1. Also note that the total number of extraction wells in all of these solutions (ranging from 3 to 6) is less than half the number of wells (15) currently operating.

Particle tracking results depicting capture in the shallow and deep zones for these solutions are presented according to the figure numbers listed above.

5.6 DISCUSSION & PREFERRED MANAGEMENT SOLUTION

Some of the interesting results of the hydraulic optimization analysis are:

- the current pumping at existing wells (7500 gpm) does not meet all constraints representing containment of the shallow 5-ppb and deep 5-ppb plume, and no combination of well rates at existing wells will satisfy those constraints (according to site managers, however, adequate remediation is believed to be occurring in areas near the toe of the plume where capture is not indicated by the model);

- containing the shallow 5-ppb plume and deep 5-ppb plume can be achieved at a substantially reduced pumping rate, with the addition of many new wells (pumping can be reduced to less than 5000 gpm if 10 or more new wells are added);

- even with the high cost of new wells ($300K/well), the addition of 10 or more new wells is cost-effective over 20 years because it permits total pumping rate to be substantially reduced;

- containing only the shallow 5-ppb plume can be achieved at an even lower total pumping rate, with the addition of new wells (as low as 2622 gpm with the addition of 7 wells), but portions of the deep 5-ppb plume are not captured by extraction wells;

- by basing the target containment zone on the 20-ppb plume rather than the 5-ppb plume (if independently demonstrated to maintain protection of human health and the environment), and adding a few new wells, total pumping could be reduced to less than 2000 gpm, with potential savings of $10M or more over 20 years compared to the present system;

- containment of only the 50-ppb plume requires 3 new wells, pumping just over 1100 gpm, and adding these wells to contain the contaminant source, as a stand-alone option, may allow portions of the aquifer down-gradient to clean up via natural attenuation; and

- adding wells to contain the 50-ppb plume (to contain the contaminant source) should also be considered in conjunction with any other strategy, since it increases the potential to clean up the aquifer (and also reduce cost by potentially decreasing the remediation timeframe).

The preferred management strategy at this site is not obvious, and to some extent depends on decisions regarding the size of the target containment zone. However, a preferred management strategy likely includes the addition of several wells close to the source area, to increase the potential for aquifer cleanup. Transport simulations and/or transport optimization may be particularly useful to evaluate cleanup potential for those scenarios.

If containment of the 20-ppb plume (rather than the 5-ppb plume) is independently determined to be protective of human health and the environment, the following strategy (presented earlier) has considerable appeal:

Scenario	# New Wells	Minimum Pumping Rate (gpm)	# Existing Wells Selected	Total Managed Cost, ($ NPV) (20 yrs, 5% discount)
contain shallow 20-ppb and 50-ppb plume, plus 500 gpm at toe of the deep 20-ppb plume	6	2620	0	$6.9M

Six new wells are required (three shallow wells near the source area, two shallow wells near the toe of the shallow 20-ppb plume, and one deep well near the toe of the deep 20-ppb plume). The area of highest concentrations (i.e., the 50-ppb plume) is contained. This increases the likelihood of ultimate (and/or quicker) cleanup in areas downgradient, by containing the source. The shallow 20-ppb plume is contained, and containment/remediation of the deep 20-ppb plume is enhanced by the addition of the new deep well. Total number of wells is reduced from 15 to 6 (60%), relative to the current system. Total pumping rate is reduced from 7500 gpm to 2620 gpm (65%), relative to the current system. Total Managed Cost over a 20-year period (which incorporates the up-front cost of $1.8M for the six new wells) is reduced from $14.7M to $6.9M (53%), relative to the current system.

It is very important to distinguish the benefits of applying hydraulic optimization technology from other benefits that may be achieved simply by "re-visiting" an existing pump-and-treat design. For Tooele, potential pumping reductions and cost savings that result from a change to a smaller target containment zone primarily result from a change in conceptual strategy. The benefit provided by hydraulic optimization is that it allows mathematical optimal solutions for each conceptual strategy to be efficiently calculated (whereas good solutions for each conceptual strategy may be difficult or impossible to achieve with trial-and-error).

The hydraulic optimization analysis indicates that additional wells are required to satisfy constraints representing plume containment for each scenario. However, before new wells are considered, additional analysis might be performed to determine if containment, in those areas not effectively captured by the present system (according to the model), is in fact required to maintain protection of human health and the environment. It is possible that improved solutions with many fewer new wells are possible, if constraints representing plume containment are relaxed in certain critical areas. Additional hydraulic optimization simulations could be performed to assess these options.

6.0 CASE #3: OFFUTT

6.1 SITE BACKGROUND

6.1.1 Site Location and Hydrogeology

The facility is located in Sarpy County, Nebraska, next to the City of Bellevue (see Figure 6-1). The specific plume evaluated in this study is in the Southern Plume within the Hardfill 2 (HF2) Composite Site at Offutt. The principal aquifer at the site consists of unconsolidated sediments resting on bedrock. The aquifer system is heterogeneous and complex. Groundwater flows easterly and southeasterly (see Figure 6-2). Depth to groundwater is generally 5 to 20 ft. The hydraulic conductivity of the alluvium varies significantly with location and depth, due the complex stratigraphy.

6.1.2 Plume Definition

Groundwater monitoring indicates that the primary contaminants are chlorinated aliphatic hydrocarbons (CAH's) including TCE, 1,2-dichloroethene (1,2-DCE), and vinyl chloride. Releases (initially as TCE) formed localized vadose zone and dissolved groundwater plumes. Subsequent groundwater transport from these multiple sources has resulted in groundwater contamination in shallow and deeper portions of the Alluvial Aquifer.

The extent of the Southern Plume is illustrated on Figure 6-3. The core zones are defined as follows:

- shallow zone: upper 20 ft of saturated zone
- shallow-intermediate zone: from 930 ft MSL to 20 ft below water table
- intermediate zone: 910 ft MSL to 930 ft MSL
- deep zone: below 910 ft MSL

The Southern Plume is approximately 2400 ft long, and extends just beyond the southern site boundary.

6.1.3 Existing Remediation System

An interim remediation system is in place, and consists of three wells (see Figure 6-3), pumping a total of 150 gpm:

- one "Toe Well" that is located within the southern plume, at 50 gpm; and
- two wells downgradient of the plume (the "LF wells"), at 100 gpm combined.

The extracted water is discharged to a POTW.

The two LF wells are associated with a landfill located downgradient from the Southern Plume boundary. The LF wells are considered part of the interim system, because they provide a degree of ultimate containment for the plume. However, allowing the plume to spread towards the LF wells is considered to be a negative long-term result.

To prevent further spreading of the Southern Plume, a long term pump-and-treat system has been designed, with the addition of a "Core Well" within the southern plume (see Figure 6-3). The design of the long-term system calls for 200 gpm total, as follows:

- one Toe well that is located within the southern plume, at 50 gpm;
- one Core well that is located within the southern plume, at 50 gpm; and
- two wells downgradient of the plume (the "LF wells"), at 100 gpm combined.

The intent is for the Toe well and Core well to prevent the Southern Plume from spreading beyond it's present extent (rather than allowing the plume to flow towards the LF wells), and also to more effectively contain the source areas (because the core well is located immediately downgradient from the source areas). Under this scenario, the LF wells are not actually providing containment or cleanup for the Southern Plume (in fact, pumping at the LF wells negatively impacts containment of the Southern Plume). The original purpose of the LF wells is not related to remediation of the Southern Plume, and it is hoped that pumping at the LF wells may be reduced (or even terminated) in the future.

6.1.4 Groundwater Flow Model

A three-dimensional, steady-state MODFLOW model was originally constructed in 1996. In addition, a solute transport model was created with the MT3D code (Zheng, 1990). The groundwater models were used to simulate various groundwater extraction scenarios. The current model has 6 layers, 77 rows, and 140 columns. Cell size varies from 25 by 25 ft to 200 x 200 ft. Layer 4 represents an alluvial sand layer, and that layer has historically been evaluated with particle tracking to determine if containment is achieved under a specific pumping scenario.

The solute transport model indicates the following:

- under the interim system, pumping will be required for more than 20 yrs to maintain containment (due to the continuing source), and concentrations near site boundary will be reduced to MCL levels within 10 to 20 yrs;

- under the long-term design, pumping will be required at the Core well for more than 20 yrs to maintain containment (due to the continuing source), but cleanup of the area downgradient of the core well will be achieved in less than 10 yrs.

In each case, some component of pumping is anticipated for "a very long time", due to continuing sources.

6.1.5 Goals of a Hydraulic Optimization Analysis

A screening analysis performed for this site (see Volume 1) suggests that little savings are likely to result from a reduction in total pumping. In that screening analysis, a pumping rate reduction of 33 percent was assumed. For this project, a hydraulic optimization analysis was nevertheless performed, to provide additional examples of hydraulic optimization techniques. The goals of the hydraulic optimization analysis are to:

(1) determine the extent to which pumping rates at the toe of the plume can actually be reduced at this site, with and without the addition of new toe wells;

(2) quantify the "containment efficiency" of the Core Well; and

(3) quantify the extent to which pumping required for containment can be reduced in response to reduced pumping rates at the downgradient LF wells.

Mathematical formulations for achieving these goals are presented below. Then "mathematical optimal solutions" for these formulations are presented, and discussed within the context of a "preferred management solution".

6.2 COMPONENTS OF MATHEMATICAL FORMULATION

6.2.1 Representation of Plume Containment

A combination of head difference constraints, gradient constraints, and relative gradient constraints were used to represent plume containment (see section 3.1.1 for an overview of the approach). For this site, this was accomplished with 4 head difference constraints, 34 gradient constraints, and 17 relative gradient constraints (see Figure 6-4). Along the southern boundary of the plume, constraints were applied along a "smoothed" approximation of the plume boundary, rather than the actual plume boundary (which has an irregular shape). Constraints were applied in layer 4 of the model, consistent with previous particle tracking analyses used to assess the interim and final design system (capture in other model layers was confirmed with particle tracking, external to the optimization algorithm).

6.2.2 Representation of Wells

Multi-aquifer wells:

The baseline scenario includes one Toe Well, one Core Well, and two LF wells. Based on the model layers and the screened interval of the wells, each is a multi-aquifer well. In MODFLOW, the amount of water discharged from a multi-aquifer well in each model layer is weighted by the relative transmissivity of each layer at the specific grid block. Balance constraints were specified in MODMAN (see section 3.1.2) to preserve the ratio of pumping between model layers for the multi-aquifer wells, as follows:

Well	MODMAN Well Numbers	Relationship	
LF Well (PW3)	Q1 (Layer 3), Q2 (Layer 4)	Q1 - 0.44Q2 = 0	(i.e., Q1/Q2 = 0.44)
LF Well (PW4)	Q3 (Layer 3), Q4 (Layer 4)	Q3 - 0.49Q4 = 0	(i.e., Q3/Q4 = 0.49)
Toe Well	Q5 (Layer 4), Q6 (Layer 6)	Q5 - 1.28Q6 = 0	(i.e., Q5/Q6 = 1.28)
Core Well	Q7 (Layer 3), Q8 (Layer 4), Q9 (Layer 6)	Q8 - 9.03Q7 = 0 Q8 - 1.31Q9 = 0	(i.e., Q8/Q7 = 9.03) (i.e., Q8/Q9 = 1.31)

Some scenarios also considered nine additional well locations near the toe of the plume. These were also multi-aquifer wells, assigned in model layers 4 and 6. Balance constraints were also specified in MODMAN for these wells, to preserve the ratio of pumping between model layers. Based on transmissivities in the model, the ratio of 1.28 calculated for the existing Toe Well was also appropriate for these additional wells.

New Well Locations Considered:

For some scenarios, up to nine additional Toe Well locations were considered. These locations are illustrated on Figure 6-4, and were only placed in locations defined as "acceptable for wells" by the installation. As previously discussed, these wells were assigned to model layers 4 and 6 (i.e., multi-aquifer wells).

Well Rate Limits:

Many MODMAN formulations were solved to evaluate the Offutt site. For each formulation, some of the well rates were "fixed". For instance, each of the LF wells might be fixed at 50 gpm for one formulation, and at 40 gpm for the next formulation. Although this can be accomplished by altering the MODMAN input file and re-executing MODMAN for each formulation, it is more efficiently performed by simply adjusting the well rate bounds in the MPS file that was originally created by MODMAN (see Appendix H).

For multi-aquifer wells, an additional calculation was made to determine the maximum rate allowed in one specific model layer, based on the maximum rate allowed for the total well.

Example: *LF Well (PW-3), max rate = 50 gpm*

Well names in MODMAN:	Q1 (Layer 1), Q2 (layer 2)
Well rate relationship:	$Q1/Q2 = 0.44$ (i.e., $Q1 = 0.44Q2$)
Max rate for total well:	$Q1 + Q2 \leq 50$ gpm
Substitute for Q1:	$Q2 + 0.44Q2 \leq 50$ gpm
Determine limit for Q16	$Q2 \leq 34.7$ gpm

Limiting the Number of New Wells Selected:

In some hydraulic optimization scenarios where additional wells were considered, integer constraints (see section 3.1.3) were specified, to allow the number of selected wells to be limited.

6.2.3 Objective Function

The objective function is "minimize total pumping in gpm". To achieve this, each pumping rate variable was multiplied by an objective function coefficient of -0.005194. The value of the coefficient converts from MODFLOW units (ft^3/d) into gpm, and the negative value of the coefficient accounts for the fact that pumping rates in MODFLOW are negative. By multiplying the negative MODFLOW rates by a negative objective function coefficient, the use of the term "minimize" becomes straightforward for the objective function.

6.3 SOLUTIONS FOR MINIMIZING PUMPING AT THE TOE WELL

6.3.1 Core Well @ 50 gpm, LF Wells @ 100 gpm (Current Design)

The current system design assumes total pumping of 100 gpm at the LF wells, and assumes 50 gpm at the Core Well. In the current design, the Toe Well pumps at 50 gpm. The purpose of this initial analysis is to determine if pumping at the Toe Well can be reduced while containment is maintained, given the assumed pumping at the LF wells and the Core Well.

The mathematical optimal solution for this case is very similar to the current design:

	Current Design (gpm)	Mathematical Optimal Solution (gpm)
LF Wells (Fixed)	100	100
Core Well (Fixed)	50	50
Toe Well	50	52
Total rate	200	202

**Note: Rate at LF wells is combined rate at two wells, divided evenly*

The rate at the Toe Well in the mathematical optimal solution is actually higher than in the current design, which is caused by approximations in the constraints representing plume containment.

These results indicate that current system design is essentially optimal, given these well locations and the assumed pumping rates for the LF wells and the Core Well.

6.3.2 Core Well @ 50 gpm, Vary Rate at LF Wells

The installation has indicated that, over time, the pumping rate at the LF wells (located downgradient of the Southern plume) will likely decline. Such decisions may impact management options for containing the Southern Plume.

These hydraulic optimization simulations are performed to determine the extent that pumping can be reduced at the existing Toe Well, if pumping at the LF wells is reduced. In each case, the Core Well is assumed to maintain a pumping rate of 50 gpm. The mathematical optimal solutions are presented below:

Fixed Rate at LF Wells (gpm)	Fixed Rate at Core Well (gpm)	Mathematical Optimal Solution at Toe Well (gpm)	Total Rate (gpm)
100	50	52	202
80	50	47	177
60	50	41	151
40	50	36	126
20	50	31	101
0	50	25	75

**Note: Rate at LF wells is combined rate at two wells, divided evenly*

The results indicate that pumping at the Toe Well can be reduced when pumping at the LF wells is reduced. For each 20 gpm reduction in combined pumping at the LF wells, a 5 gpm reduction in Toe Well pumping can be realized. This is extremely useful information from a management perspective. Each 5 gpm reduction in Toe Well pumping reduces discharge costs by approximately $2000/yr. Therefore, if pumping at the LF wells is reduced from 100 gpm to zero, a corresponding rate reduction of approximately 25 gpm at the existing Toe Well is possible, with a savings of $10,000/yr.

6.3.3 Vary rate at Core Well, LF Wells @ 100 gpm

The current design includes 50 gpm at the Core Well, to accelerate mass removal. In general, containment is most efficient when pumping wells remove water near the toe of the plume. However, pumping in the core of the plume may also contribute to overall plume containment, such that the addition of core pumping may permit pumping near the toe of the plume to be reduced, without compromising plume containment. Hydraulic optimization can be used to quantify that relationship.

For these simulations, the LF wells are assumed to pump at total of 100 gpm (as in the baseline system). The mathematical optimal solutions are as follows:

Fixed Rate at Core Well (gpm)	Mathematical Optimal Solution at Toe Well (gpm)	Total Pumping at Toe Well Plus Core Well (gpm)
50	52	102
40	56	96
30	61	91
20	65	85
10	69	79
0	74	74

The results indicate that for each increase of 10 gpm at the Core Well, required pumping at the Toe Well is decreased by approximately 4.5 gpm. As discussed in Section 3.3.3, this can be expressed as "containment efficiency" of the Core Well:

$$\text{containment efficiency} = 4.5/10.0 = 45\%$$

The results provided by MODMAN allow additional annual costs associated with core well pumping to be quantified. If the Core Well is not pumped, only 74 gpm at is required to contain the plume (in addition to the 100 gpm at the LF wells). If the Core Well is pumped at 50 gpm, and the Toe well pumping is reduced to 52 gpm, a net pumping increase of 28 gpm is incurred. This extra pumping increases discharge costs by approximately $11,000/yr. This is a relatively small cost, considering that accelerated mass removal (and potentially a reduced remediation timeframe for a portion of the plume) is provided by the pumping at the Core Well.

6.3.4 Vary rate at Core Well, LF Wells @ 0 gpm

These simulations are nearly identical to those just presented, except that for these simulations the LF wells are assumed to pump at total of 0 gpm as (instead of 100 gpm). This allows the impacts of the Core Well pumping on total pumping rate to be assessed for conditions that might occur in the future.

The mathematical optimal solutions are as follows:

Fixed Rate at Core Well (gpm)	Mathematical Optimal Solution at Toe Well (gpm)	Total Pumping at Toe Well Plus Core Well (gpm)
50	25	75
40	29	69
30	34	64
20	38	58
10	43	53
0	47	47

These results also indicate that for each increase of 10 gpm at the Core Well, required pumping at the Toe Well is decreased by approximately 4.5 gpm (containment efficiency of 45%). Note these are the same general results as determined for the case where the LF wells are pumping at 100 gpm. This indicates that, in this case, that pumping at the LF wells does not impact the containment efficiency of the Core Well.

6.4 CONSIDER NINE ADDITIONAL WELL LOCATIONS AT PLUME TOE

6.4.1 Solutions for a Single Toe Well

The purpose of these simulations is to determine if a better location for a single Toe Well might have been found if mathematical optimization had been performed during the original design process. In

addition to the existing Toe Well, nine additional locations (referred to as NW-1 through NW-9) were specified as potential well locations. These locations are illustrated in Figure 6.4, and were only placed in locations defined as "acceptable for wells" by the installation. Integer constraints were specified to limit the number of toe wells actively pumping to one (out of 10 potential locations including the existing Toe Well).

Mathematical optimal solutions were determined for each of the following scenarios:

- Core Well = 50 gpm, LF wells = 100 gpm (baseline scenario)
- Core Well = 50 gpm, LF wells = 0 gpm
- Core Well = 0 gpm, LF wells = 100 gpm
- Core Well = 0 gpm, LF wells = 0 gpm

The results are as follows:

Scenario	Mathematical Optimal Solution for Existing Toe Well (gpm)	Mathematical Optimal Solution For Any One of the 10 Toe Wells (gpm)	Reduction in Toe Pumping Using Alternate Well
Core Well = 50 gpm LF Wells = 100 gpm	52 (Existing Toe Well)	38 (NW-4)	14 gpm (28%)
Core Well = 50 gpm LF Wells = 0 gpm	25 (Existing Toe Well	21 (NW-4)	4 gpm (18%)
Core Well = 0 gpm LF Wells = 100 gpm	74 (Existing Toe well)	74 (Existing Toe Well)	0 gpm (0%)
Core Well = 0 gpm LW Wells = 0 gpm	47 (Existing Toe Well)	46 (NW-1)	1 gpm (1%)

*note: percentage reductions in last column calculated with non-rounded values

These results indicate that no single Toe Well location is best for all scenarios. For scenarios without pumping in the core of the plume, the location of the existing Toe Well is essentially optimal. However, for cases where there is pumping at the Core Well, a different location (NW-4) is optimal, with a potential reduction in pumping near the toe of the plume of approximately 4 to 14 gpm (18-28%).

6.4.2 Solutions for Multiple Toe Wells

Figure 6-5 illustrates a variety of mathematical optimal solutions for each of the following scenarios:

- Core Well = 50 gpm, LF wells = 100 gpm
- Core Well = 50 gpm, LF wells = 0 gpm
- Core Well = 0 gpm, LF wells = 100 gpm
- Core Well = 0 gpm, LF wells = 0 gpm

These figures present the optimal total rate at the selected Toe Wells for solutions with 1 to 5 Toe wells. Note that there are diminishing returns (in terms of pumping rate reduction) as more Toe Wells are allowed.

For scenarios with 50 gpm at the Core Well, there is little benefit to increasing the number of wells. For instance, the maximum reduction in total Toe Well pumping afforded by adding one well is approximately 5 gpm, which translates to a savings in discharge costs of approximately $2,000/yr. This does not compare favorably with the up-front costs of installing a new well (approximately $40,000).

For scenarios without pumping at the Core Well, greater reductions in total Toe Well pumping are afforded by adding a second well. Potential pumpage reductions of approximately 15 to 20 gpm are possible by adding a second well, which translates to a savings in discharge costs of $6,000 to $8,000/yr. However, this yields marginal benefits when one considers the up-front costs of installing a new well (approximately $40,000).

6.5 DISCUSSION & PREFERRED MANAGEMENT SOLUTION

For the current system design (a Core Well at 50 gpm, a Toe Well at 50 gpm, and two dowgradient LF wells at a combined rate of 100 gpm), the hydraulic optimization results indicate that the pumping rate at the Toe Well is essentially optimal for achieving containment (given the fixed rates at the other wells). This might be expected, because the benefits of hydraulic optimization are diminished in cases where only a few well locations are evaluated. In those cases, a good modeler may achieve near-optimal (or optimal) solutions by performing trial-and-error simulations.

The existing Toe Well location plus nine additional Toe Well locations were considered with hydraulic optimization, in conjunction with various combinations of well rates assigned for the Core Well and the LF wells. First, only one Toe Well location was allowed. For scenarios without pumping in the core of the plume, the location of the existing Toe Well was essentially optimal. However, for cases with pumping at the Core Well, a different location was optimal, with a potential reduction in pumping near the toe of the plume of approximately 4 to 14 gpm (18-28%). Had hydraulic optimization been performed during the design process, a different Toe Well location may have been selected on the basis of these results. However, the annual savings in discharge costs that would have resulted would have been relatively minor (less than $6K/yr). When selection of two Toe Well locations was allowed, results indicated that potential pumping rate reductions (and corresponding reductions in discharge costs) would be marginal, relative to the costs of installing a new well.

Hydraulic optimization allows sensitivity of mathematical optimal solutions to be quantified with respect to other non-managed stresses. In this case, the pumping rates at the LF wells are managed separately from the plume management wells, yet increased pumping at the LF wells negatively impacts the ability of plume management wells to contain the plume. Results of the hydraulic optimization analyses indicate that, for each 20 gpm reduction at the LF wells, a corresponding reduction of 5 gpm can be implemented at the Toe Well. This is useful information from a management perspective.

The containment efficiency of the Core Well was quantified (45 percent). For each 10 gpm increase at the Core Well, containment can be maintained with a corresponding reduction of 4.5 gpm at the Toe Well. For this site, core zone pumping yields benefits (source area containment, allowing potential cleanup of downgradient portions of the plume). The additional annual cost of operating a core well (due to increased total pumping required for containment) is small at this site, and a strategy that includes a Core Wells seems preferable to a "containment-only" strategy.

The preferred management strategy at this site is to implement the current system design. Little or no benefit would be achieved by adding an additional Toe Well. However, if pumping rates at the LF wells

are reduced in the future, corresponding rate reductions can be made at the existing Toe Well (for each 20 gpm reduction at the LF wells, a corresponding reduction of 5 gpm can be implemented at the Toe Well).

These conclusions are consistent with the screening analysis performed in Volume 1, which indicated that little potential costs savings would result from reductions in pumping rate of as much as 33 percent. The reason is that, at this site, annual O&M costs directly related to pumping rates are quite low (approximately $400/gpm/yr). Therefore, even when improved pumping rate solutions are obtained with hydraulic optimization, the cost benefits are marginal. Nevertheless, the strategies for applying hydraulic optimization demonstrated for this site can be applied at other sites, particularly where net cost benefits are likely to be greater.

7.0 DISCUSSION AND CONCLUSIONS

Hydraulic optimization couples simulations of groundwater flow with optimization techniques such as linear and mixed-integer programming. Hydraulic optimization allows all potential combinations of well rates at specific locations to be mathematically evaluated with respect to an objective function (e.g., minimize total pumping) and series of constraints (e.g., the plume must be contained). The hydraulic optimization code quickly determines the best set of well rates, such that the objective function is minimized and all constraints are satisfied.

For this document, the term "optimization" for pump-and-treat design was refined as follows:

> *Mathematical Optimal Solution.* The best solution, determined with a mathematical optimization technique, for a specific mathematical formulation (defined by a specific objective function and set of constraints); and
>
> *Preferred Management Solution.* A preferred management strategy based on a discrete set of mathematical optimal solutions, as well as on factors (e.g., costs, risks, uncertainties, impediments to change) not explicitly considered in those mathematical solutions.

For this demonstration project, hydraulic optimization was applied at three sites with existing pump-and-treat systems. For each case study, many mathematical formulations were developed, and many mathematical optimal solutions were determined. For each site, a preferred management solution was then suggested. The three sites can be summarized as follows:

Site	Existing Pumping Rate	Cost Per gpm	Potential Savings from System Modification
Kentucky	Moderate	High	$Millions
Tooele	High	Low	$Millions
Offutt	Low	Low	Little or None

At two of the sites (Kentucky and Tooele), pumping solutions were obtained that have the potential to yield millions of dollars of savings, relative to costs associated with the current pumping rates.

In cases where only a few well locations are considered, the benefits of hydraulic optimization are diminished. In those cases, a good modeler may achieve near-optimal (or optimal) solutions by performing trial-and-error simulations. This was demonstrated by the Offutt case study. However, as the number of potential well locations increases, it becomes more likely that hydraulic optimization will yield improved pumping solutions, relative to a trial-and-error approach. This was demonstrated by potential pumping rate reductions suggested by the hydraulic optimization results for the Kentucky and Tooele case studies.

These case studies illustrate a variety of strategies for evaluating pump-and-treat designs with hydraulic optimization. Components of mathematical formulations demonstrated with these case studies include:

Item Demonstrated	Kentucky	Tooele	Offutt
objective function minimizes total pumping	X	X	X
objective function minimizes cost		X	
multi-aquifer wells		X	X
plume containment with head limits	X		
plume containment with head difference limits		X	X
plume containment with relative gradient limits		X	X
integer constraints (limiting # of wells selected)	X	X	X
sensitivity of solutions to # of wells selected	X	X	X
scenario for "containment only"	X	X	X
scenarios with core zone extraction	X	X	X
"containment efficiency" of core zone wells evaluated	X		X
multiple target containment zones		X	
reinjection of treated water		X	
sensitivity of solutions to conservatism of constraints	X		
sensitivity of solution to non-managed stresses			X

For each of the three case studies, an analysis was performed to illustrate the sensitivity of mathematical optimal solutions to limits placed on the number of wells. For each of the three case studies, an analysis was also performed to evaluate changes in the mathematical optimal solution when new well locations were considered. For the Kentucky site, an analysis was performed to illustrate the sensitivity of the mathematical optimal solution to conservatism in the constraints representing plume containment. All of these types of analyses can be efficiently conducted with hydraulic optimization techniques. In most cases, these types of analyses are difficult (if not impossible) to comprehensively perform with a trial-and-error approach. It is important to note that the case studies presented in this report are for facilities with existing pump-and-treat systems. Mathematical optimization techniques can also be applied during initial system design, to generate improved solutions versus a trial-and-error approach.

Hydraulic optimization cannot incorporate simulations of contaminant concentrations or cleanup time. For that reason, hydraulic optimization is generally most applicable to problems where plume containment is the prominent goal. However, two of the case studies (Kentucky and Offutt) illustrate that hydraulic optimization can be used to determine the "containment efficiency" of wells placed in the core zone of a plume. This type of analysis can be performed to compare a "containment only" strategy to a strategy with additional core zone wells (to accelerate mass removal). The "containment efficiency" of the core zone wells, determined with hydraulic optimization, quantifies potential pumping

reductions at containment wells when the core zone pumping is added, such that containment is maintained. These pumping reductions (also difficult or impossible to determine with a trial-and-error approach) can potentially yield considerable savings, as demonstrated for the Kentucky site.

It is very important to distinguish the benefits of applying hydraulic optimization technology from other benefits that may be achieved simply by "re-visiting" an existing pump-and-treat design. In some cases, the underlying benefits associated with a system modification may be primarily due to a modified conceptual strategy. For instance, the Tooele case study includes analyses for different target containment zones. The potential pumping reductions and cost savings that result from a change to a smaller target containment zone primarily result from the change in conceptual strategy. The benefit provided by hydraulic optimization is that it allows mathematical optimal solutions for each conceptual strategy to be efficiently calculated and compared (whereas good solutions for each conceptual strategy may be difficult or impossible to achieve with trial-and-error).

The case studies demonstrate that there are a large variety of objective functions, constraints, and application strategies potentially available within the context of hydraulic optimization. Therefore, the development of a "preferred management solution" for a specific site depends not only on the availability of hydraulic optimization technology, but also on the ability to formulate meaningful mathematical formulations. That ability is a function of the skill and experience of the individuals performing the work, as well as the quality of site-specific information available to them.

These case studies demonstrate ways in which hydraulic optimization techniques can be applied to evaluate pump-and-treat designs. The types of analyses performed for these three sites can be applied to a wide variety of sites where pump-and-treat systems currently exist or are being considered. However, the results of any particular hydraulic optimization analysis are highly site-specific, and are difficult to generalize. For instance, a hydraulic optimization analysis at one site may indicate that the installation of new wells yields little benefit. That result cannot be generally applied to all sites. Rather, a site-specific analysis for each site is required. A spreadsheet-based screening analysis (presented in Volume 1 of this report) can be used to quickly determine if significant cost savings are likely to be achieved at a site by reducing total pumping rate. Those sites are good candidates for a hydraulic optimization analysis.

8.0 REFERENCES AND DOCUMENTS PROVIDED BY SITES

Colarullo, S.J., M. Heidari, and T. Maddock, III, 1984. *Identification of an optimal groundwater strategy in a contaminated aquifer*. Water Resources Bulletin, 20(5): 747-760.

Gorelick, S.M., 1987. *Sensitivity analysis of optimal groundwater contaminant capture curves: spatial variability and robust solutions*, in Solving Groundwater Problems With Models, Nat. Water Well Assoc., Feb. 10-12, 133-146.

Gorelick, S.M., and B.J. Wagner, 1986. *Evaluating strategies for groundwater contaminant plume stabilization and removal*, selected papers in the Hydrologic Sciences, U.S. Geological Survey, Water-Supply Series 2290, 81-89.

Dames & Moore, 1997. *Plantwide Corrective Action Program, Evaluation of Effectiveness, Second Half 1997, Kentucky Site (December 30, 1997)*.

Dames & Moore (date unknown). *Isoconcentration Maps, September 1996* (Draft).

Gorelick, S.M., R.A. Freeze, D. Donohue, and J.F. Keely, 1993. *Groundwater Contamination: Optimal Capture and Containment*, Lewis Publishers, 385 p.

Greenwald, R.M., 1998a. *Documentation and User's Guide: MODMAN, an Optimization Module for MODFLOW, Version 4.0*, HSI GeoTrans, Freehold, New Jersey.

Greenwald, R.M., 1998b. *MODMAN 4.0 Windows-Based Preprocessor, Preprocessor Version 1.0*, HSI GeoTrans, Freehold, New Jersey.

Harbaugh, A.W. and McDonald, M.G., 1996a. *User's documentation for MODFLOW-96, An update to the U.S. Geological Survey modular finite-difference ground-water flow model*, U.S. Geological Survey Open-File Report 96-485, 56 p.

Harbaugh, A.W. and McDonald, M.G., 1996b. *Programmer's documentation for MODFLOW-96, An update to the U.S. Geological Survey modular finite-difference ground-water flow model*, U.S. Geological Survey Open-File Report 96-486, 220 p.

Kleinfelder, Inc. 1998. *Draft, Southeastern Boundary Groundwater Investigation, Report of Findings, Tooele Army Depot (TEAD, Tooele, Utah, Volume 1* (Draft Report, February 13, 1998).

Lefkoff, L.J., and S.M. Gorelick, 1987. *AQMAN: Linear and quadratic programming matrix generator using two-dimensional groundwater flow simulation for aquifer management modeling*, U.S. Geological Survey, Water Resources Investigations Report, 87-4061, 164 pp.

Lefkoff, L.J., and S.M. Gorelick, 1986. *Design and cost of rapid aquifer restoration systems using flow simulation and quadratic programming*, Ground Water, 24(6): 777-790.

Lindo Systems, 1996. *LINDO Users Manual*, Lindo Systems, Chicago, Illinois.

McDonald, M.G., and A.W. Harbaugh, 1988. *A modular three-dimensional finite-difference groundwater flow model*, U.S. Geological Survey, Techniques of Water-Resources Investigations, Book 6, Chapter A1.

Trescott, P.C., et al., 1976. *Finite-difference model for aquifer simulation in two-dimensions with results of numerical experiments*, U.S. Geological Survey, Techniques for Water Resources Investigations, Book 7, Chapter C1, 116-0118.

Woodward-Clyde, 1997. *Draft Feasibility Study, Hardfill 2 Composite Site (SS-40), Offutt Air Force Base, Nebraska* (Draft Report, August 28, 1997)

Woodward Clyde, 1998. *Pre-Draft, Pump Cycling Report, Landfill 4, Offutt Air Force Base, Nebraska* (Pre-Draft Report, August 1998).

Zheng, Chunmiao, 1990. *A modular Three-Dimensional Transport Model for Simulation of Advection, Dispersion, and Chemical Reactions of Contaminants in Groundwater Systems*. S.S. Papadopulos and Associates, Inc.

FIGURES

H012009A.DWG

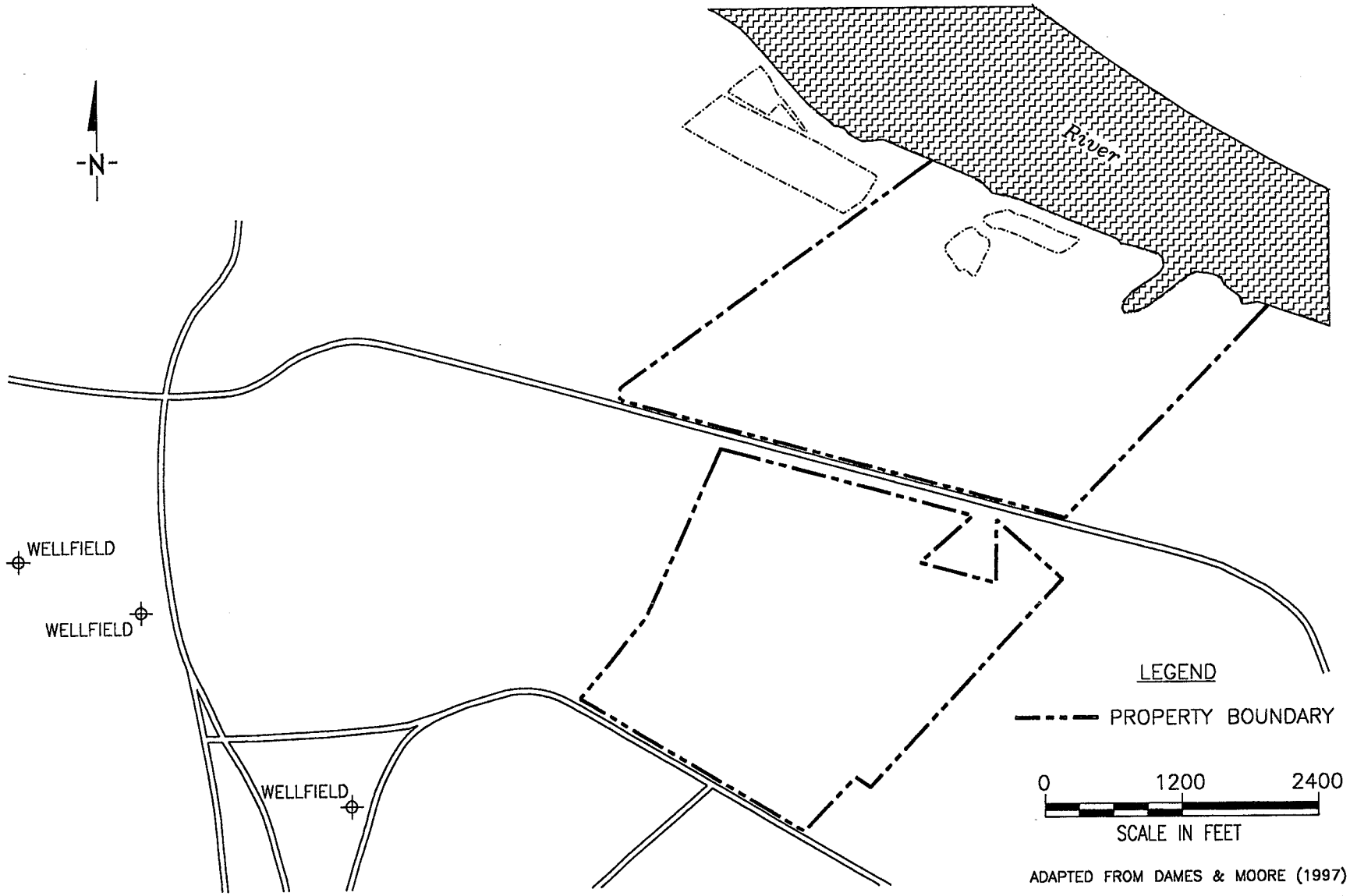


Figure 4-1. Site location map, Kentucky.

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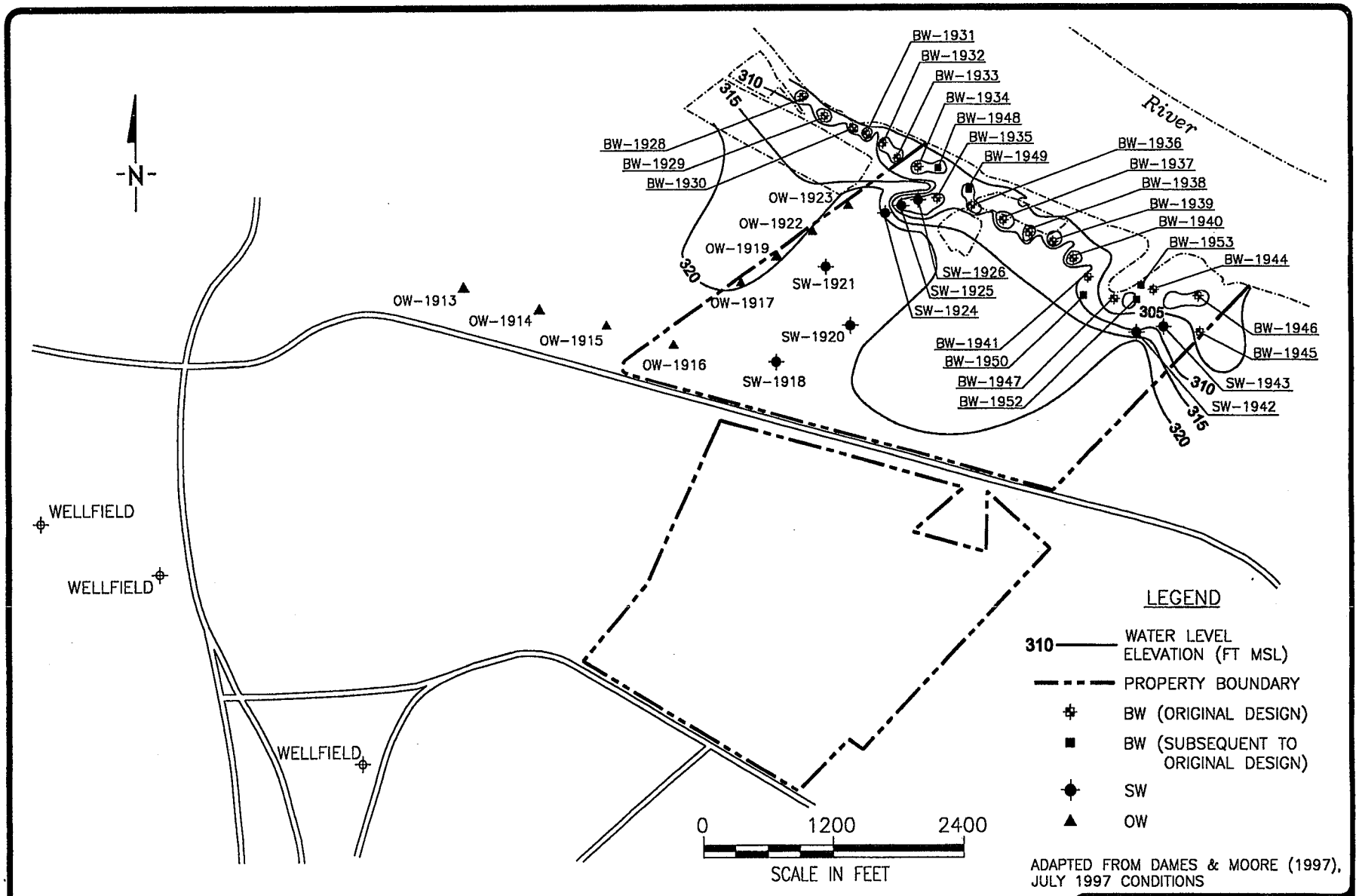

NOTE: REMEDIATION WELLS ARE ILLUSTRATED ON THIS FIGURE. ALL WATER LEVEL DATA POINTS NOT SHOWN.

Figure 4-2. Groundwater elevation contours, Kentucky.

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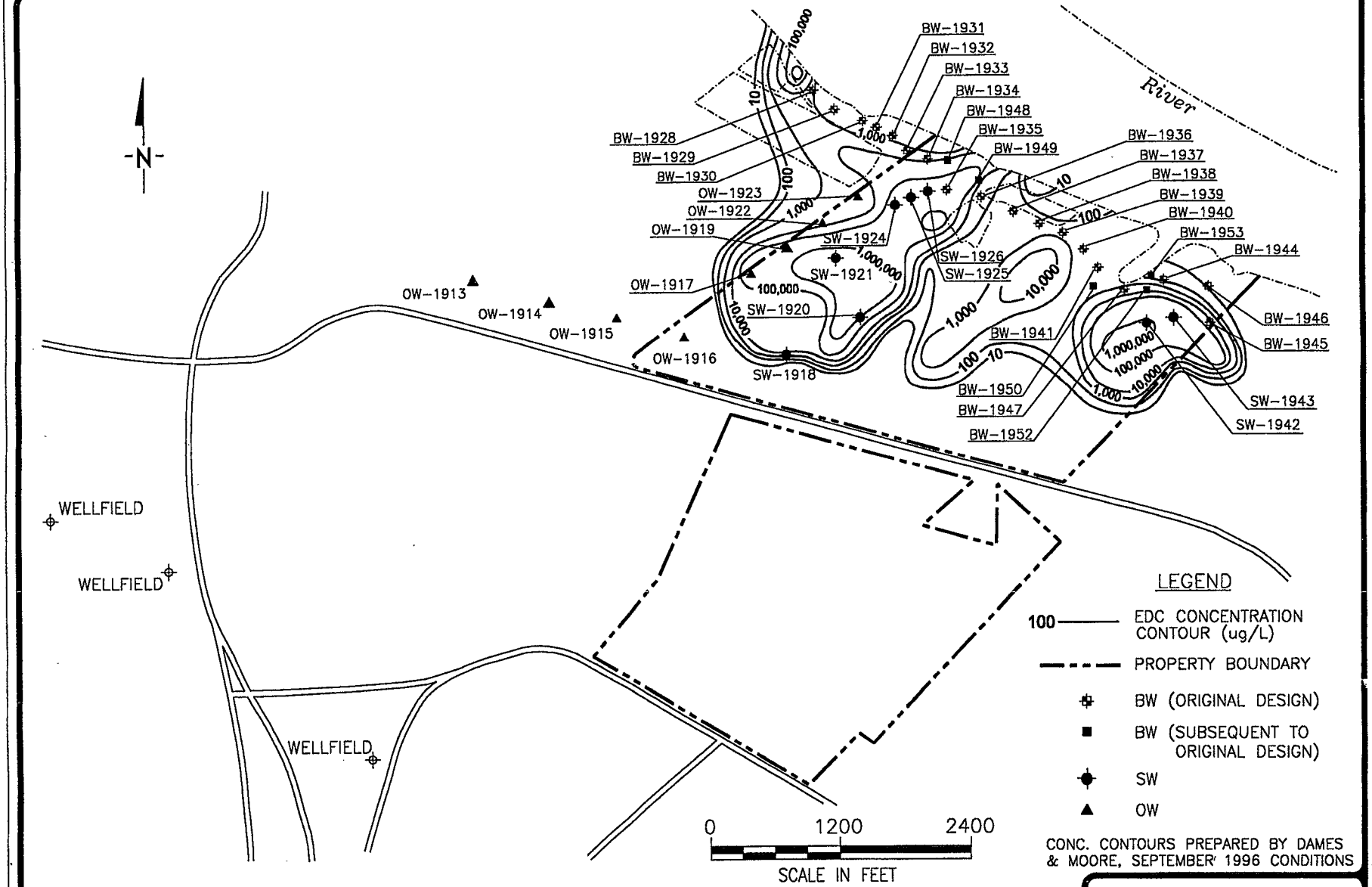

Figure 4-3. EDC concentrations and current remediation wells, Kentucky.

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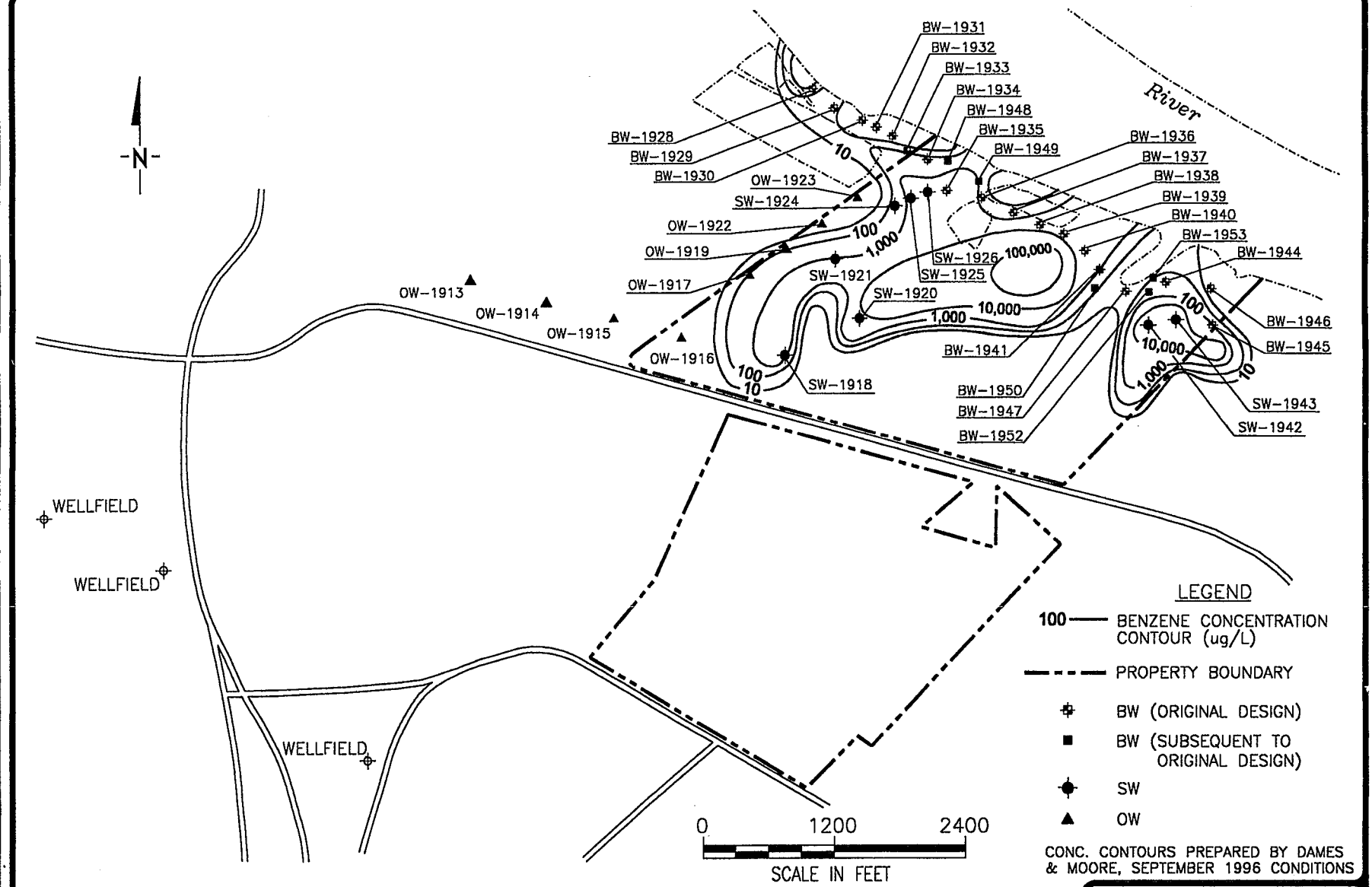

Figure 4-4. Benzene concentrations and current remediation wells, Kentucky.

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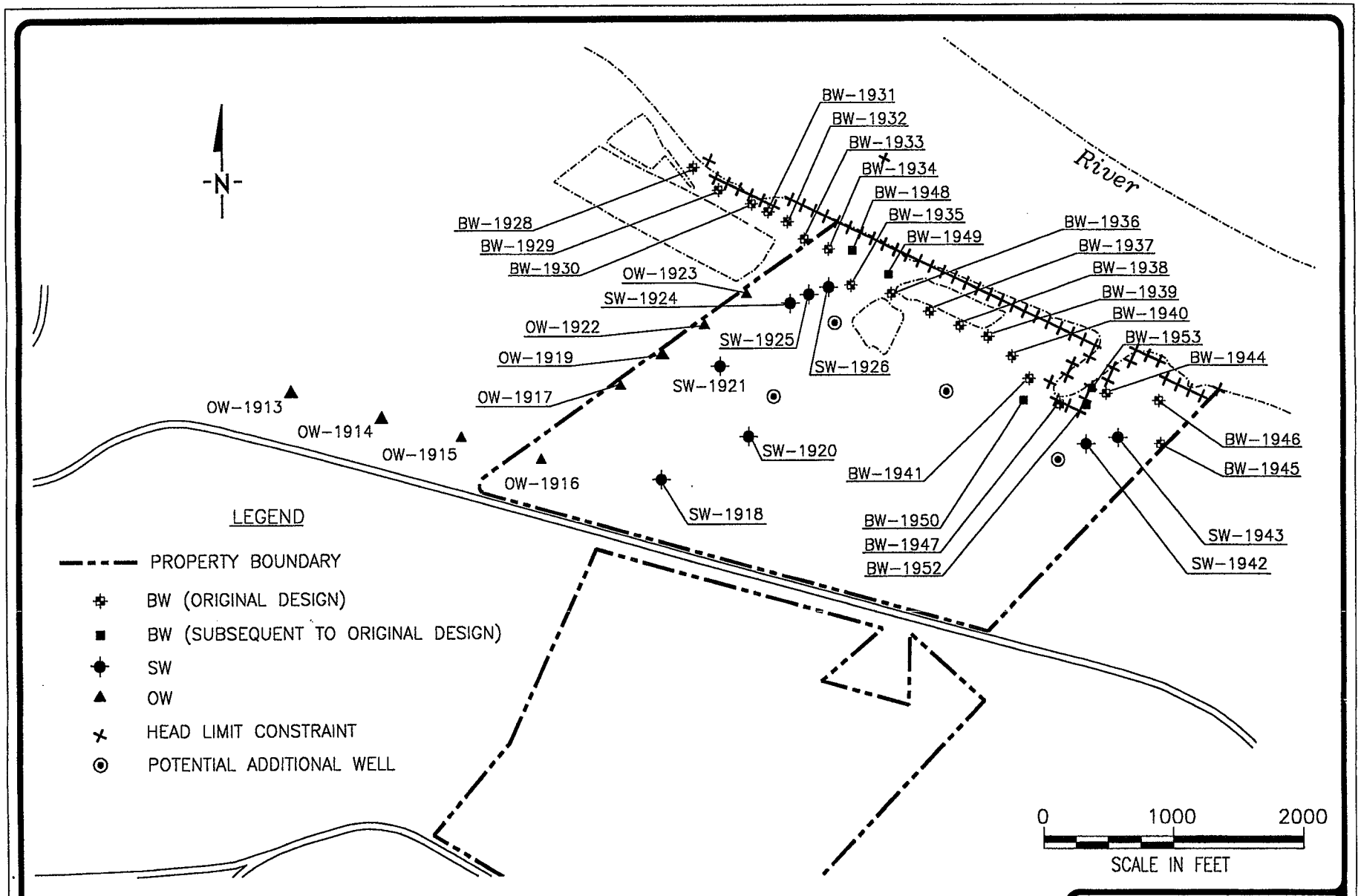

Figure 4-5. Constraint locations and potential additional wells, Kentucky.

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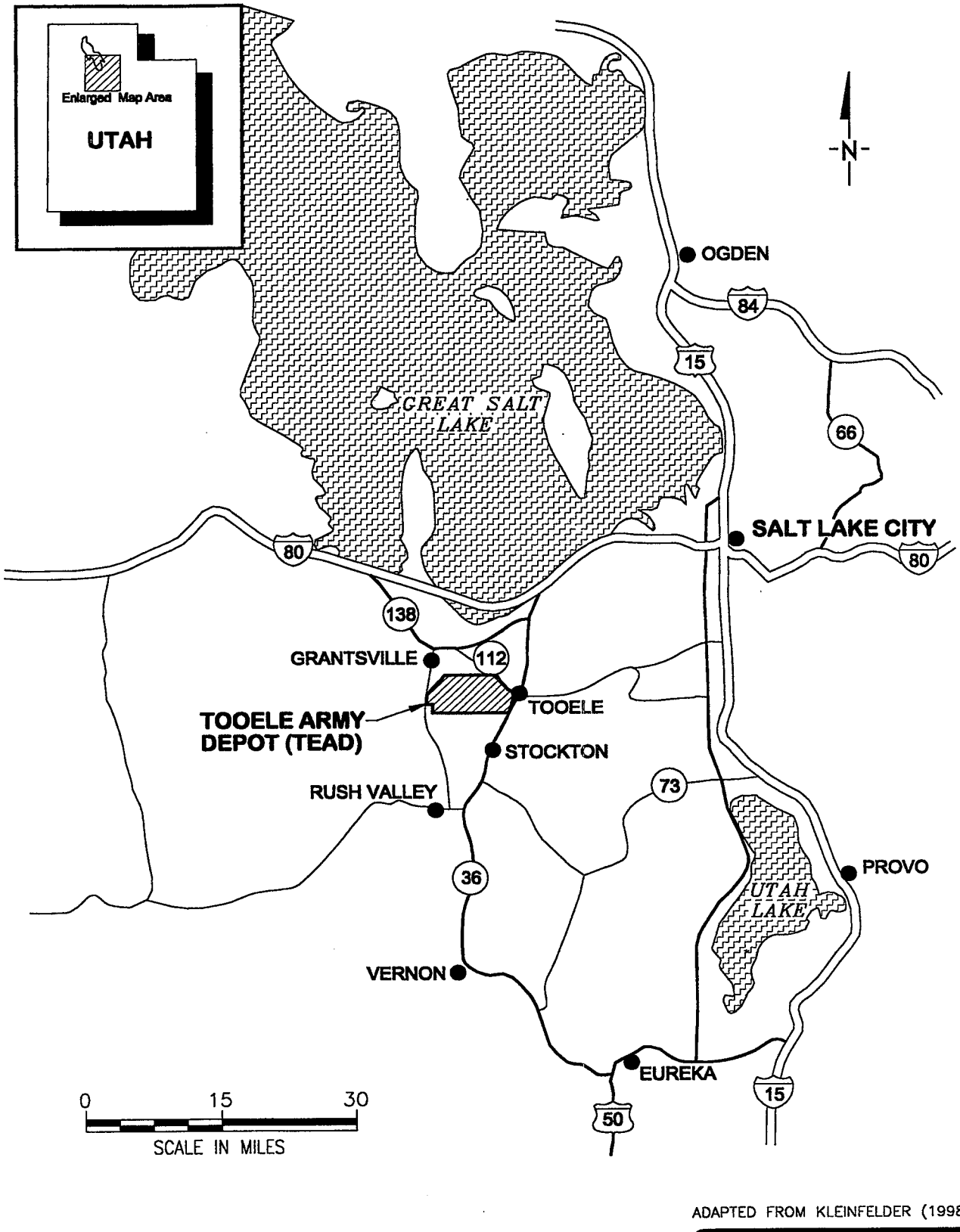

ADAPTED FROM KLEINFELDER (1998)

Figure 5-1. Site location map, Tooele.

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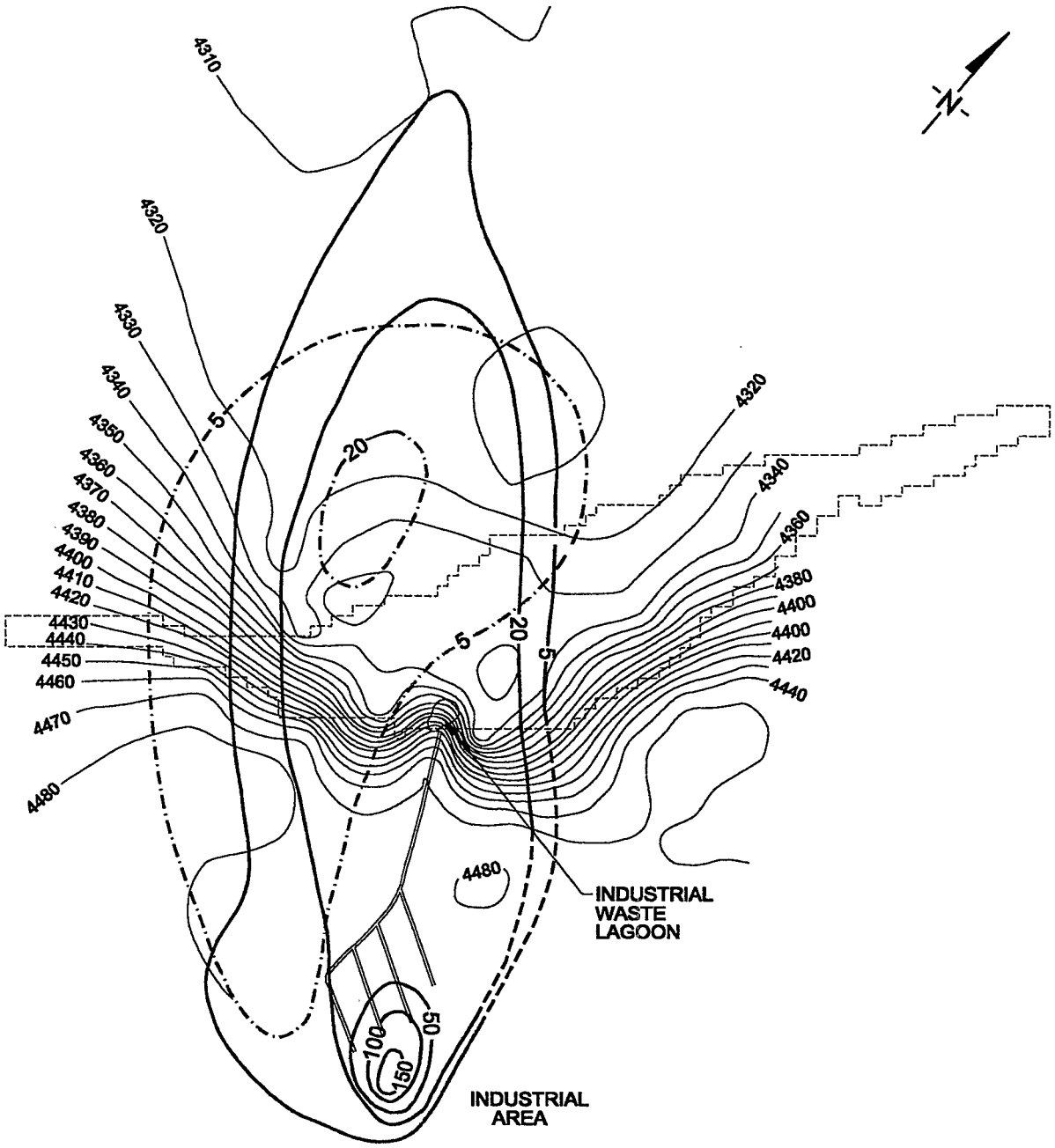

LEGEND

DEEP-TCE CONTOUR

SHALLOW TCE CONTOUR (DASHED WHERE INFERRED)

BEDROCK BLOCK AS IMPLEMENTED IN MODEL

4480 GROUNDWATER ELEVATION CONTOUR

0 3000 6000

SCALE IN FEET

WATER LEVELS, MARCH 1997, TAKEN FROM KLEINFELDER (1998)

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Figure 5–2. Groundwater elevation contours, Tooele.

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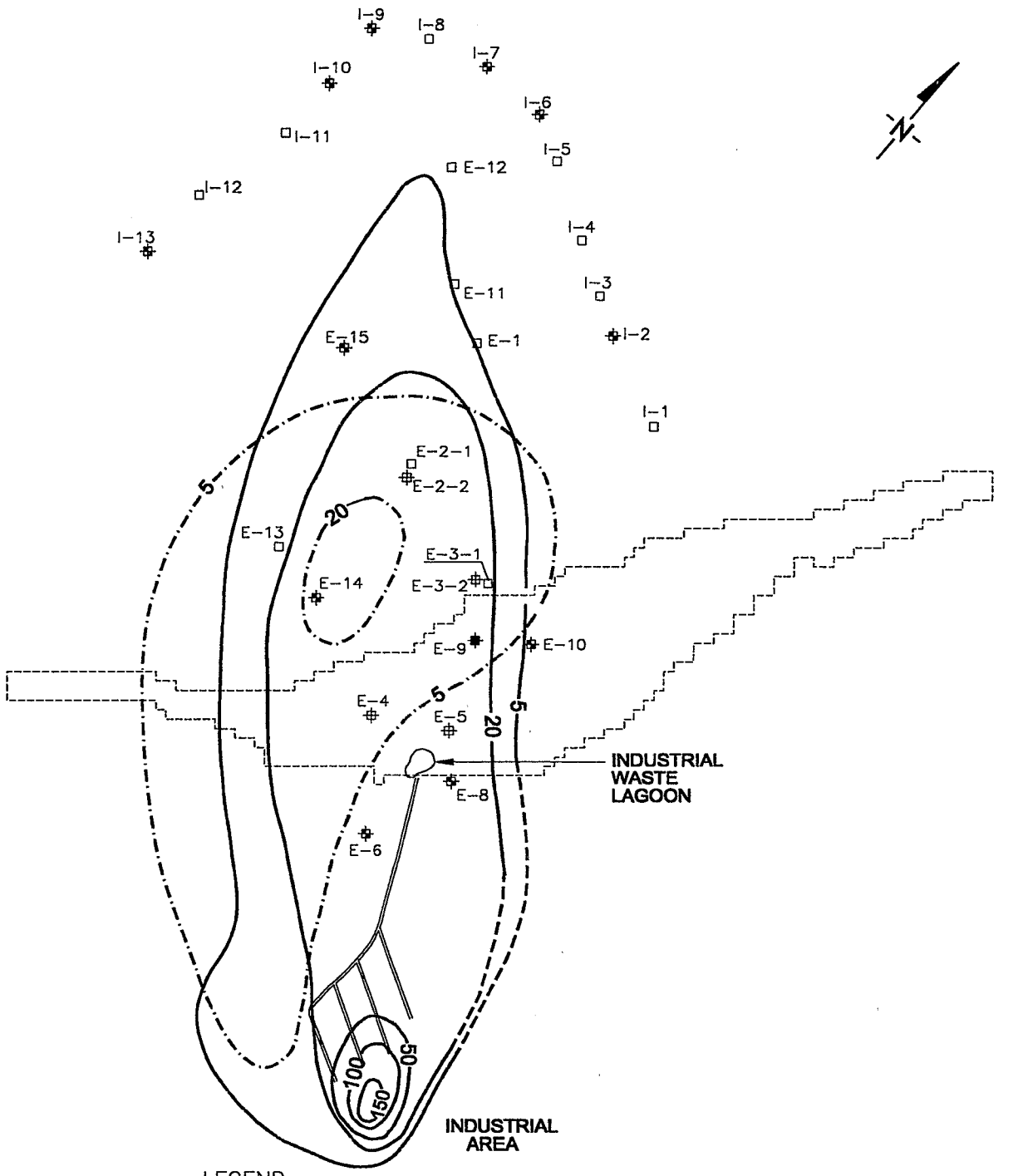

LEGEND

I-4 INJECTION WELL

E-4 EXTRACTION WELL

EX. WELL IN LAYER 1

EX. WELL IN LAYER 2

EX. WELL IN LAYERS 1 & 2

EX. WELL IN LAYERS 1, 2 & 3

DEEP TCE CONTOUR (ug/L or ppb)

SHALLOW TCE CONTOUR (ug/L or ppb) (DASHED WHERE INFERRED)

UNLINED DITCH

BEDROCK BLOCK AS IMPLEMENTED IN MODEL

0 3000 6000

SCALE IN FEET

ADAPTED FROM KLEINFELDER (1998)

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Figure 5-3. TCE concentrations and current remediation wells, Tooele.

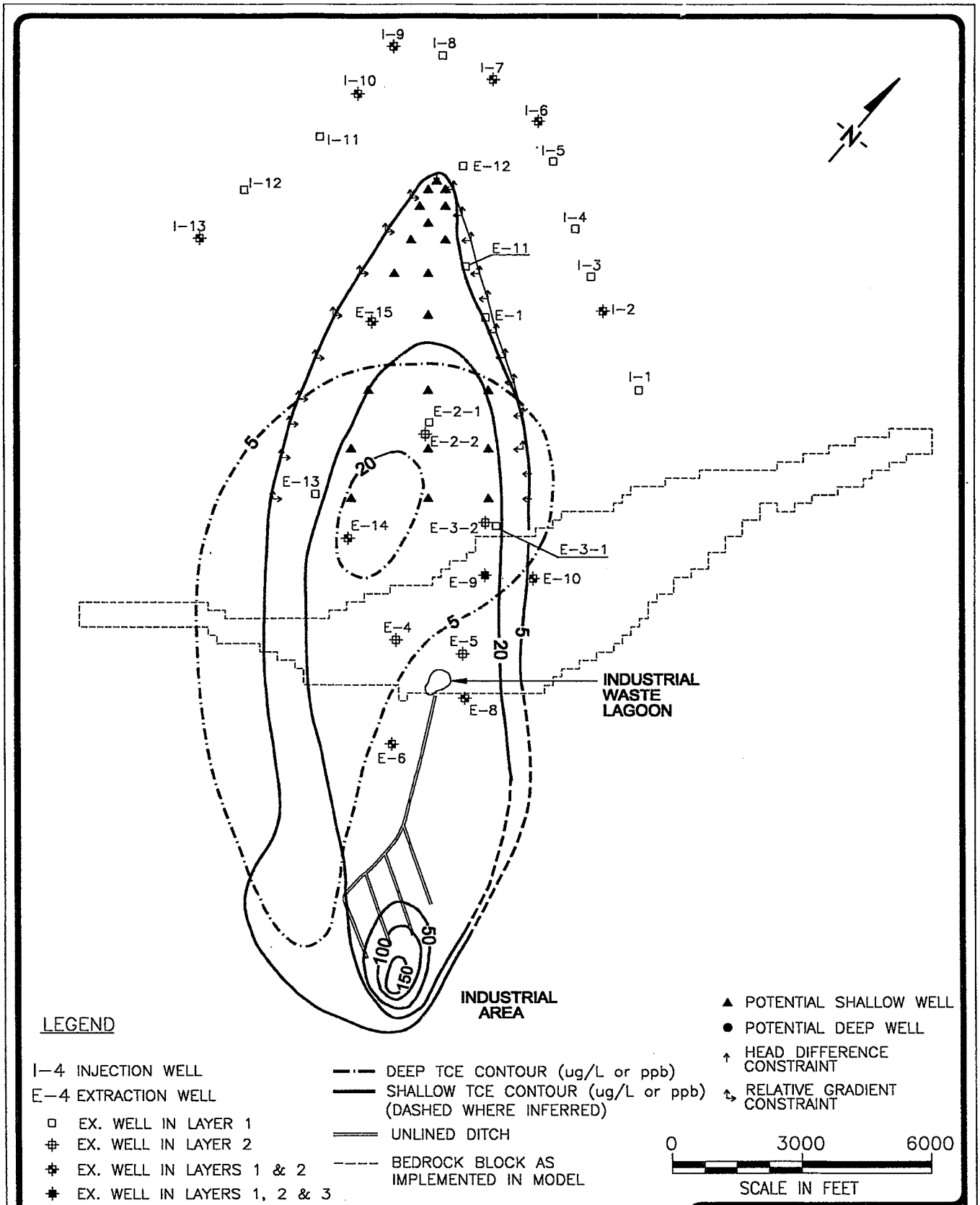

Figure 5-4. Contraint locations and potential additional wells, shallow 5-ppb plume, Tooele.

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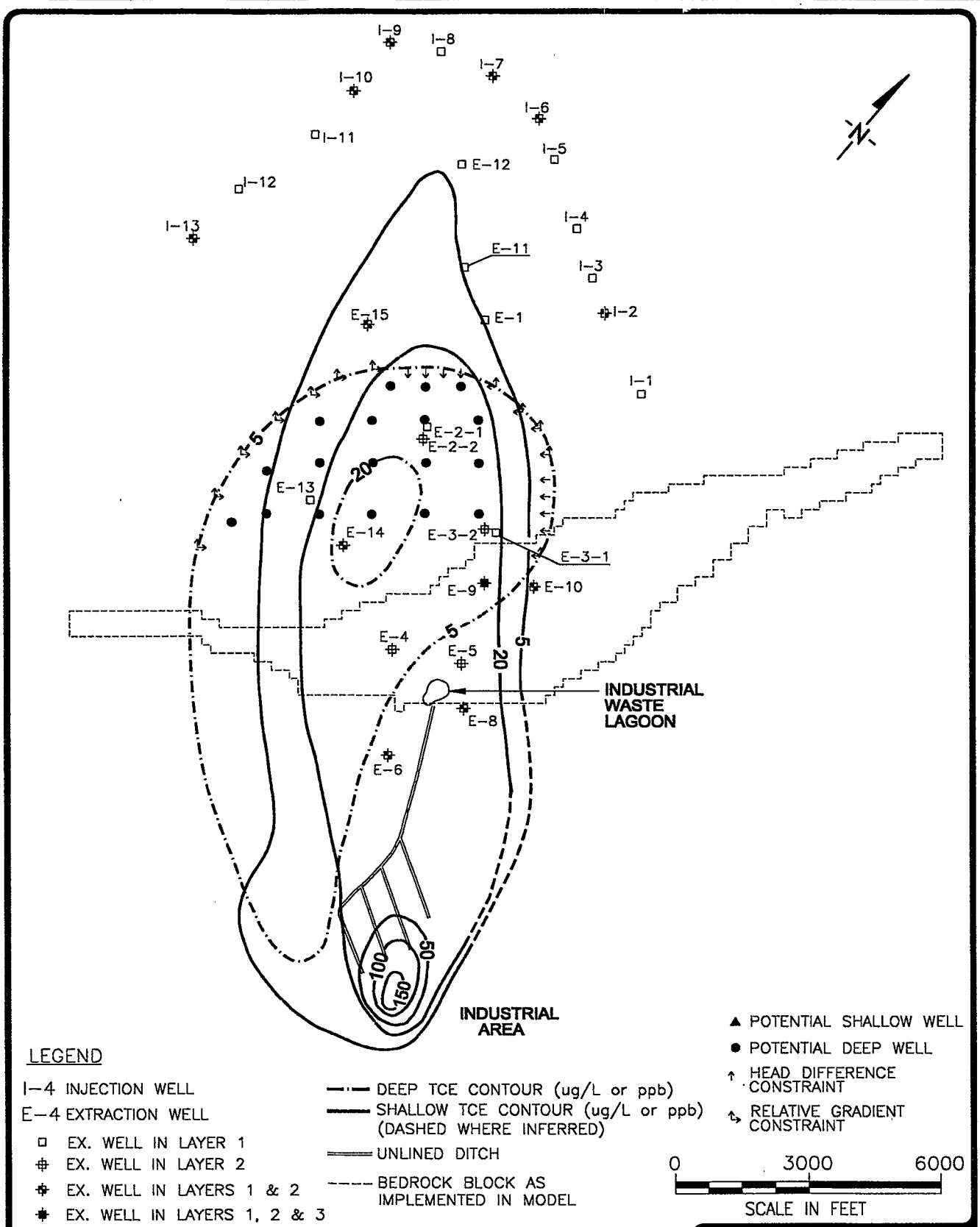

Figure 5-5. Contraint locations and potential additional wells, deep 5-ppb plume, Tooele.

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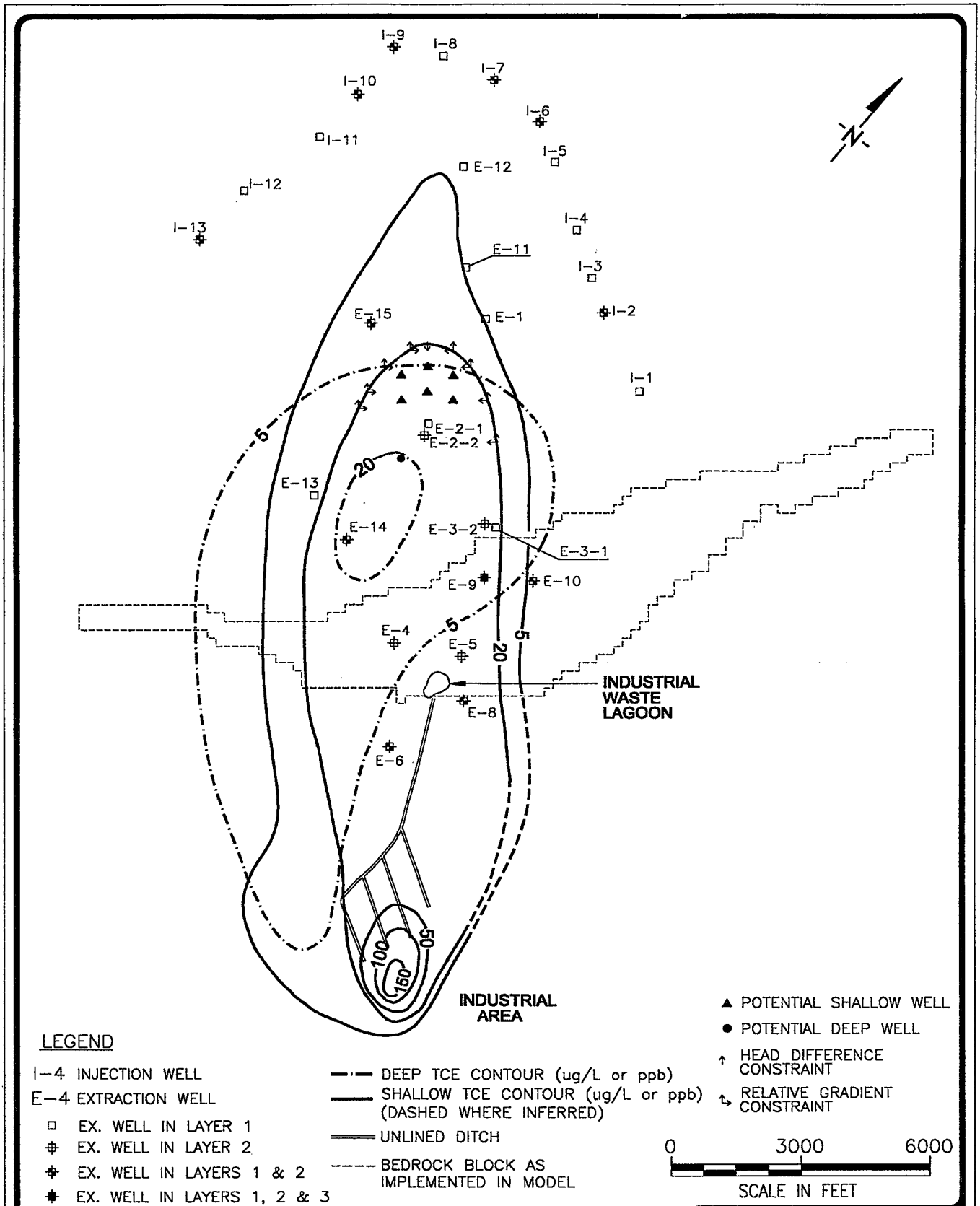

Figure 5-6. Contraint locations and potential additional wells, shallow 20-ppb plume, Tooele.

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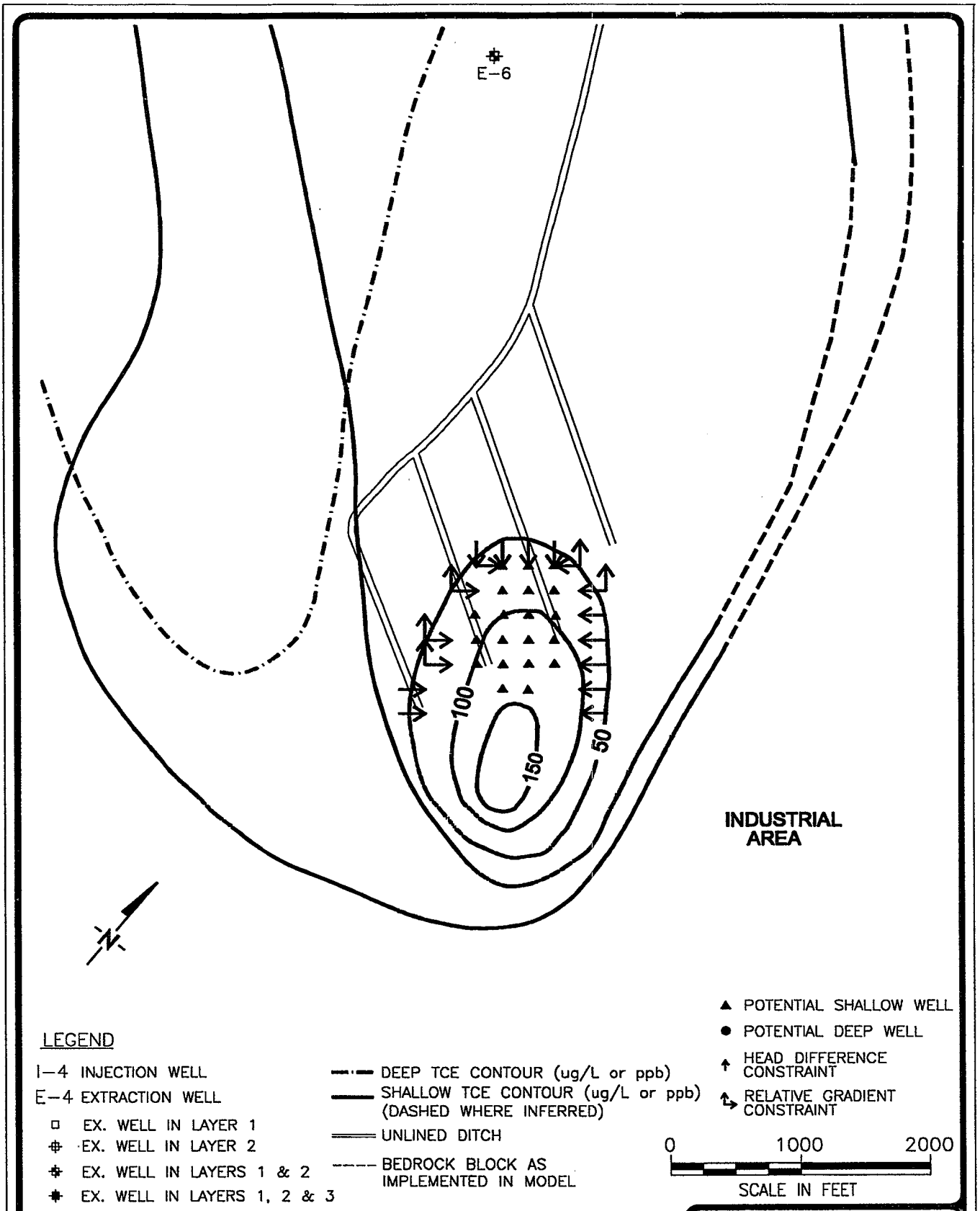

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Figure 5-7. Contraint locations and potential additional wells, 50-ppb plume, Tooele.

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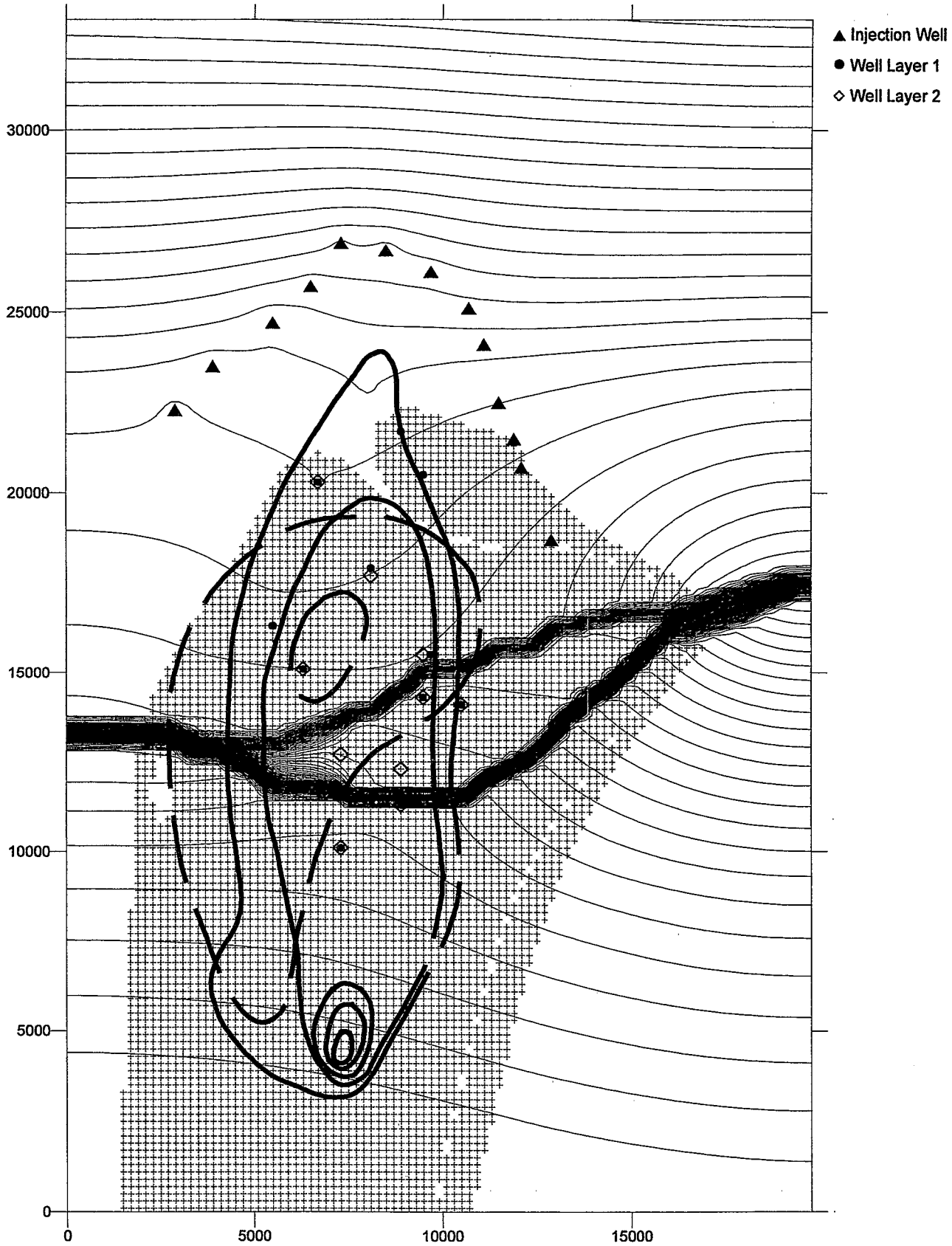
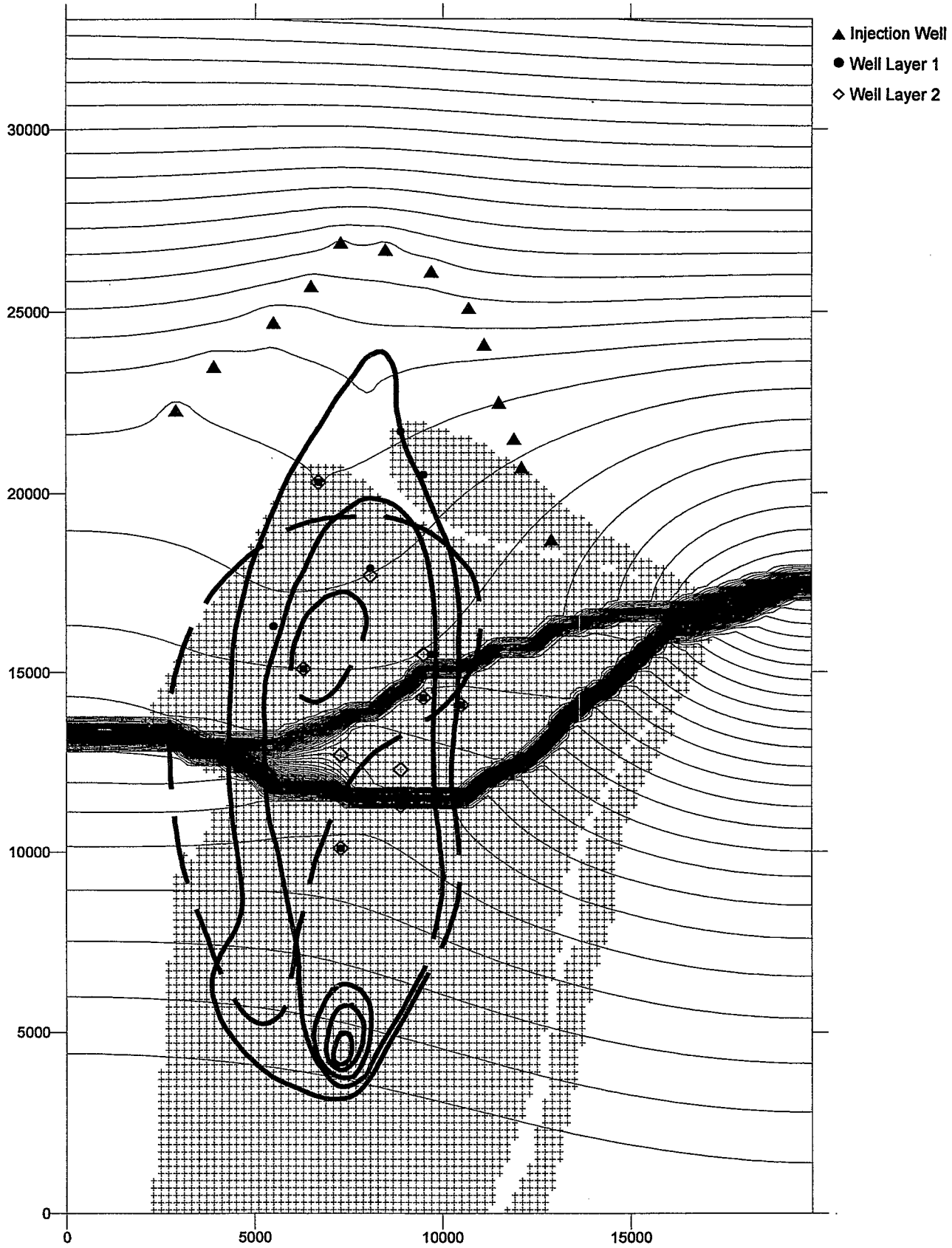
Figure 5-8: Shallow Particles, Layer 1 heads, Pumping on April 6, 1998
(~7460 gpm, 15 existing wells)



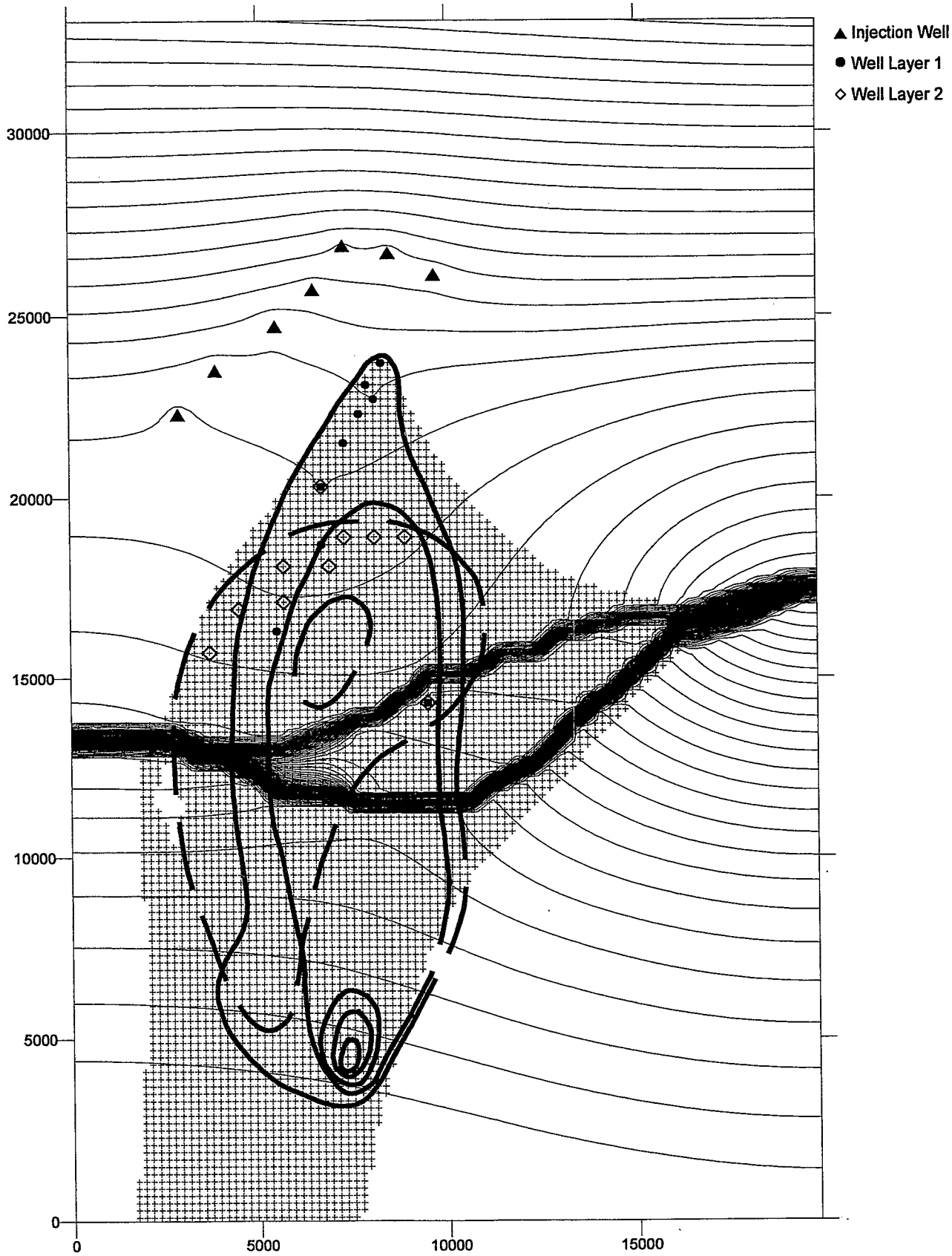
A "+" symbol indicates that a particle starting at that location is captured by one of the remediation wells, based on particle tracking with MODPATH. Shallow particles originate half-way down in layer 1.

Figure 5-9: Deep Particles, Layer 1 heads, Pumping on April 6, 1998
(~7460 gpm, 15 existing wells)



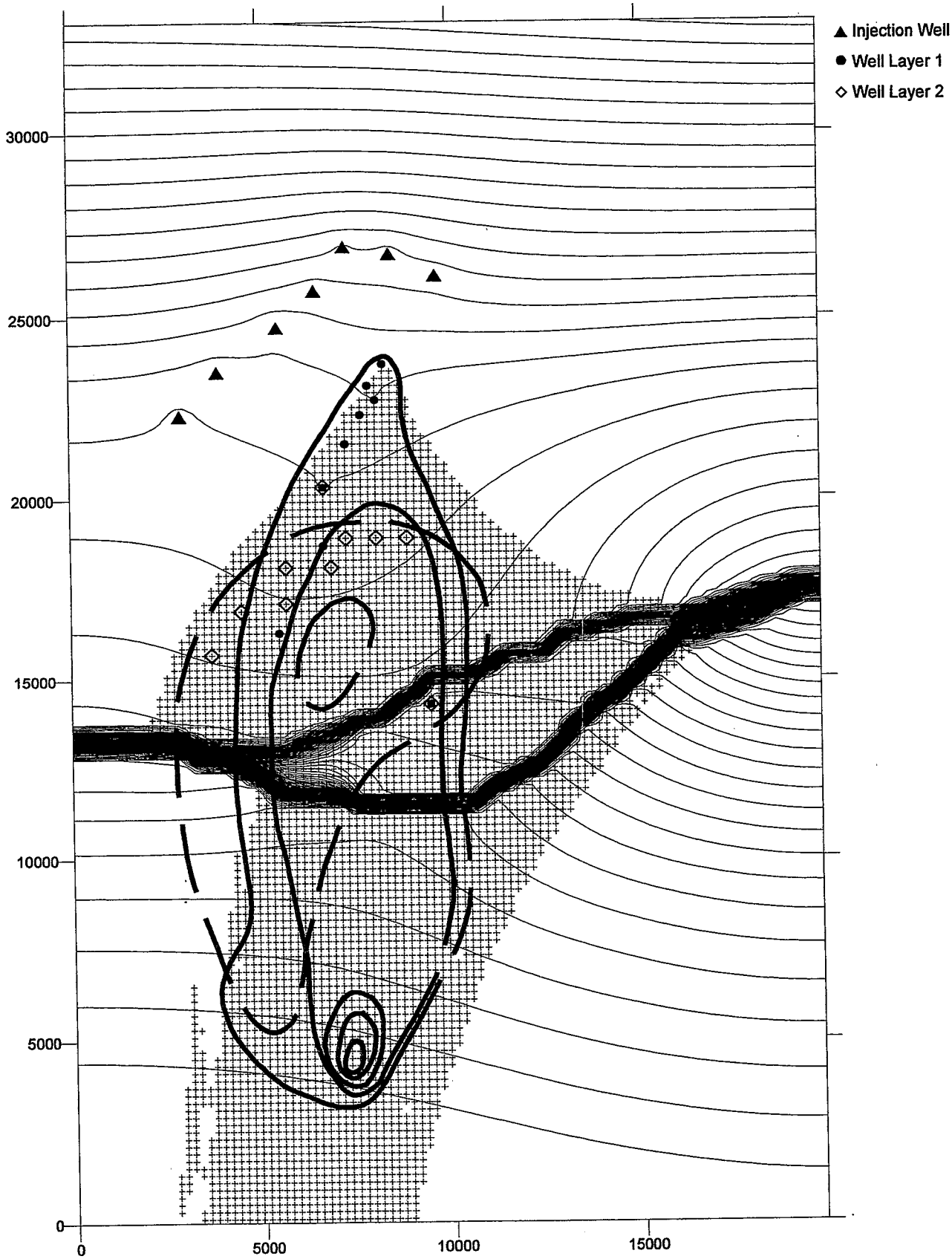
A "+" symbol indicates that a particle starting at that location is captured by one of the remediation wells, based on particle tracking with MODPATH. Deep particles originate half-way down in layer 2.

Figure 5-10: Shallow Particles, Contain Shallow & Deep 5-ppb Plume
(4163 gpm, 14 new wells, 3 existing wells)



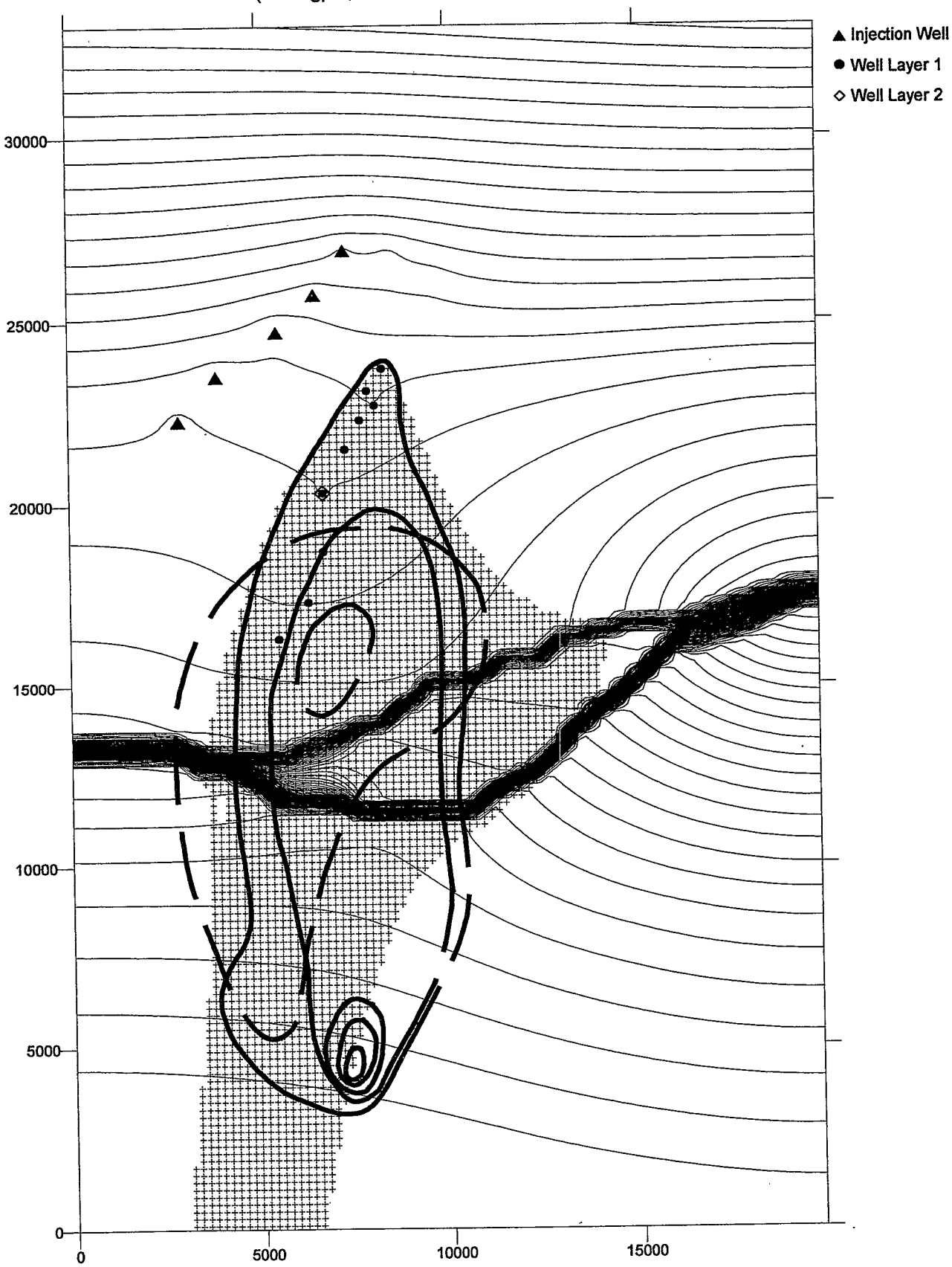
A "+" symbol indicates that a particle starting at that location is captured by one of the remediation wells, based on particle tracking with MODPATH. Shallow particles originate half-way down in layer 1.

Figure 5-11: Deep Particles, Contain Shallow & Deep 5-ppb Plume
(4163 gpm, 14 new wells, 3 existing wells)



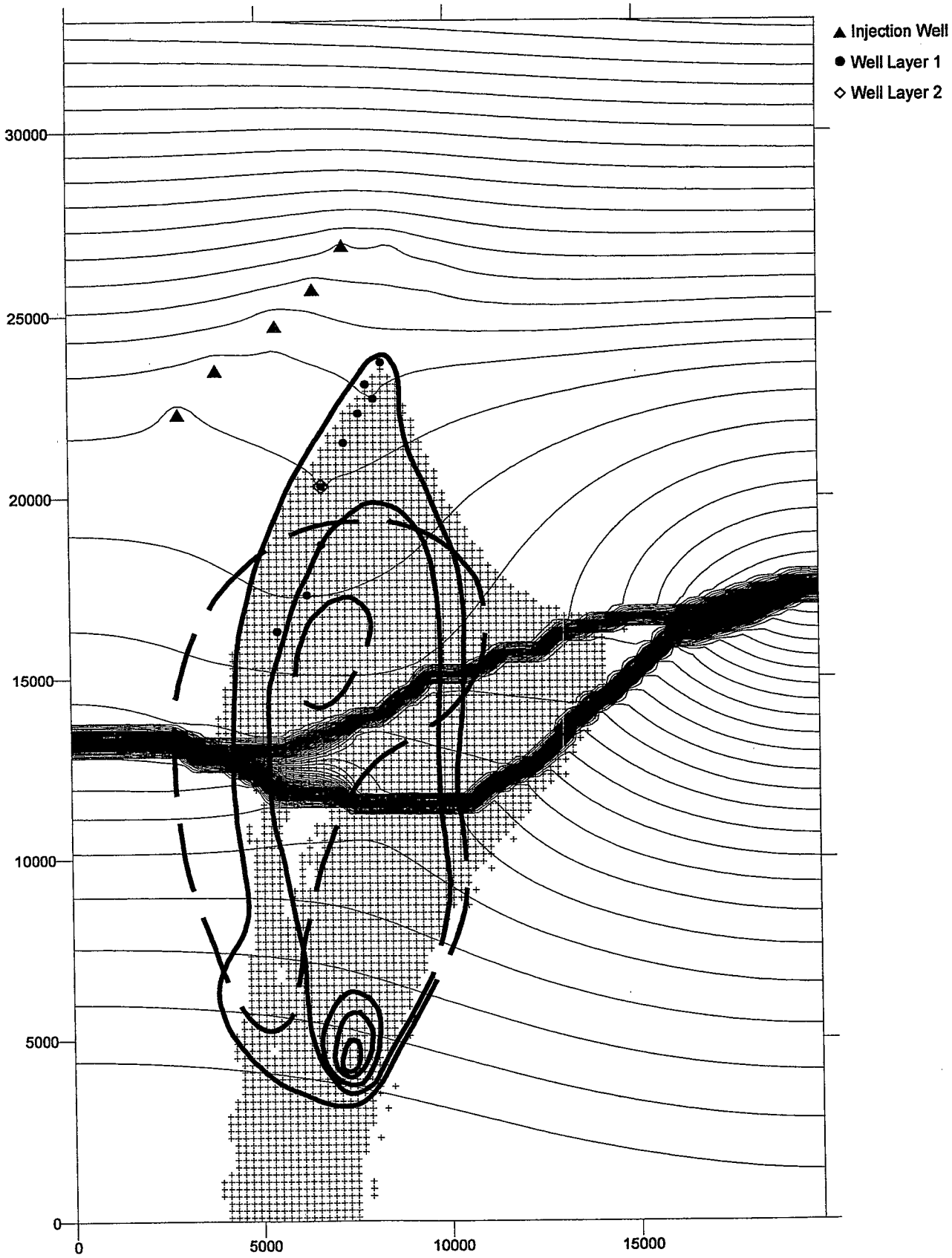
A "+" symbol indicates that a particle starting at that location is captured by one of the remediation wells, based on particle tracking with MODPATH. Deep particles originate half-way down in layer 2.

Figure 5-12: Shallow Particles, Contain Shallow 5-ppb Plume
(2622 gpm, 7 new wells, 2 existing wells)



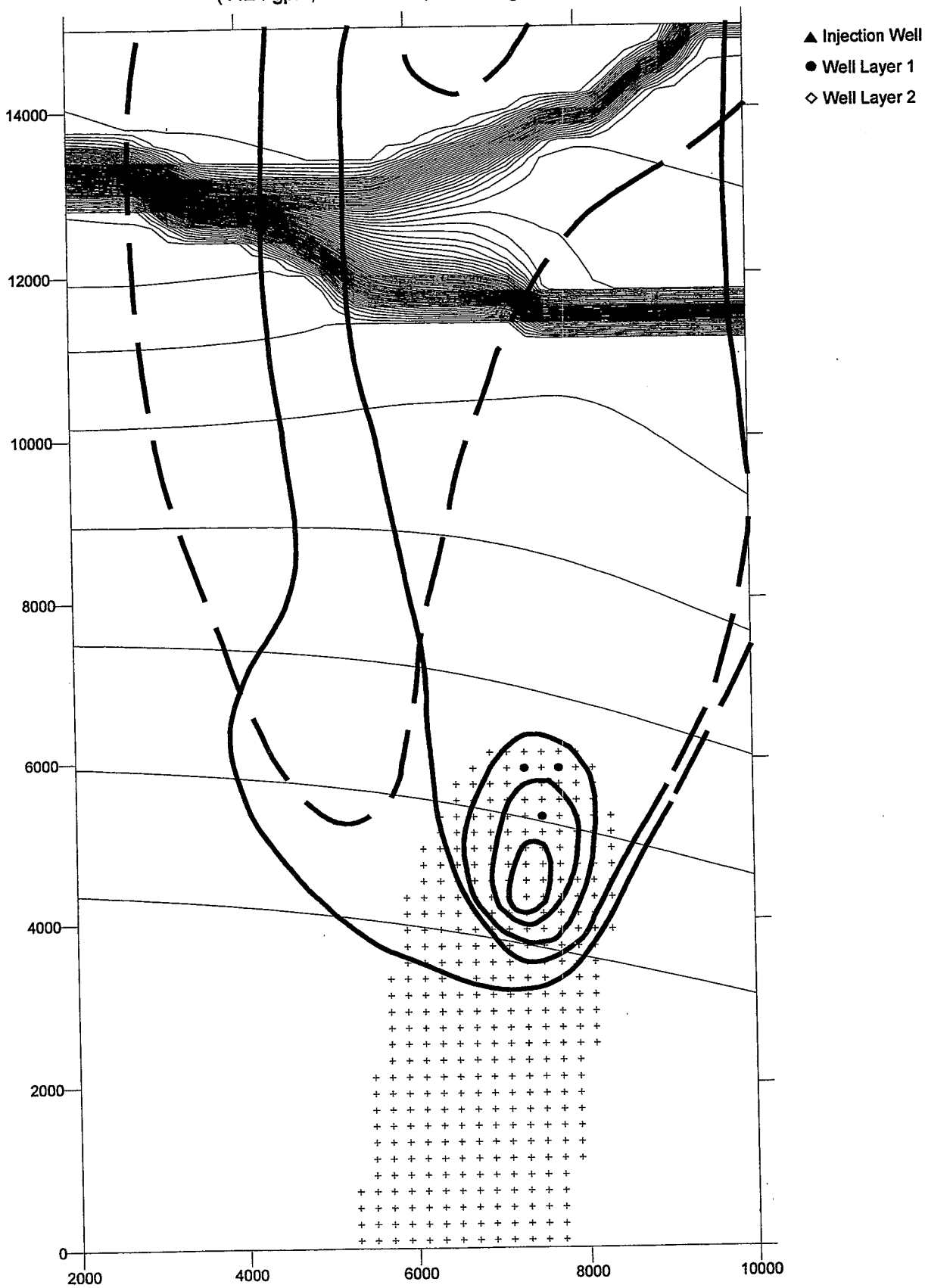
A "+" symbol indicates that a particle starting at that location is captured by one of the remediation wells, based on particle tracking with MODPATH. Shallow particles originate half-way down in layer 1.

Figure 5-13: Deep Particles, Contain Shallow 5-ppb Plume
(2622 gpm, 7 new wells, 2 existing wells)



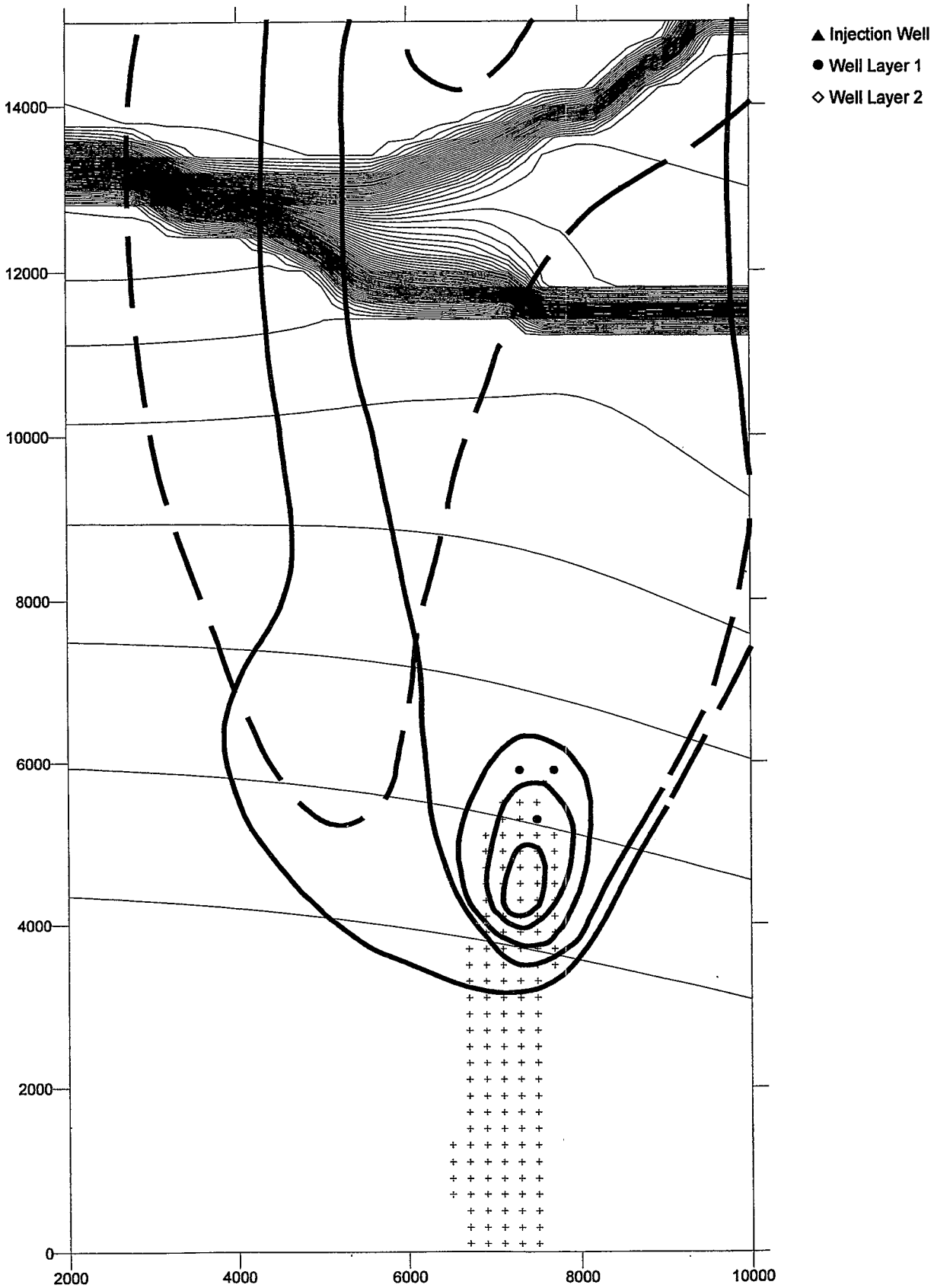
A "+" symbol indicates that a particle starting at that location is captured by one of the remediation wells, based on particle tracking with MODPATH. Deep particles originate half-way down in layer 2.

Figure 5-14: Shallow Particles, Contain Shallow 50-ppb Plume
(1124 gpm, 3 new wells, 0 existing wells)



A "+" symbol indicates that a particle starting at that location is captured by one of the remediation wells, based on particle tracking with MODPATH. Shallow particles originate half-way down in layer 1.

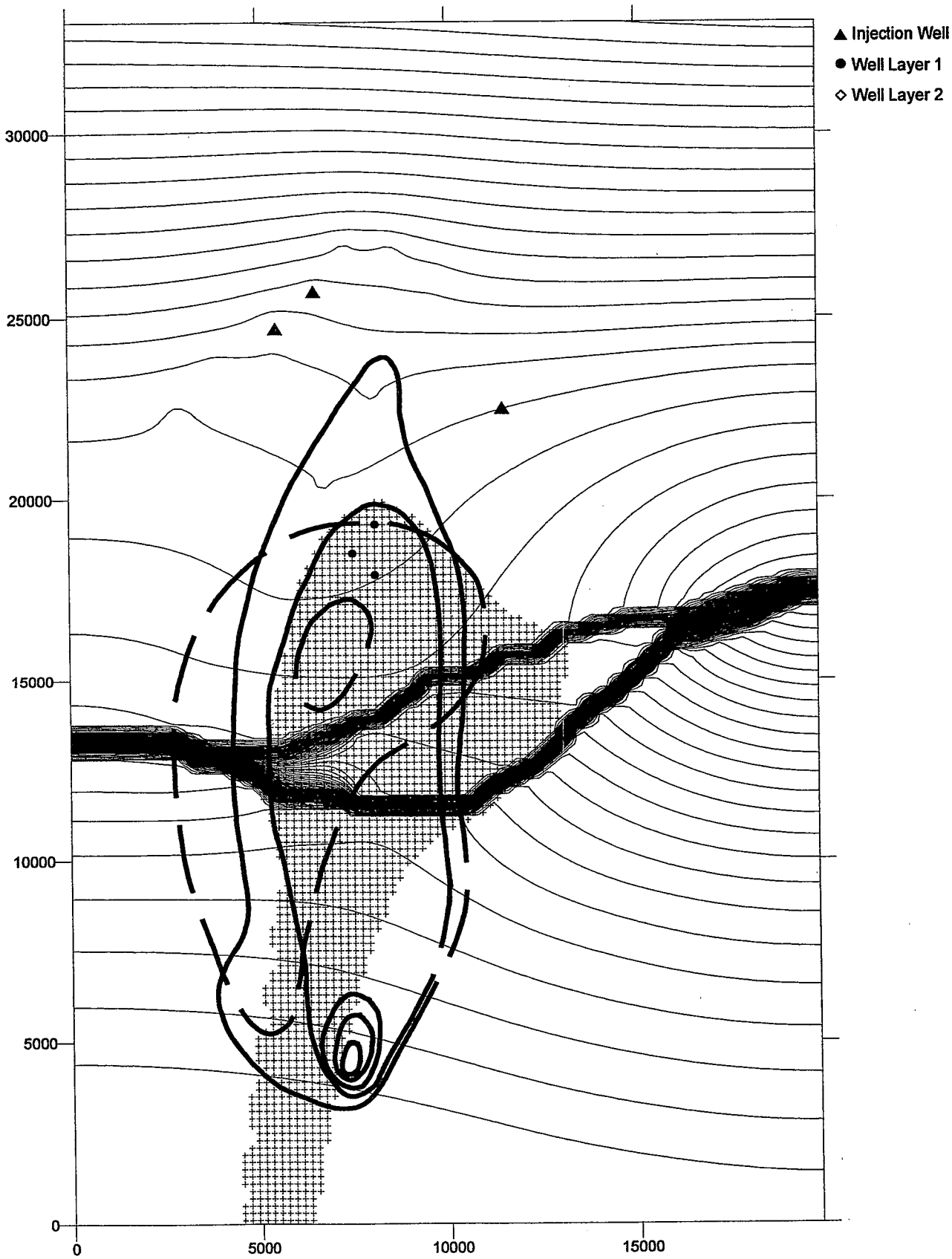
Figure 5-15: Deep Particles, Contain Shallow 50-ppb Plume
(1124 gpm, 3 new wells, 0 existing wells)



A "+" symbol indicates that a particle starting at that location is captured by one of the remediation wells, based on particle tracking with MODPATH. Deep particles originate half-way down in layer 2.

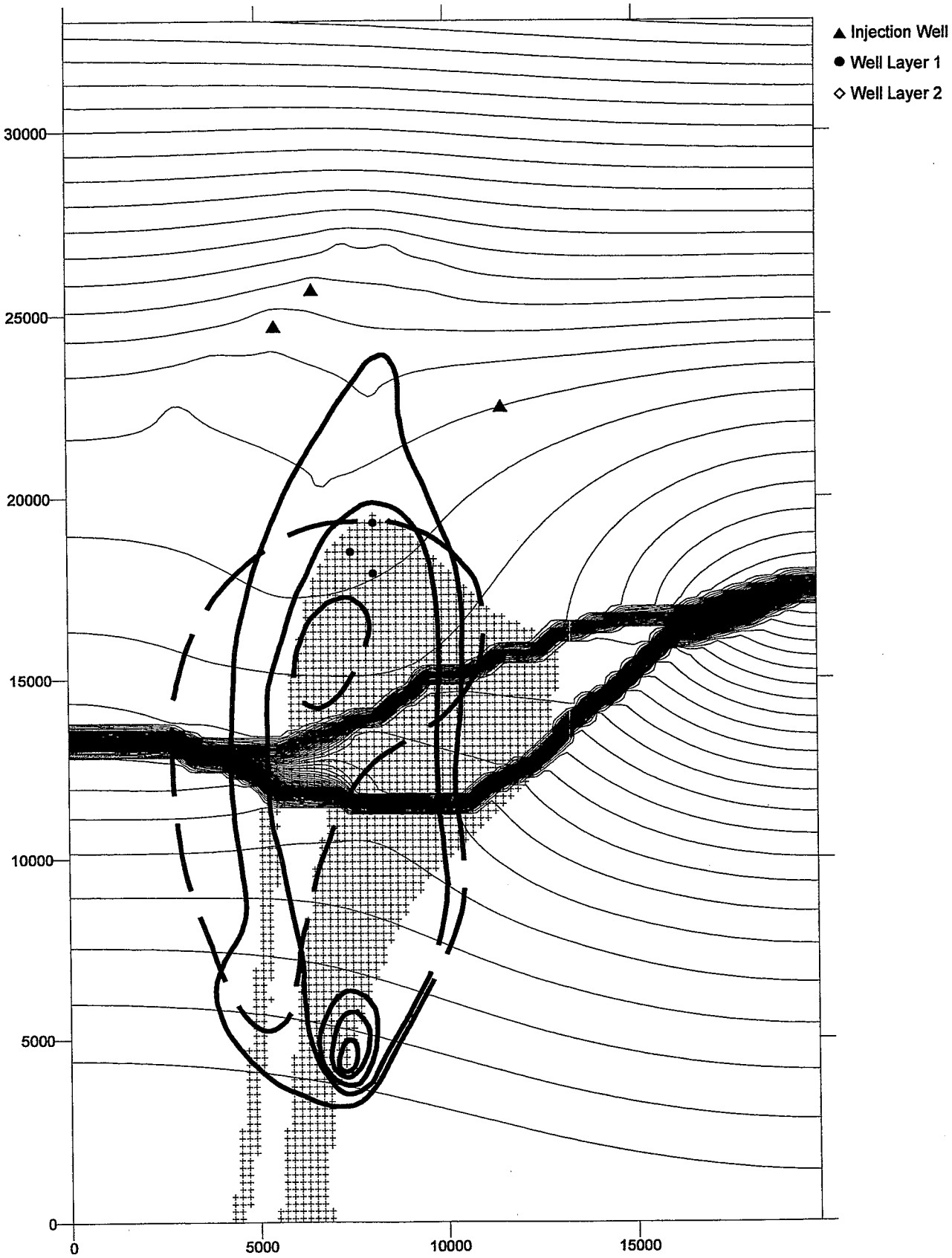
Figure 5-16: Shallow Particles, Contain Shallow 20-ppb Plume

(1377 gpm, 2 new wells, 1 existing well)



A "+" symbol indicates that a particle starting at that location is captured by one of the remediation wells, based on particle tracking with MODPATH. Shallow particles originate half-way down in layer 1.

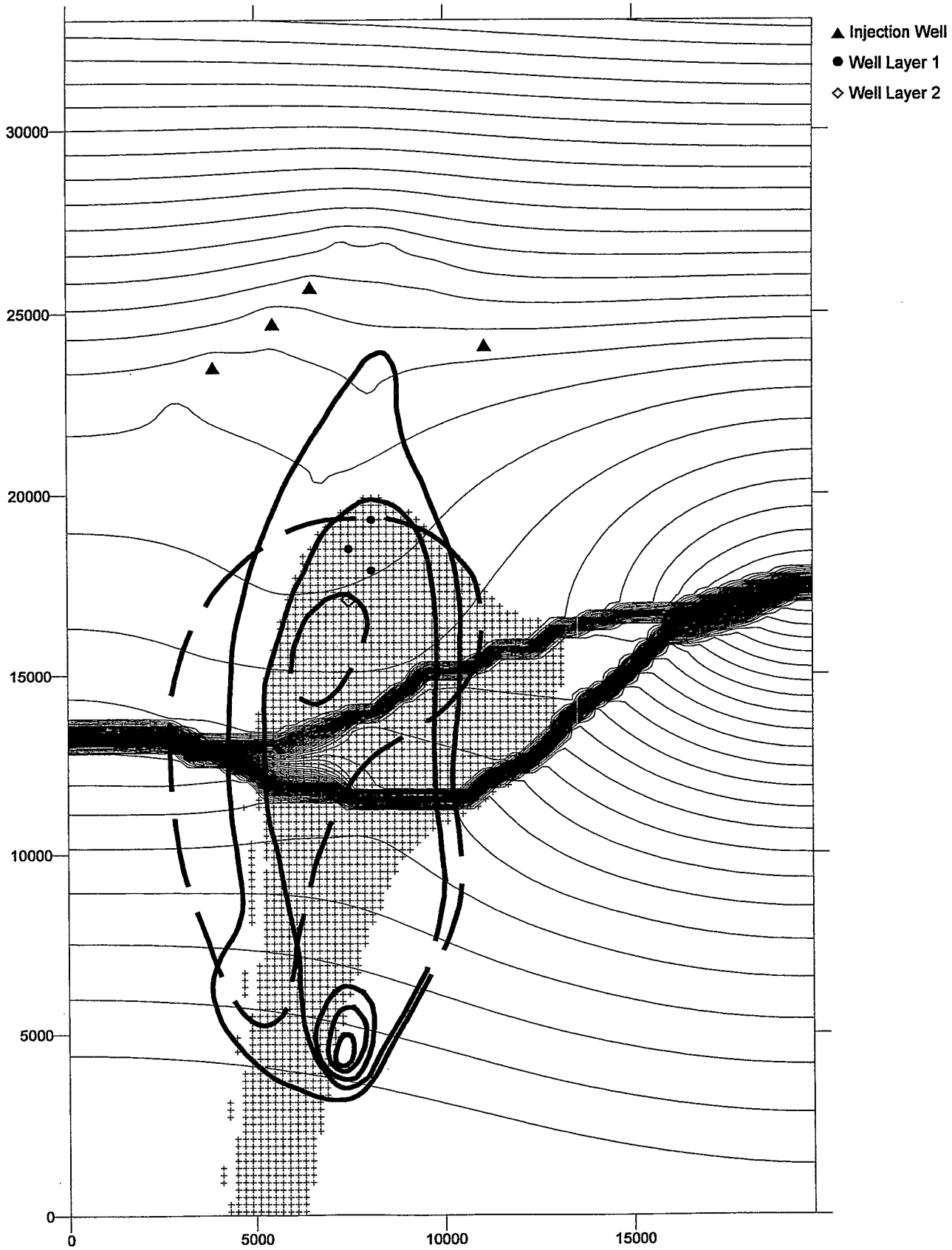
Figure 5-17: Deep Particles, Contain Shallow 20-ppb Plum e
(1377 gpm, 2 new wells, 1 existing well)



A "+" symbol indicates that a particle starting at that location is captured by one of the remediation wells, based on particle tracking with MODPATH. Deep particles originate half-way down in layer 2.

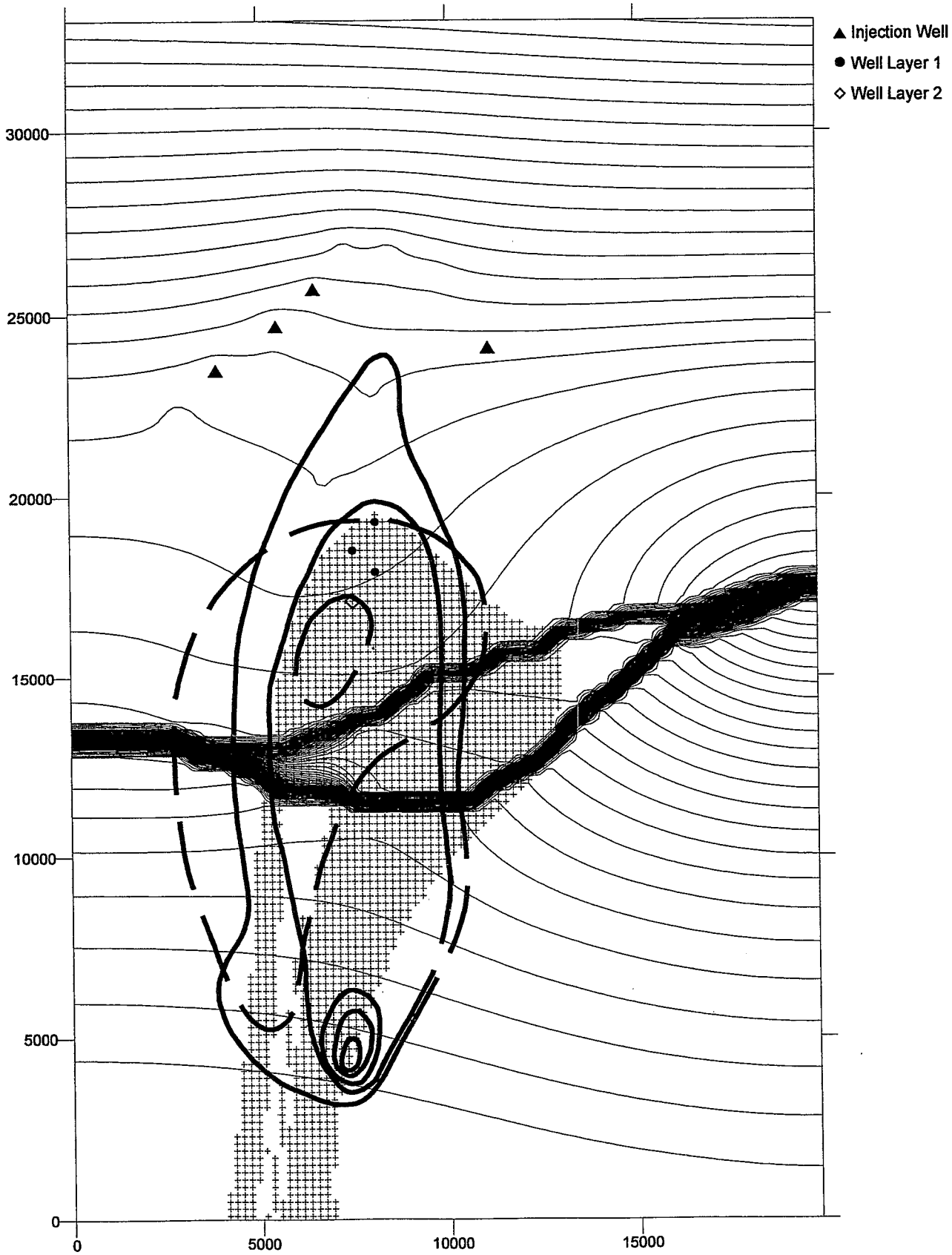
Figure 5-18: Shallow Particles, Contain Shallow 20-ppb Plume, & 500 gpm for Deep 20-ppb plume

(1573 gpm, 3 new wells, 1 existing well)



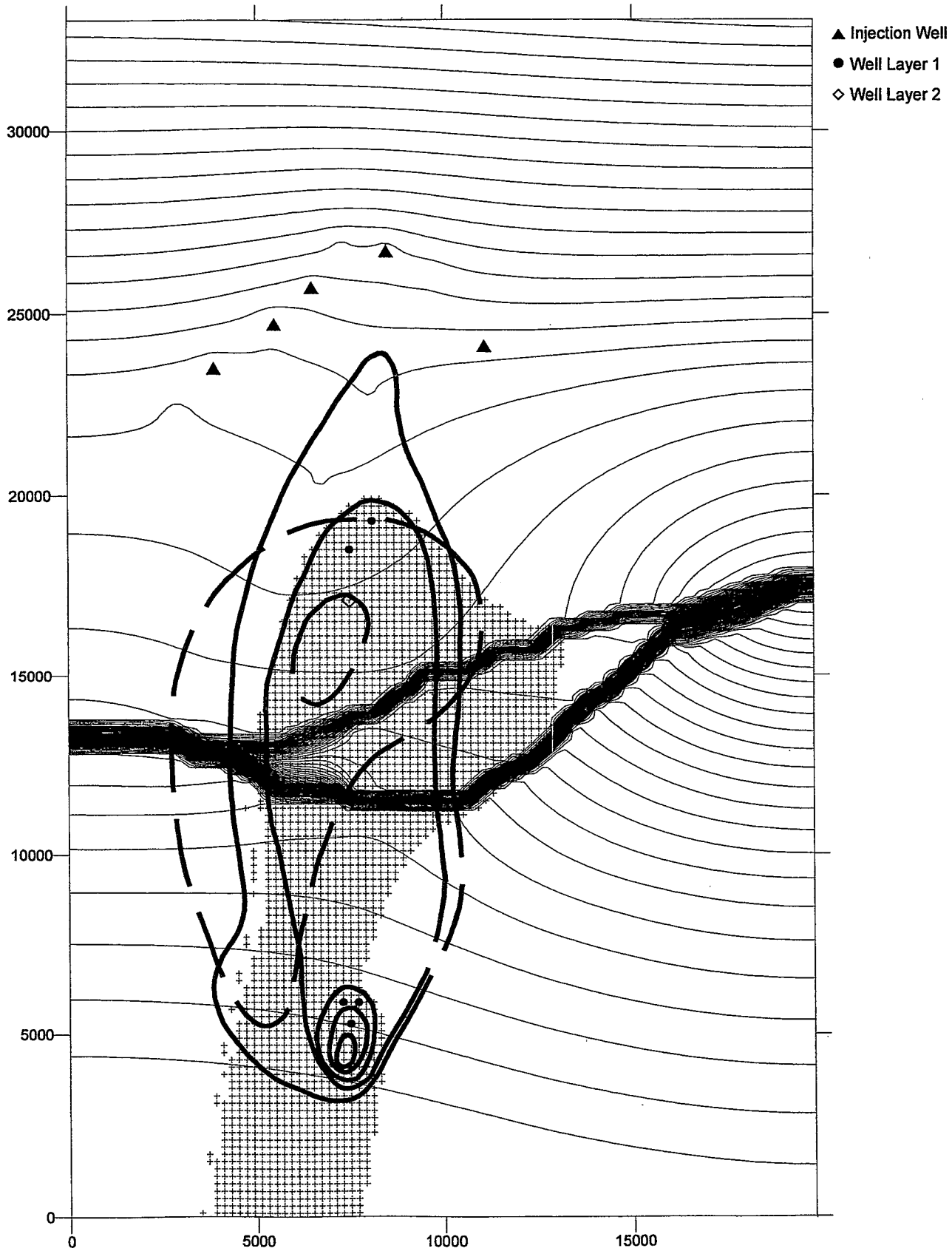
A "+" symbol indicates that a particle starting at that location is captured by one of the remediation wells, based on particle tracking with MODPATH. Shallow particles originate half-way down in layer 1.

Figure 5-19: Deep Particles, Contain Shallow 20-ppb Plume, & 500 gpm for Deep 20-ppb plume
(1573 gpm, 3 new wells, 1 existing well)



A "+" symbol indicates that a particle starting at that location is captured by one of the remediation wells, based on particle tracking with MODPATH. Deep particles originate half-way down in layer 2.

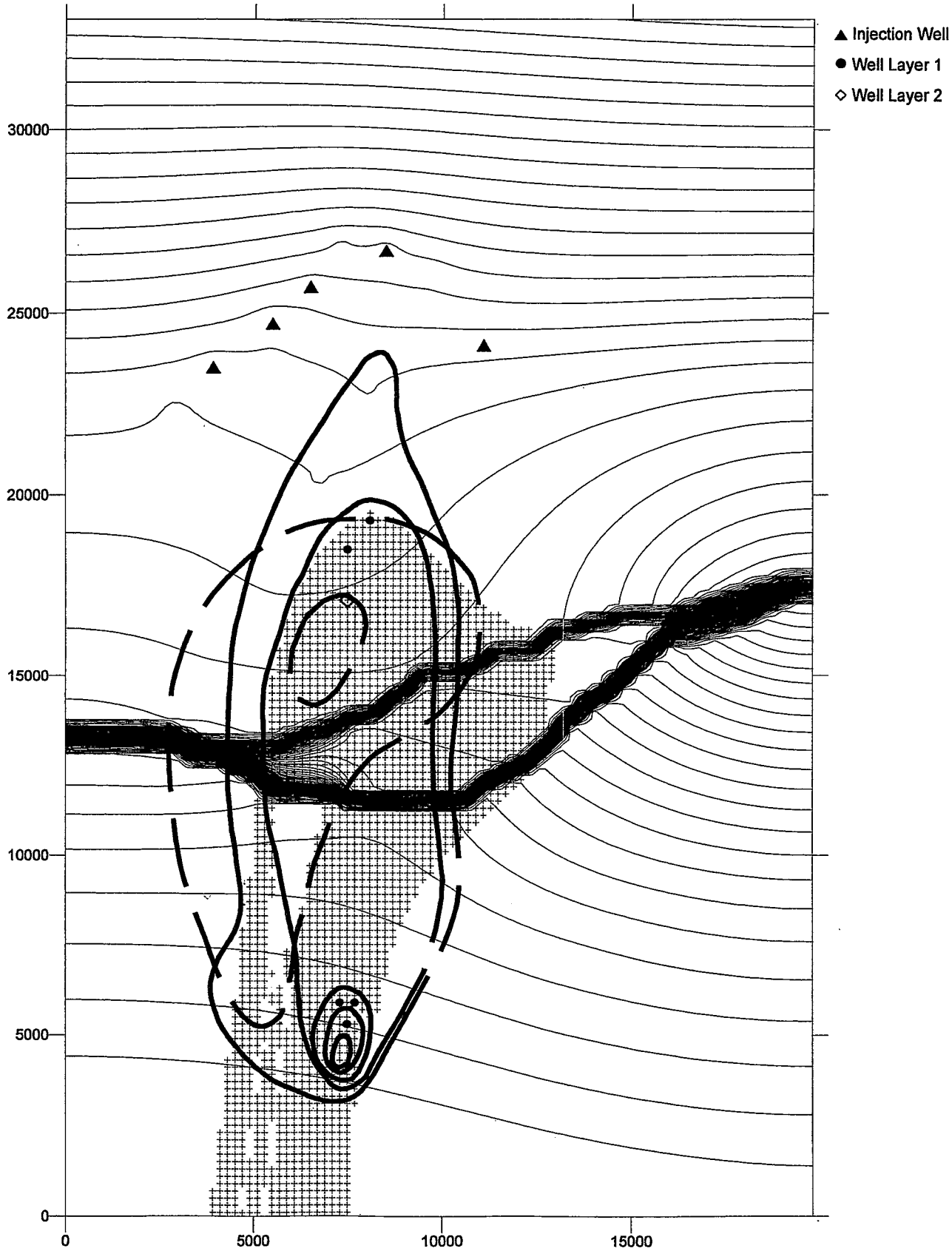
Figure 5-20: Shallow Particles, Contain Shallow 20-ppb & 50-ppb Plumes, & 500 gpm for Deep 20-ppb plume
(2620 gpm, 6 new wells, 0 existing wells)



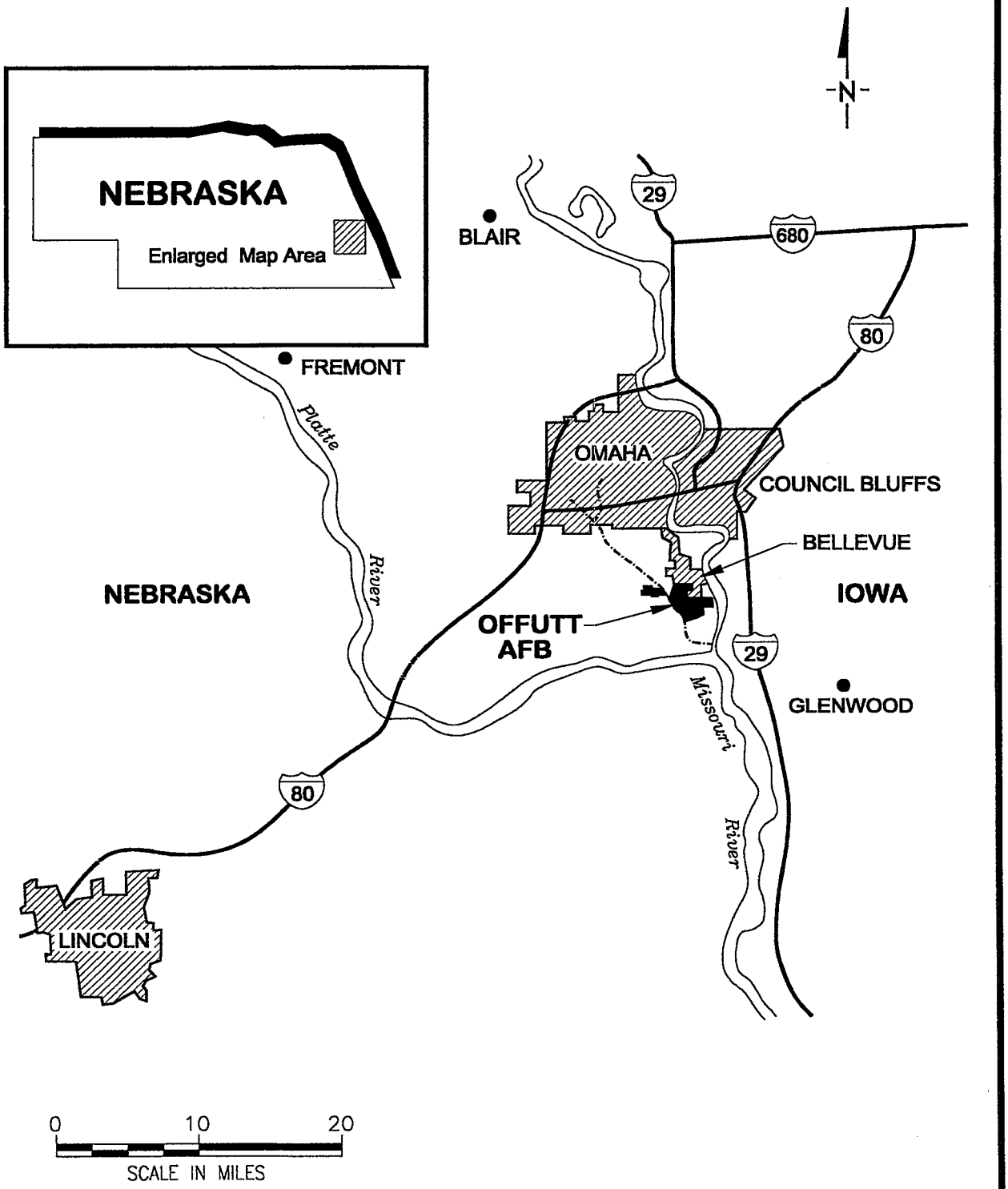
A "+" symbol indicates that a particle starting at that location is captured by one of the remediation wells, based on particle tracking with MODPATH. Shallow particles originate half-way down in layer 1.

Figure 5-21: Deep Particles, Contain Shallow 20-ppb & 50-ppb Plumes, & 500 gpm for Deep 20-ppb plume

(2620 gpm, 6 new wells, 0 existing wells)



A "+" symbol indicates that a particle starting at that location is captured by one of the remediation wells, based on particle tracking with MODPATH. Deep particles originate half-way down in layer 2.



ADAPTED FROM WOODWARD–CLYDE (1998)

H012013A.DWG

Figure 6–1. Site location map, Offutt.

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H012014A.DWG

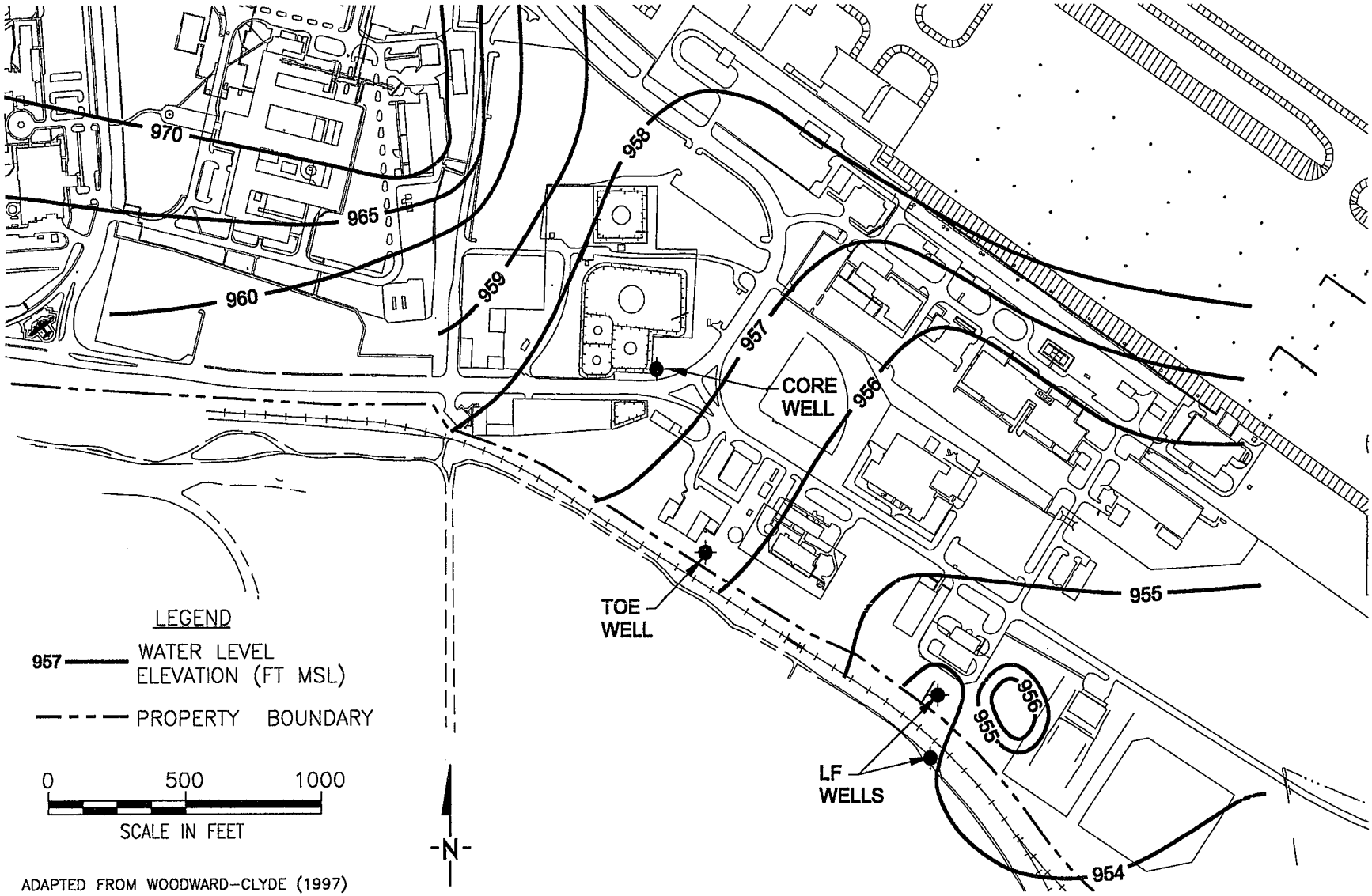

Figure 6-2. Groundwater elevation contours, Offutt.

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H012015A.DWG

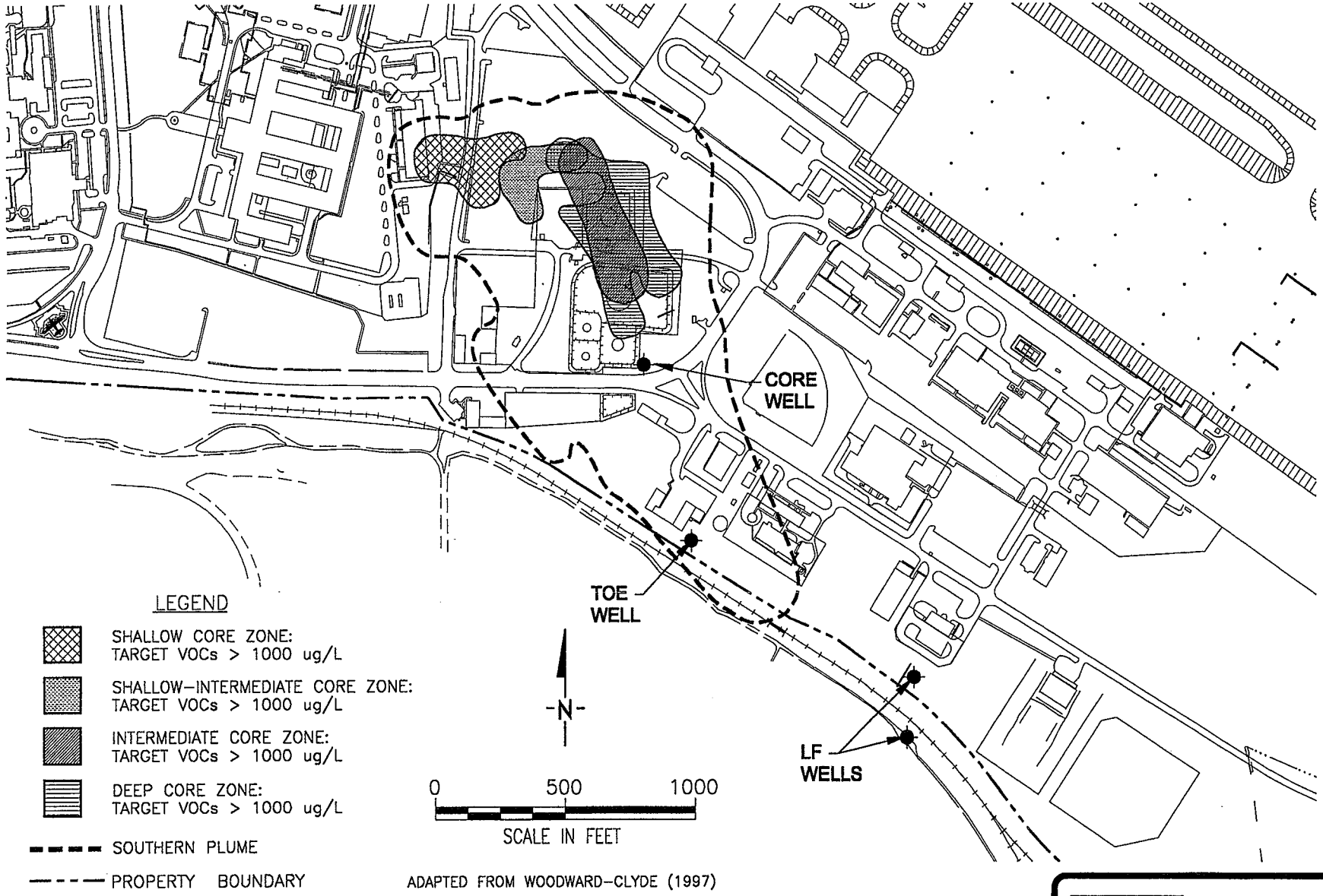

Figure 6–3. Southern plume and current remediation wells, Offutt.

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H012017A.DWG

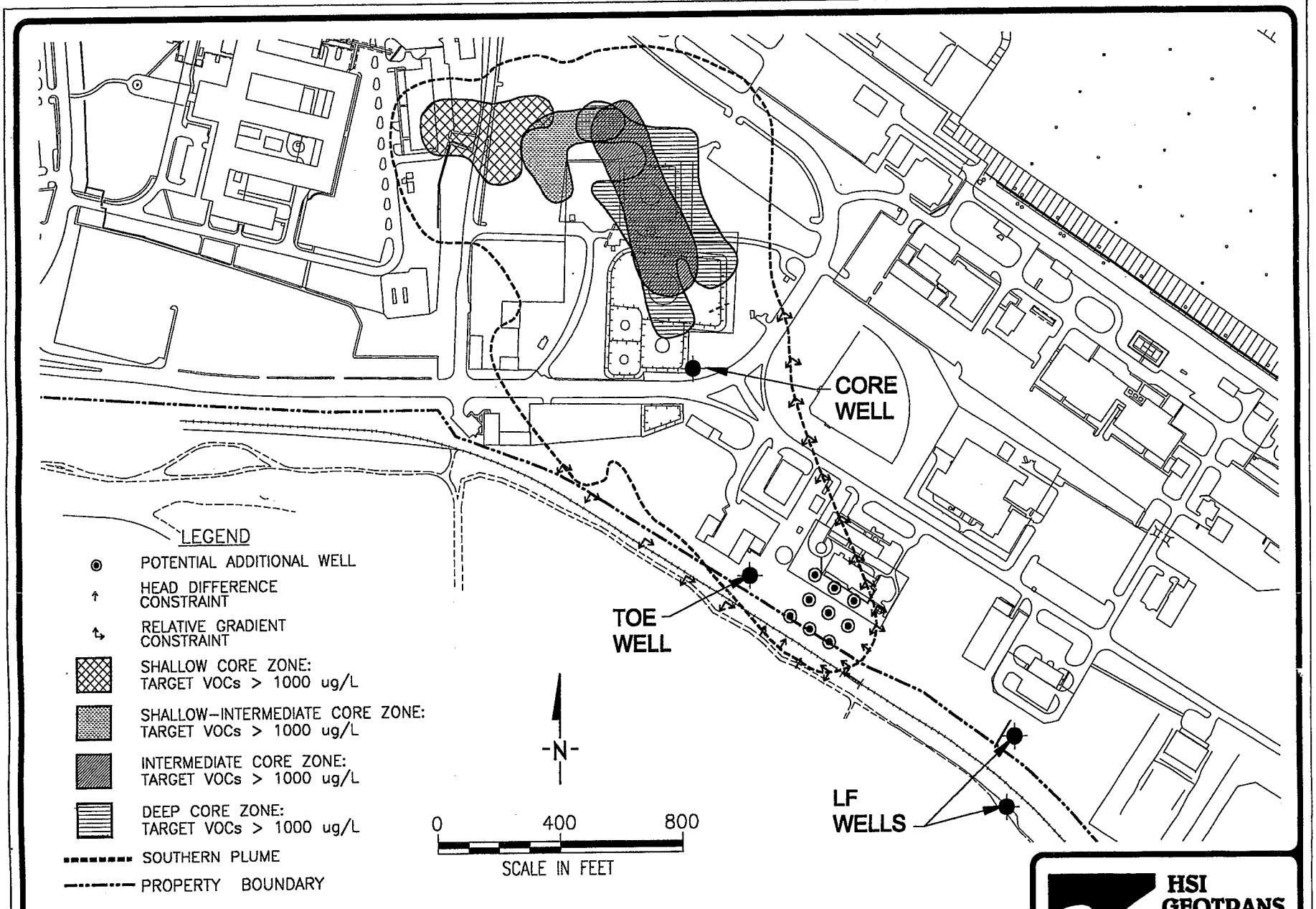
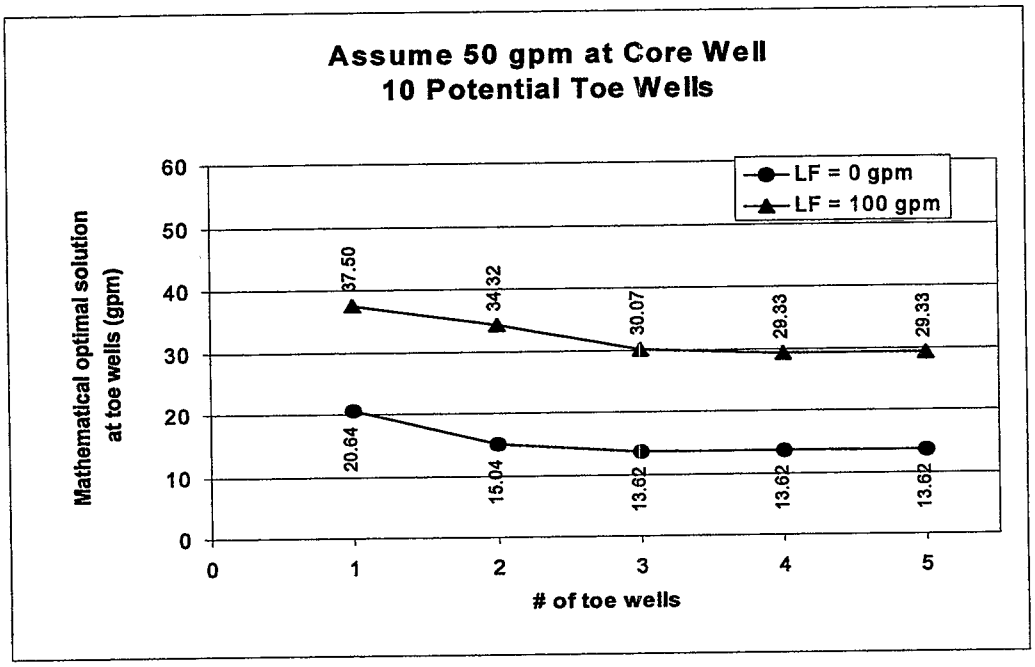
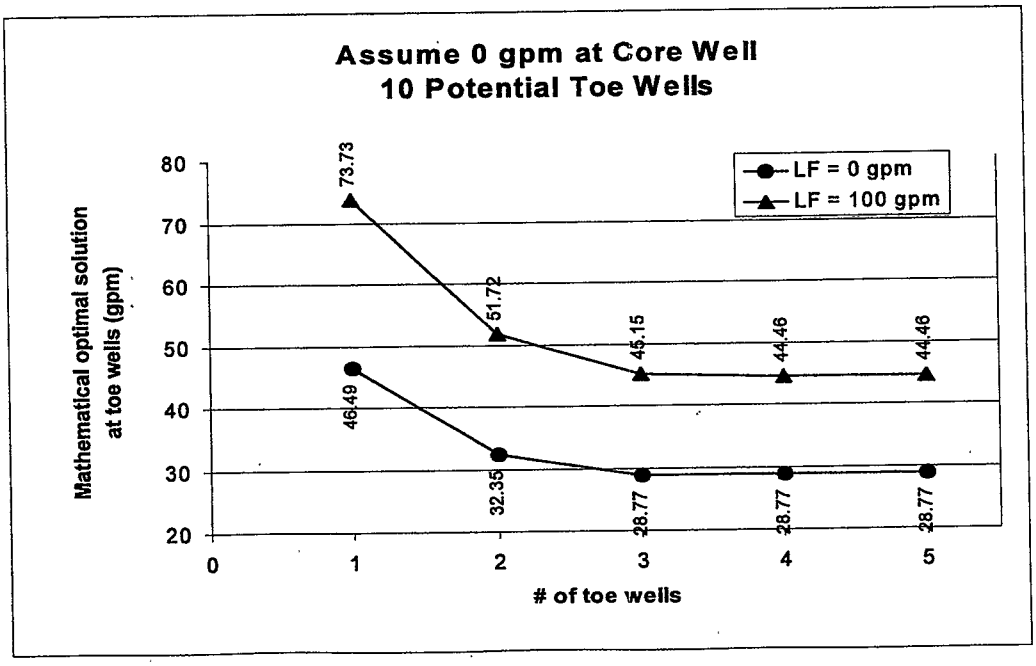


Figure 6-4. Constraint locations and potential additional wells, Offutt.

Figure 6-5. Solutions for multiple toe wells, Offutt.





TABLES

Table 4-1. Current system, Kentucky.

Screening Analysis

Site: **Kentucky**
Scenario: **Current System**

Discount Rate: 0.05

	Up-Front Costs	Annual Costs	# Years	Total of Annual Costs	Total Costs
O&M Costs					
-Electric	$0	$200,000	20	$2,617,064	$2,617,064
-Materials (pH adjustment)	$0	$100,000	20	$1,308,532	$1,308,532
-Maintenance	$0	$50,000	20	$654,266	$654,266
-Discharge Fees	$0	$0	20	$0	$0
-Annual O&M	$0	$250,000	20	$3,271,330	$3,271,330
-Analytical	$0	$0	20	$0	$0
-Steam	$0	$1,200,000	20	$15,702,385	$15,702,385
-Other 2	$0	$0	20	$0	$0
-Other 3	$0	$0	20	$0	$0
Costs of Analysis					
-Flow Modeling	$0	$0		$0	$0
-Transport Modeling	$0	$0		$0	$0
-Optimization	$0	$0		$0	$0
-Other 1	$0	$0		$0	$0
System Modification Costs					
-Engineering Design	$0	$0		$0	$0
-Regulatory Process	$0	$0		$0	$0
-New wells/pipes/equipment	$0	$0		$0	$0
-Increased Monitoring	$0	$0		$0	$0
-Other 1	$0	$0		$0	$0
-Other 2	$0	$0		$0	$0
-Other 3	$0	$0		$0	$0
Total Costs	**$0**	**$1,800,000**		**$23,553,578**	**$23,553,578**

Note: All costs are in present-day dollars. The discount rate is applied to annual costs to calculate the Net Present Value (NPV). The PV function in Microsoft Excel was utilized to calculate NPV, with payments applied at the beginning of each year.

Assumptions
Analytical costs not included.

Table 4-2. Summary of design well rates and maximum observed well rates (6/97 to 11/97), Kentucky.

Well	Design Rate (gpm)	Max Rate (gpm)	Comments
bw-1928	7.84	18.16	
bw-1929	36.67	15.62	
bw-1930	12.16	25.11	
bw-1931	2.73	15.56	
bw-1932	7.69	18.10	
bw-1933	48.57	36.55	
bw-1934	43.58	43.11	
bw-1935	42.59	32.42	
bw-1936	58.54	62.87	
bw-1937	62.90	61.84	
bw-1938	54.44	36.19	
bw-1939	29.71	34.63	
bw-1940	35.74	35.42	
bw-1941	37.97	33.36	
bw-1944	19.74	34.80	
bw-1945	19.79	35.21	
bw-1946	20.05	35.56	
bw-1947	8.78	35.99	
bw-1948	N/A	11.64	Installed after original design
bw-1949	N/A	29.78	Installed after original design
bw-1950	N/A	36.56	Installed after original design
bw-1952	N/A	2.04	Installed after original design
bw-1953	N/A	10.09	Installed after original design
BW Subtotal	*549.49*	*700.61*	
sw-1918	21.14	7.97	
sw-1920	8.26	20.80	
sw-1921	7.90	13.03	
sw-1924	81.29	63.84	
sw-1925	13.77	6.29	
sw-1926	4.00	10.61	
sw-1942	21.19	36.64	
sw-1943	13.04	30.91	
SW Subtotal	*170.59*	*190.01*	
ow-1914	12.00	6.96	
ow-1915	11.90	6.84	
ow-1916	12.41	7.22	
ow-1917	14.91	11.13	
ow-1919	21.82	20.11	
ow-1922	14.70	43.83	
ow-1923	31.69	39.96	
OW Subtotal	*131.67*	*143.17*	

Note: Max Rate refers to maximum observed rate between 6/97 and 11/97, based on daily measurements.

Table 5-1. Current system, Tooele.

Screening Analysis

Site: **Tooele**
Scenario: **Current System**

Discount Rate: 0.05

	Up-Front Costs	Annual Costs	# Years	Total of Annual Costs	Total Costs
O&M Costs					
-Electric	$0	$1,000,000	20	$13,085,321	$13,085,321
-Materials (Sodium Metaphosphate)	$0	$200,000	20	$2,617,064	$2,617,064
-Maintenance	$0	$30,000	20	$392,560	$392,560
-Discharge Fees	$0	$0	20	$0	$0
-Annual O&M	$0	$500,000	20	$6,542,660	$6,542,660
-Analytical	$0	$80,000	20	$1,046,826	$1,046,826
-Other 1	$0	$0	20	$0	$0
-Other 2	$0	$0	20	$0	$0
-Other 3	$0	$0	20	$0	$0
Costs of Analysis					
-Flow Modeling	$0	$0		$0	$0
-Transport Modeling	$0	$0		$0	$0
-Optimization	$0	$0		$0	$0
-Other 1	$0	$0		$0	$0
System Modification Costs					
-Engineering Design	$0	$0		$0	$0
-Regulatory Process	$0	$0		$0	$0
-New wells/pipes/equipment	$0	$0		$0	$0
-Increased Monitoring	$0	$0		$0	$0
-Other 1	$0	$0		$0	$0
-Other 2	$0	$0		$0	$0
-Other 3	$0	$0		$0	$0
Total Costs	**$0**	**$1,810,000**		**$23,684,431**	**$23,684,431**

Note: All costs are in present-day dollars. The discount rate is applied to annual costs to calculate the Net Present Value (NPV). The PV function in Microsoft Excel was utilized to calculate NPV, with payments applied at the beginning of each year.

<u>Assumptions</u>
None

Table 5-2. Example calculation for "Total Managed Cost", Tooele.

Calculate Total Managed Cost (Example)

Site: **Tooele**
Scenario: **12 new wells, total of 4200 gpm**

New Wells 12
Pumping Rate (gpm) 4200
Discount Rate: 0.05

	Up-Front Costs	Annual Costs	# Years	Total of Annual Costs	Total Costs
New Wells ($300K/well)	$3,600,000	$0	0	$0	$3,600,000
Managed Annual Costs ($150/yr/gpm)	$0	$630,000	20	$8,243,752	$8,243,752
Total Costs	**$3,600,000**	**$630,000**		**$8,243,752**	**$11,843,752**

Note: All costs are in present-day dollars. The discount rate is applied to annual costs to calculate the Net Present Value (NPV). The PV function in Microsoft Excel was utilized to calculate NPV, with payments applied at the beginning of each year.

Table 6-1. Current system, Offutt: one new core well, 100 gpm at LF wells.

Screening Analysis

Site: **Offutt**
Scenario: **Current System (Add 1 new core zone well, pump 200 gpm from 4 wells)**

Discount Rate: 0.05

	Up-Front Costs	Annual Costs	# Years	Total of Annual Costs	Total Costs
O&M Costs					
-Electric	$0	$2,000	20	$26,171	$26,171
-Materials	$0	$0	20	$0	$0
-Maintenance (Labor)	$0	$12,000	20	$157,024	$157,024
-Discharge (Core & LF 150 gpm, 20 yrs)	$0	$60,000	20	$785,119	$785,119
-Annual O&M	$0	$3,000	20	$39,256	$39,256
-Analytical	$0	$25,000	20	$327,133	$327,133
-Discharge (Toe Well, 50 gpm, 10 yrs)	$0	$20,000	10	$162,156	$162,156
-Other 2	$0	$0	20	$0	$0
-Other 3	$0	$0	20	$0	$0
Costs of Analysis					
-Flow Modeling	$0	$0		$0	$0
-Transport Modeling	$0	$0		$0	$0
-Optimization	$0	$0		$0	$0
-Other 1	$0	$0		$0	$0
System Modification Costs					
-Fixed Construction/All Scenarios	$47,000	$0		$0	$47,000
-Regulatory Process	$0	$0		$0	$0
-New wells/pipes/equipment	$40,000	$0		$0	$40,000
-Increased Monitoring	$0	$0		$0	$0
-Other 1	$0	$0		$0	$0
-Other 2	$0	$0		$0	$0
-Other 3	$0	$0		$0	$0
Total Costs	**$87,000**	**$122,000**		**$1,496,859**	**$1,583,859**

Note: All costs are in present-day dollars. The discount rate is applied to annual costs to calculate the Net Present Value (NPV).
The PV function in Microsoft Excel was utilized to calculate NPV, with payments applied at the beginning of each year.

Assumptions
Toe well can be shut off in 10 yrs

APPENDIX A:

OVERVIEW OF MODMAN

MODMAN Code History

MODMAN (Greenwald, 1998a) is a FORTRAN code developed by HSI GeoTrans that adds optimization capability to the U.S.G.S. finite-difference model for groundwater flow simulation in three dimensions, called MODFLOW-96 (Harbaugh and McDonald, 1996a,b). MODMAN, in conjunction with optimization software, yields answers to the following groundwater management questions: (1) where should pumping and injection wells be located, and (2) at what rate should water be extracted or injected at each well? The optimal solution maximizes or minimizes a user-defined objective function and satisfies all user-defined constraints. A typical objective may be to maximize the total pumping rate from all wells, while constraints might include upper and lower limits on heads, gradients, and pumping rates. A variety of objectives and constraints are available to the user, allowing many types of groundwater management issues to be considered.

MODMAN Version 1.5 was originally developed for the South Florida Water Management District (SFWMD) in 1989-1990. Emphasis was placed on the solution of water supply problems. The majority of code conceptualization, code de-bugging, and code documentation to date has been performed under contract to SFWMD. MODMAN Version 2.0, developed for the USEPA in 1990, included additional features for the solution of groundwater management problems related to plume containment and plume removal. MODMAN Version 2.1 was developed in 1992 for SFWMD to allow wells to be constrained to pump or inject only at their upper or lower allowable rates, if they are selected to pump at all in the optimal solution. MODMAN Version 3.0 was linked to a version of MODFLOW distributed by the International Ground Water Modeling Center (IGWMC). The current version, MODMAN Version 4.0, has been developed for the USEPA and is linked directly with the MODFLOW-96 code. A preprocessor for reading and writing MOMAN input files, and running MODMAN and LINDO from a user shell, is also now available (Greenwald, 1998b). This preprocessor runs in the Microsoft Windows environment.

The MODMAN code logic is an extension of AQMAN (Lefkoff and Gorelick, 1987), a code developed by the U.S. Geological Survey for two-dimensional groundwater management modeling. However, MODMAN is a significantly more comprehensive package than AQMAN, offering a large variety of management options and input/output features not available with the AQMAN code.

Flowchart for Executing MODMAN

A flowchart describing the optimization process is presented in Figure A-1. First, a groundwater model is calibrated with MODFLOW. A management problem is formulated and a MODMAN input file indicating user-defined choices for the objective function and constraints is created by the user. The decision variables are the pumping and/or injection rates at potential well locations. MODMAN utilizes the response matrix technique to transform the groundwater management problem into a linear or mixed-integer program. To perform the response matrix technique, a slightly modified version of MODFLOW is called repeatedly as a subroutine. The linear or mixed-integer program is written to an ASCII file in MPS (Mathematical Programming System) format. At this point, the execution of MODMAN in "mode 1" is complete.

The next step is to solve the linear or mixed-integer program. The MPS file is read into the optimization code LINDO (Lindo Systems, 1996) to determine the optimal solution. Specific LINDO commands generate an output file containing the optimal solution. MODMAN is then executed a second time ("mode 2") to read this file and post-process the optimal results. As part of the post-processing, MODMAN automatically inserts the optimal well rates into MODFLOW, performs a simulation based on the optimal well rates, indicates which constraints are "binding" (exactly satisfied by the optimal solution), and indicates if nonlinearities have significantly affected the optimization process. A methodology is suggested in the User's Guide (Greenwald, 1998a) to solve problems where nonlinearities significantly affect optimal results.

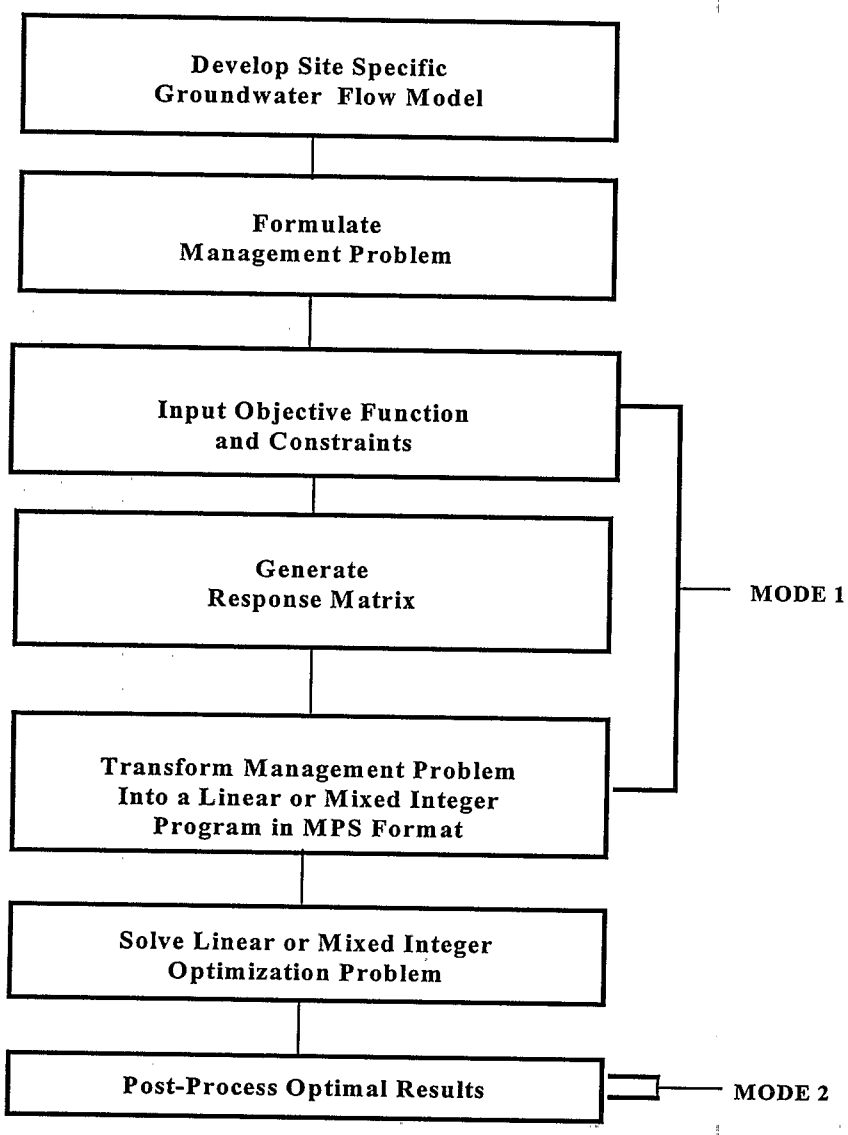


Figure A-1. General flowchart for executing MODMAN.

Linear Response Theory in Groundwater Systems Upon Which MODMAN is Based

Linear response theory in groundwater systems is based on the principle of linear superposition. The principle of linear superposition is two-fold in nature:

- multiplication of a well rate by a factor increases drawdown induced by that well by the same factor; and
- drawdown induced by more than one well is equal to the sum of drawdowns induced by each individual well.

Linear superposition, when applicable, is valid for both steady-state and transient groundwater systems. Linear superposition is not strictly applicable in unconfined systems, but often may be reasonably applied. Likewise, in some systems where river leakage, drains, or evapotranspiration are significant components, linear superposition is not strictly applicable but may often be reasonably applied. A detailed explanation of linear versus nonlinear responses in groundwater systems is presented in the User's Guide (Greenwald, 1998a).

Concept Of The Response Matrix

A response matrix, generated on the basis of linear superposition, allows drawdown induced by one or more wells to be calculated with matrix multiplication. For example, drawdown at three control locations, induced by two wells in a steady-state system, is calculated as follows:

$$\begin{bmatrix} s_1 \\ s_2 \\ s_3 \end{bmatrix} = \begin{bmatrix} R_{1A} & R_{1B} \\ R_{2A} & R_{2B} \\ R_{3A} & R_{3B} \end{bmatrix} \begin{bmatrix} Q_A \\ Q_B \end{bmatrix}$$

DRAWDOWN VECTOR **RESPONSE MATRIX** **WELL-RATE VECTOR**

where

s_i = drawdown at control location i (1, 2, or 3)
Q_j = rate at well j (A or B)
R_{ij} = drawdown response at location i to a unit stress at well j

Once the response matrix is known, any set of well rates may be entered and the resulting drawdowns calculated.

With a response matrix, drawdowns induced by wells are defined as linear combinations of well rates. This allows implementation of linear programming methodology, with well rates as the decision variables. The objective function and each constraint are written in terms of well rates, either directly or in terms of drawdowns (which are linearly determined from well rates). Constraints pertaining to heads, head differences, gradients and velocities may all be defined in terms of drawdown, and therefore be included in the optimization process.

The first step for generating the response matrix is to define control locations. These are locations where one or more hydrogeologic constraints, such as limits on head, will be applied. The second step is to define the location of each managed well (i.e., each decision well). Wells where rates are fixed, and therefore not part of the decision-

making process, are not managed wells and are called fixed wells. The third step is to compute the unmanaged head (explained below), in each stress period, at each control location. Then, one groundwater flow simulation is performed for each managed well location, to determine the coefficients for the response matrix.

Unmanaged Heads

Unmanaged heads refer to simulated heads resulting from unmanaged (i.e., background) flow conditions. Unmanaged flow conditions are created when all managed wells are turned off for the entire simulation. Unmanaged heads are a function of fixed well rates, boundary conditions, initial conditions (in transient cases), and hydrogeologic properties.

Unmanaged heads must be calculated before the response matrix can be generated. The reason is that drawdowns induced by each managed well must be discernible from drawdowns due to other factors, such as fixed wells. For instance, to determine drawdown induced by a well, it is first necessary to simulate heads with no pumping at the well (unmanaged head). Drawdown induced by rate Q at the well is the difference between heads resulting from rate Q and the unmanaged heads. All boundary effects, fixed wells, and hydrogeologic conditions are accounted for in both simulations. Then the drawdown induced by any rate at that particular well can be calculated, using the principle of linear superposition.

Concept Of A Unit Stress And Scaling

The coefficients in the response matrix are calculated for each managed well by applying a stress at that well, and determining the drawdown at each control location induced by that stress. The stress applied at a managed well to generate these coefficients is called the unit stress, or unit rate. The drawdown at each control location induced by the unit stress is called the drawdown response:

drawdown response	=	unmanaged head	-	head resulting from the unit stress

The unit response is defined as:

unit response = drawdown response / unit rate

and is interpreted as drawdown induced by a rate of one unit. Drawdown due to any other well rate is then calculated as:

induced drawdown = unit response * well rate.

The magnitude of the unit stress can be quite significant with regard to scaling. In general, a unit rate should be chosen that is the same magnitude as expected well rates. For example, if actual well rates are constrained to be between -1000 and -6000 units, a unit rate of -1000 units is much better than a unit rate of -1 unit. One reason is that a unit rate of -1 unit may yield such small drawdown responses that FORTRAN precision errors and MODFLOW convergence criteria become significant. Another reason is that a small unit rate will produce very small coefficients in the response matrix, which is not good for the LP/MIP solver (coefficients close to one are preferred for matrix inversions used to solve the LP or MIP). Both of these situations would be termed "scaling problems".

Repeated Simulations (Steady-State and Transient Cases)

To determine response coefficients for a managed well in a steady-state case, a unit rate is applied at that well while all other managed wells are turned off (rate of zero). This procedure is repeated for each managed well, with one simulation for each managed well.

For transient cases the same procedure is followed, but the unit rate is only applied in stress period 1. All stress periods are required to be of equal length. Drawdown responses in all periods are calculated in terms of a unit rate applied in stress period 1. The reason is that drawdown in each period is not only induced by pumping in that period, but also by pumping in previous periods. For instance, drawdown in period 2 is due to pumping in period 2 and pumping in period 1. Because stress periods are of equal length, drawdown in period 3 due to a stress in period 2 is the same as drawdown in period 2 due to the same stress in period 1. This feature allows the entire response matrix for transient systems to be constructed with one simulation per managed well, by applying unit stresses in period 1 only.

This concept is best illustrated with an example. Suppose there are two wells (A and B), two control locations (x and y), and three stress periods. First, unmanaged heads are calculated with MODFLOW, setting rates at wells A and B to zero for all three stress periods. Then drawdown responses for well A are calculated with MODFLOW, for the entire three periods, with a unit rate applied at well A during period 1 only, and no pumping at well B. The process is repeated for well B, with well A not pumping. Suppose the drawdown responses, at the end of each stress period, are as follows:

		DRAWDOWN RESPONSE IN STRESS PERIOD:		
LOCATION	PUMPING WELL	1 (pumping on)	2 (pumping off)	3 (pumping off)
x	A	-0.50	-0.20	-0.10
x	B	-0.75	-0.40	-0.25
y	A	-0.15	-0.05	-0.01
y	B	-1.50	-1.00	-0.60

Note that drawdown responses are negative. The sign convention for drawdown is positive for head lowered below a datum and negative for head raised above a datum. The sign convention for pumpage is negative for withdrawal and positive for injection. A negative pumpage (withdrawal) will create a positive drawdown and vice versa. Accordingly, the drawdown responses (matrix generated from a unit stress) will always be negative. The response matrix for this example, in matrix notation, is:

$$\begin{bmatrix} S_{x,1} \\ S_{x,2} \\ S_{x,1} \\ S_{x,2} \\ S_{x,1} \\ S_{x,2} \end{bmatrix} = \begin{bmatrix} -0.50 & -0.75 & 0.00 & 0.00 & 0.00 & 0.00 \\ -0.15 & -1.50 & 0.00 & 0.00 & 0.00 & 0.00 \\ -0.20 & -0.40 & -0.50 & -0.75 & 0.00 & 0.00 \\ -0.05 & -1.00 & -0.15 & -1.50 & 0.00 & 0.00 \\ -0.10 & -0.25 & -0.20 & -0.40 & -0.50 & -0.75 \\ -0.01 & -0.60 & -0.05 & -1.00 & -0.15 & -1.50 \end{bmatrix} \begin{bmatrix} Q_{A,1} \\ Q_{B,1} \\ Q_{A,2} \\ Q_{B,2} \\ Q_{A,3} \\ Q_{B,3} \end{bmatrix}$$

Managed drawdown, s, at each of the control points (x or y) can be calculated from the response matrix for any time period. For instance, managed drawdown at point x after period 2 is:

$$s_{x,2} = \underbrace{-0.20Q_{A,1} + -0.40Q_{B,1}}_{\text{---due to pumping in---}\ \textit{stress period 1}} + \underbrace{-0.50Q_{A,2} + -0.75Q_{B,2}}_{\text{---due to pumping in---}\ \textit{stress period 2}}$$

Note the predominance of zeroes above the main diagonal of the response matrix. This results because drawdown is due to current and previous pumpage, but not future pumpage. In the above example, drawdowns in time period 1 only depend on pumping in period 1, while drawdowns in period 2 are based on pumping in periods 1 and 2. Note the repetition of blocks within the response matrix. This structure is made possible by the fact that stress periods are of equal length, and allows efficient storage of the response matrix in the MODMAN code. Also note that the response matrix is fully generated by applying a unit stress, at each decision well, in the first stress period only.

APPENDIX B:

OVERVIEW OF SIMULATION-MANAGEMENT METHODS INCORPORATING TRANSPORT SIMULATIONS

Hydraulic optimization is based on simulation of groundwater flow. In many cases, the management objectives or constraints at a site may involve terms that cannot be rigorously evaluated with a groundwater flow model, such as contaminant concentrations and/or cleanup time. In those cases, solute transport models can be developed to predict contaminant concentrations over space and/or time, and simulation-management techniques based on the results of the contaminant transport simulations can be applied.

Many hydraulic optimization techniques (e.g., those employed by MODMAN) utilize the principle of linear superposition to transform the groundwater management problem into a linear program (see Appendix A). This is possible because, when linear superposition applies, drawdown is directly proportional to pumping rate. Unfortunately, there is no such linear relationship between concentrations and pumping rates. Increasing pumping rate by a factor of two does not decrease concentrations by a factor of two. Therefore, simulation-management problems involving contaminant transport require optimization techniques that are significantly more complex than linear programming.

Since the mid-1980's, a large number of transport-based simulation-management approaches have been described in the literature. These techniques are typically computer-intensive, but with improved algorithms and constantly improving computer speeds, these techniques are likely to become more mainstream within the next several years. A full review of transport-based simulation-management modeling is well beyond the scope of this report. The interested reader can begin with some of the references indicated in Appendix I of this report. A partial listing of researchers that are particularly active in code development for transport-based simulation-management modeling is as follows:

David Dougherty
Richard Peralta
Christine Shoemaker
Brian Wagner
Chunmiao Zheng

Contact information for these individuals is presented in Appendix I.

APPENDIX C:

OVERVIEW OF SIMULATION-MANAGEMENT METHODS INCORPORATING UNCERTAINTY AND/OR RISK

The applications of hydraulic optimization presented in this study are based on deterministic groundwater flow simulations (i.e., model parameters are assumed to be known precisely). Impacts to mathematical optimal solutions from uncertainties associated with the groundwater flow model are not accounted for. Stochastic groundwater management tools are required to account for:

(1) parameter uncertainty; and/or
(2) spatially variable aquifer properties that can only be represented statistically.

Coupling of stochastic techniques with simulation-management models can allow uncertainty and risk to be incorporated into the optimization algorithm. For example, one can specify that constraints be satisfied within a specified reliability (e.g., constraints satisfied with 95% reliability). Another example is to specify constraints that satisfy multiple potential realizations for spatial distribution of key aquifer parameters (e.g., hydraulic conductivity), rather than one realization in a deterministic model. Stochastic approaches to simulation-management modeling have been applied to both hydraulic optimization and transport optimization problems.

A full review of this topic is well beyond the scope of this report. A brief description is provided in Appendix B of Gorelick et. al. (1993). An excellent resource for this area of research is Brian Wagner at the U.S.G.S. (see Appendix I for contact information).

APPENDIX D:

PARTIAL LISTING OF MODMAN APPLICATIONS

Douthitt, Jeff W. And Bruce E. Phillips, 1994, "*Model Assisted Design of a Groundwater Pump and Treat System at the Paducah Gaseous Diffusion Plant*", Toxic Substances and the Hydrologic Sciences, American Institute of Hydrology, pp. 346 to 365.

Greenwald, Robert M. and Joost C. Herweijer, Ira Star, Mark Gallagher, and Allan L. Dreher, 1992, "*Optimization of Well Locations and Rates for Containment of Contaminants Utilizing an Automated Management Routine Coupled to MODFLOW: A Case History*", Solving Ground Water Problems With Models, Dallas, Texas, February 1992.

Hagemeyer, Todd R., Peter F. Andersen, Robert M. Greenwald, and Jay L. Clausen, 1993, "*Evaluation of Alternative Plume Containment Designs at the Paducah Gaseous Diffusion Plant Using MODMAN, A Well Pumpage Optimization Module for MODFLOW*", IGWMC Modeling Conference, Golden, Colorado, June 1993.

Johnson, Kevin D. and James D. Bowen, 1993, "*Trade-Offs Between Pumping and Slurry Walls Under Changing Hydraulic Parameters*", IGWMC Modeling Conference, Golden, Colorado, June 1993.

McCready, Roger W. And Robert M. Greenwald, 1997, "*Pump-and-Treat Well Location and Rate Optimization Using MODFLOW and MODMAN: A Case Study*", Midwest Groundwater Conference, Coralville, Iowa, October 1997 (Abstract Only).

Russell, K.T. and A.J. Rabideau, "*Decision Analysis for Pump-and-Treat Design*", Ground Water Monitoring and Remediation (in press).

Russell, K.T. and A.J. Rabideau, "*Simulating the Reliability of Pump-and-treat Systems*", Ground Water Monitoring and Remediation (in review).

APPENDIX E:

SAMPLE MODMAN INPUT: KENTUCKY

```
grmm2a-1.INP:  Apples to Apples, Kentucky
SET0: General Parameters
   1(MODE)       .01       .01       .01    1.E-03       .01         1
SET1: Time Parameters
         1      1.00         1      1.00
SET2: Well Information
  43   0  43
         1         1         8        28          -1000.00          /bw-1928
         2         1         9        30          -1000.00          /bw-1929
         3         1         9        32          -1000.00          /bw-1930
         4         1         9        34          -1000.00          /bw-1931
         5         1         9        35          -1000.00          /bw-1932
         6         1         9        37          -1000.00          /bw-1933
         7         1         9        39          -1000.00          /bw-1934
         8         1        11        42          -1000.00          /bw-1935
         9         1        10        45          -1000.00          /bw-1936
        10         1        10        48          -1000.00          /bw-1937
        11         1        10        51          -1000.00          /bw-1938
        12         1        10        53          -1000.00          /bw-1939
        13         1        10        55          -1000.00          /bw-1940
        14         1        11        57          -1000.00          /bw-1941
        15         1        13        59          -1000.00          /bw-1947
        16         1        11        64          -1000.00          /bw-1944
        17         1         9        68          -1000.00          /bw-1946
        18         1        12        69          -1000.00          /bw-1945
        19         1        12        40          -1000.00          /sw-1926
        20         1        13        39          -1000.00          /sw-1925
        21         1        14        38          -1000.00          /sw-1924
        22         1        20        36          -1000.00          /sw-1921
        23         1        25        40          -1000.00          /sw-1920
        24         1        30        35          -1000.00          /sw-1918
        25         1        13        66          -1000.00          /sw-1943
        26         1        14        64          -1000.00          /sw-1942
        27         1        15        35          -1000.00          /ow-1923
        28         1        18        33          -1000.00          /ow-1922
        29         1        22        31          -1000.00          /ow-1919
        30         1        25        29          -1000.00          /ow-1917
        31         1        33        26          -1000.00          /ow-1916
        32         1        35        19          -1000.00          /ow-1915
        33         1        36        13          -1000.00          /ow-1914
        34         1        37         6          -1000.00          /ow-1913
        35         1         8        41          -1000.00          /bw-1948 (not used this run)
        36         1         8        44          -1000.00          /bw-1949 (not used this run)
        37         1        13        58          -1000.00          /bw-1950 (not used this run)
        38         1        11        62          -1000.00          /bw-1952 (not used this run)
        39         1        10        62          -1000.00          /bw-1953 (not used this run)
        40         1        16        62          -1000.00          /new-1   (not used this run)
        41         1        15        52          -1000.00          /new-2   (not used this run)
        42         1        14        42          -1000.00          /new-3   (not used this run)
        43         1        21        40          -1000.00          /new-4   (not used this run)
   1         1         M          -3496.04    0.E+00         /bw-1928
   1         2         M          -3007.06    0.E+00         /bw-1929
   1         3         M          -4834.01    0.E+00         /bw-1930
   1         4         M          -2995.51    0.E+00         /bw-1931
   1         5         M          -3484.49    0.E+00         /bw-1932
   1         6         M          -7036.36    0.E+00         /bw-1933
   1         7         M          -8299.25    0.E+00         /bw-1934
   1         8         M          -6241.28    0.E+00         /bw-1935
   1         9         M         -1.21E+04    0.E+00         /bw-1936
   1        10         M        -1.191E+04    0.E+00         /bw-1937
   1        11         M          -6967.06    0.E+00         /bw-1938
   1        12         M          -6666.74    0.E+00         /bw-1939
   1        13         M          -6818.82    0.E+00         /bw-1940
   1        14         M          -6422.25    0.E+00         /bw-1941
   1        15         M          -6928.56    0.E+00         /bw-1947
   1        16         M          -6699.47    0.E+00         /bw-1944
   1        17         M          -6845.78    0.E+00         /bw-1946
   1        18         M          -6778.40    0.E+00         /bw-1945
   1        19         M           -770.00   -770.00         /sw-1926
   1        20         M          -2650.00  -2650.00         /sw-1925
```

1	21	M	-1.565E+04	-1.565E+04	/sw-1924	
1	22	M	-1520.00	-1520.00	/sw-1921	
1	23	M	-1590.00	-1590.00	/sw-1920	
1	24	M	-4070.00	-4070.00	/sw-1918	
1	25	M	-2510.00	-2510.00	/sw-1943	
1	26	M	-4080.00	-4080.00	/sw-1942	
1	27	M	-6100.00	-6100.00	/ow-1923	
1	28	M	-2830.00	-2830.00	/ow-1922	
1	29	M	-4200.00	-4200.00	/ow-1919	
1	30	M	-2870.00	-2870.00	/ow-1917	
1	31	M	-2390.00	-2390.00	/ow-1916	
1	32	M	-2290.00	-2290.00	/ow-1915	
1	33	M	-2310.00	-2310.00	/ow-1914	
1	34	M	-2360.00	-2360.00	/ow-1913	
1	35	M	0.E+00	0.E+00	/bw-1948	(not used this run)
1	36	M	0.E+00	0.E+00	/bw-1949	(not used this run)
1	37	M	0.E+00	0.E+00	/bw-1950	(not used this run)
1	38	M	0.E+00	0.E+00	/bw-1952	(not used this run)
1	39	M	0.E+00	0.E+00	/bw-1953	(not used this run)
1	40	M	0.E+00	0.E+00	/new-1	(not used this run)
1	41	M	0.E+00	0.E+00	/new-2	(not used this run)
1	42	M	0.E+00	0.E+00	/new-3	(not used this run)
1	43	M	0.E+00	0.E+00	/new-4	(not used this run)

SET3: Control Locations

52

1	1	6	64
2	1	6	65
3	1	6	66
4	1	6	71
5	1	7	28
6	1	7	35
7	1	7	36
8	1	7	37
9	1	7	38
10	1	7	39
11	1	7	40
12	1	7	41
13	1	7	42
14	1	7	43
15	1	7	44
16	1	7	45
17	1	7	46
18	1	7	47
19	1	7	48
20	1	7	49
21	1	7	50
22	1	7	51
23	1	7	52
24	1	7	53
25	1	7	54
26	1	7	55
27	1	7	56
28	1	7	57
29	1	7	58
30	1	7	59
31	1	7	60
32	1	7	61
33	1	7	64
34	1	7	67
35	1	7	68
36	1	7	69
37	1	7	70
38	1	8	29
39	1	8	30
40	1	8	31
41	1	8	32
42	1	8	33
43	1	8	34
44	1	8	61
45	1	8	63
46	1	9	60
47	1	9	63
48	1	10	60
49	1	10	62
50	1	11	59
51	1	11	62

```
        52          1         12         62
SET4: Head Limits
  52
         1          1          1    0.E+00    301.99
         2          1          2    0.E+00    301.99
         3          1          3    0.E+00    301.99
         4          1          4    0.E+00    301.99
         5          1          5    0.E+00    301.99
         6          1          6    0.E+00    301.99
         7          1          7    0.E+00    301.99
         8          1          8    0.E+00    301.99
         9          1          9    0.E+00    301.99
        10          1         10    0.E+00    301.99
        11          1         11    0.E+00    301.99
        12          1         12    0.E+00    301.99
        13          1         13    0.E+00    301.99
        14          1         14    0.E+00    301.99
        15          1         15    0.E+00    301.99
        16          1         16    0.E+00    301.99
        17          1         17    0.E+00    301.99
        18          1         18    0.E+00    301.99
        19          1         19    0.E+00    301.99
        20          1         20    0.E+00    301.99
        21          1         21    0.E+00    301.99
        22          1         22    0.E+00    301.99
        23          1         23    0.E+00    301.99
        24          1         24    0.E+00    301.99
        25          1         25    0.E+00    301.99
        26          1         26    0.E+00    301.99
        27          1         27    0.E+00    301.99
        28          1         28    0.E+00    301.99
        29          1         29    0.E+00    301.99
        30          1         30    0.E+00    301.99
        31          1         31    0.E+00    301.99
        32          1         32    0.E+00    301.99
        33          1         33    0.E+00    301.99
        34          1         34    0.E+00    301.99
        35          1         35    0.E+00    301.99
        36          1         36    0.E+00    301.99
        37          1         37    0.E+00    301.99
        38          1         38    0.E+00    301.99
        39          1         39    0.E+00    301.99
        40          1         40    0.E+00    301.99
        41          1         41    0.E+00    301.99
        42          1         42    0.E+00    301.99
        43          1         43    0.E+00    301.99
        44          1         44    0.E+00    301.99
        45          1         45    0.E+00    301.99
        46          1         46    0.E+00    301.99
        47          1         47    0.E+00    301.99
        48          1         48    0.E+00    301.99
        49          1         49    0.E+00    301.99
        50          1         50    0.E+00    301.99
        51          1         51    0.E+00    301.99
        52          1         52    0.E+00    301.99
SET5: Head Difference Limits
   0
SET6: Drawdown Limits
   0
SET7A: Gradient Limits
   0
SET7B: Velocity Limits
   0
SET7C: Relative Gradient Limits
   0
SET8: Balance Constraints
   0
SET9: Integer Constraints
   1
         1          B          1          L         18         18          /limit # BW wells to 18 or less
   1
   2
   3
   4
   5
   6
```

```
 7
 8
 9
10
11
12
13
14
15
16
17
18
SET10: Objective Function
        1        43                                  /* convert to positive gpm
 1   1  -5.194E-03
 1   2  -5.194E-03
 1   3  -5.194E-03
 1   4  -5.194E-03
 1   5  -5.194E-03
 1   6  -5.194E-03
 1   7  -5.194E-03
 1   8  -5.194E-03
 1   9  -5.194E-03
 1  10  -5.194E-03
 1  11  -5.194E-03
 1  12  -5.194E-03
 1  13  -5.194E-03
 1  14  -5.194E-03
 1  15  -5.194E-03
 1  16  -5.194E-03
 1  17  -5.194E-03
 1  18  -5.194E-03
 1  19  -5.194E-03
 1  20  -5.194E-03
 1  21  -5.194E-03
 1  22  -5.194E-03
 1  23  -5.194E-03
 1  24  -5.194E-03
 1  25  -5.194E-03
 1  26  -5.194E-03
 1  27  -5.194E-03
 1  28  -5.194E-03
 1  29  -5.194E-03
 1  30  -5.194E-03
 1  31  -5.194E-03
 1  32  -5.194E-03
 1  33  -5.194E-03
 1  34  -5.194E-03
 1  35  -5.194E-03
 1  36  -5.194E-03
 1  37  -5.194E-03
 1  38  -5.194E-03
 1  39  -5.194E-03
 1  40  -5.194E-03
 1  41  -5.194E-03
 1  42  -5.194E-03
 1  43  -5.194E-03
```

APPENDIX F:

SAMPLE MODMAN INPUT: TOOELE

```
TOMM1-1:  5 ppb plume, shallow and deep
SET0: General Parameters
   1(MODE)        .01        .01        .01    1.E-03        .01          1
SET1: Time Parameters
          1       1.00          1       1.00
SET2: Well Information
  80    0  80
          1          1         63         48          -9.626E+04  e1-1
          2          1         76         41          -9.626E+04  e2-1
          3          2         77         41          -9.626E+04  e2-2
          4          1         88         49          -9.626E+04  e3-1
          5          2         88         48          -9.626E+04  e3-2
          6          2        102         37          -9.626E+04  e4-2
          7          2        104         45          -9.626E+04  e5-2
          8          1        115         37          -9.626E+04  e6-1
          9          2        115         37          -9.626E+04  e6-2
         10          1        109         45          -9.626E+04  e8-1
         11          2        109         45          -9.626E+04  e8-2
         12          1         94         48          -9.626E+04  e9-1
         13          2         94         48          -9.626E+04  e9-2
         14          3         94         48          -9.626E+04  e9-3
         15          1         95         53          -9.626E+04  e10-1
         16          2         95         53          -9.626E+04  e10-2
         17          1         57         45          -9.626E+04  e11-1
         18          1         45         45          -9.626E+04  e12-1
         19          1         84         28          -9.626E+04  e13-1
         20          1         90         32          -9.626E+04  e14-1
         21          2         90         32          -9.626E+04  e14-2
         22          1         64         34          -9.626E+04  e15-1
         23          2         64         34          -9.626E+04  e15-2
         24          1         72         65           9.626E+04  i1-1
         25          1         62         61           9.626E+04  i2-1
         26          2         62         61           9.626E+04  i2-2
         27          1         58         60           9.626E+04  i3-1
         28          1         53         58           9.626E+04  i4-1
         29          1         45         56           9.626E+04  i5-1
         30          1         40         54           9.626E+04  i6-1
         31          2         40         54           9.626E+04  i6-2
         32          1         35         49           9.626E+04  i7-1
         33          2         35         49           9.626E+04  i7-2
         34          1         32         43           9.626E+04  i8-1
         35          1         31         37           9.626E+04  i9-1
         36          2         31         37           9.626E+04  i9-2
         37          1         37         33           9.626E+04  i10-1
         38          2         37         33           9.626E+04  i10-2
         39          1         42         28           9.626E+04  i11-1
         40          1         48         20           9.626E+04  i12-1
         41          1         54         15           9.626E+04  i13-1
         42          2         54         15           9.626E+04  i13-2
         43          1         52         41          -9.626E+04  /* new s1
         44          1         54         39          -9.626E+04  /* new s2
         45          1         54         43          -9.626E+04  /* new s3
         46          1         58         37          -9.626E+04  /* new s4
         47          1         58         41          -9.626E+04  /* new s5
         48          1         63         41          -9.626E+04  /* new s6
         49          1         72         34          -9.626E+04  /* new s7
         50          1         72         41          -9.626E+04  /* new s8
```

51	1	72	48	-9.626E+04	/* new s9
52	1	79	32	-9.626E+04	/* new s10
53	1	79	41	-9.626E+04	/* new s11
54	1	79	48	-9.626E+04	/* new s12
55	1	85	32	-9.626E+04	/* new s13
56	1	85	41	-9.626E+04	/* new s14
57	1	85	48	-9.626E+04	/* new s15
58	1	47	42	-9.626E+04	/* new s16
59	1	48	41	-9.626E+04	/* new s17
60	1	48	43	-9.626E+04	/* new s18
61	1	50	40	-9.626E+04	/* new s19
62	1	50	43	-9.626E+04	/* new s20
63	2	71	37	-9.626E+04	/* new d1/21
64	2	71	41	-9.626E+04	/* new d2/22
65	2	71	45	-9.626E+04	/* new d3/23
66	2	75	29	-9.626E+04	/* new d4/24
67	2	75	35	-9.626E+04	/* new d5/25
68	2	75	41	-9.626E+04	/* new d6/26
69	2	75	47	-9.626E+04	/* new d7/27
70	2	80	29	-9.626E+04	/* new d8/28
71	2	80	35	-9.626E+04	/* new d9/29
72	2	80	41	-9.626E+04	/* new d10/30
73	2	80	47	-9.626E+04	/* new d11/31
74	2	86	23	-9.626E+04	/* new d12/32
75	2	86	29	-9.626E+04	/* new d13/33
76	2	86	35	-9.626E+04	/* new d14/34
77	2	86	41	-9.626E+04	/* new d15/35
78	2	86	47	-9.626E+04	/* new d16/36
79	2	87	19	-9.626E+04	/* new d17/37
80	2	81	23	-9.626E+04	/* new d18/38

1	1	M	-9.626E+04	0.E+00	e1-1
1	2	M	-9.626E+04	0.E+00	e2-1
1	3	M	-9.626E+04	0.E+00	e2-2
1	4	M	-9.626E+04	0.E+00	e3-1
1	5	M	-9.626E+04	0.E+00	e3-2
1	6	M	-1.296E+05	0.E+00	e4-2
1	7	M	-1.388E+05	0.E+00	e5-2
1	8	M	-9.626E+04	0.E+00	e6-1
1	9	M	-1.637E+04	0.E+00	e6-2
1	10	M	-9.626E+04	0.E+00	e8-1
1	11	M	-3.85E+04	0.E+00	e8-2
1	12	M	-9.626E+04	0.E+00	e9-1
1	13	M	-9.968E+04	0.E+00	e9-2
1	14	M	-9.626E+04	0.E+00	e9-3
1	15	M	-9.626E+04	0.E+00	e10-1
1	16	M	-1.196E+05	0.E+00	e10-2
1	17	M	-9.626E+04	0.E+00	e11-1
1	18	M	-9.626E+04	0.E+00	e12-1
1	19	M	-1.119E+05	0.E+00	e13-1
1	20	M	-9.626E+04	0.E+00	e14-1
1	21	M	-7.523E+04	0.E+00	e14-2
1	22	M	-8.424E+04	0.E+00	e15-1
1	23	M	-9.626E+04	0.E+00	e15-2
1	24	M	0.E+00	9.626E+04	i1-1
1	25	M	0.E+00	9.626E+04	i2-1
1	26	M	0.E+00	2.12E+04	i2-2
1	27	M	0.E+00	9.626E+04	i3-1
1	28	M	0.E+00	1.315E+05	i4-1
1	29	M	0.E+00	1.996E+05	i5-1
1	30	M	0.E+00	5.548E+04	i6-1
1	31	M	0.E+00	9.626E+04	i6-2
1	32	M	0.E+00	1.131E+05	i7-1
1	33	M	0.E+00	9.626E+04	i7-2
1	34	M	0.E+00	1.222E+05	i8-1
1	35	M	0.E+00	8.94E+04	i9-1
1	36	M	0.E+00	9.626E+04	i9-2

```
1        37        M            0.E+00 7.754E+04      i10-1
1        38        M            0.E+00 9.626E+04      i10-2
1        39        M            0.E+00 1.398E+05      i11-1
1        40        M            0.E+00 9.626E+04      i12-1
1        41        M            0.E+00 9.626E+04      i13-1
1        42        M            0.E+00 1.925E+04      i13-2
1        43        M        -9.626E+04    0.E+00      /* new s1
1        44        M        -9.626E+04    0.E+00      /* new s2
1        45        M        -9.626E+04    0.E+00      /* new s3
1        46        M        -9.626E+04    0.E+00      /* new s4
1        47        M        -9.626E+04    0.E+00      /* new s5
1        48        M        -9.626E+04    0.E+00      /* new s6
1        49        M        -9.626E+04    0.E+00      /* new s7
1        50        M        -9.626E+04    0.E+00      /* new s8
1        51        M        -9.626E+04    0.E+00      /* new s9
1        52        M        -9.626E+04    0.E+00      /* new s10
1        53        M        -9.626E+04    0.E+00      /* new s11
1        54        M        -9.626E+04    0.E+00      /* new s12
1        55        M        -9.626E+04    0.E+00      /* new s13
1        56        M        -9.626E+04    0.E+00      /* new s14
1        57        M        -9.626E+04    0.E+00      /* new s15
1        58        M        -9.626E+04    0.E+00      /* new s16
1        59        M        -9.626E+04    0.E+00      /* new s17
1        60        M        -9.626E+04    0.E+00      /* new s18
1        61        M        -9.626E+04    0.E+00      /* new s19
1        62        M        -9.626E+04    0.E+00      /* new s20
1        63        M        -9.626E+04    0.E+00      /* new d1/21
1        64        M        -9.626E+04    0.E+00      /* new d2/22
1        65        M        -9.626E+04    0.E+00      /* new d3/23
1        66        M        -9.626E+04    0.E+00      /* new d4/24
1        67        M        -9.626E+04    0.E+00      /* new d5/25
1        68        M        -9.626E+04    0.E+00      /* new d6/26
1        69        M        -9.626E+04    0.E+00      /* new d7/27
1        70        M        -9.626E+04    0.E+00      /* new d8/28
1        71        M        -9.626E+04    0.E+00      /* new d9/29
1        72        M        -9.626E+04    0.E+00      /* new d10/30
1        73        M        -9.626E+04    0.E+00      /* new d11/31
1        74        M        -9.626E+04    0.E+00      /* new d12/32
1        75        M        -9.626E+04    0.E+00      /* new d13/33
1        76        M        -9.626E+04    0.E+00      /* new d14/34
1        77        M        -9.626E+04    0.E+00      /* new d15/35
1        78        M        -9.626E+04    0.E+00      /* new d16/36
1        79        M        -9.626E+04    0.E+00      /* new d17/37
1        80        M        -9.626E+04    0.E+00      /* new d18/38
SET3: Control Locations
 114
        1        1        85        23                /*shallow 5-ppb
        2        1        84        23
        3        1        85        24
        4        1        80        24
        5        1        79        24
        6        1        80        25
        7        1        76        25
        8        1        75        25
        9        1        76        26
       10        1        73        26
       11        1        72        26
       12        1        73        27
       13        1        68        28
       14        1        67        28
       15        1        68        29
       16        1        63        30
       17        1        62        30
       18        1        63        31
       19        1        58        33
       20        1        57        33
```

21	1	58	34	
22	1	53	36	
23	1	52	36	
24	1	53	37	
25	1	49	39	
26	1	48	39	
27	1	49	40	
28	1	46	42	
29	1	47	42	
30	1	52	44	
31	1	51	44	
32	1	52	43	
33	1	51	45	
34	1	50	45	
35	1	51	44	
36	1	54	46	
37	1	53	46	
38	1	54	45	
39	1	58	47	
40	1	57	47	
41	1	58	46	
42	1	61	48	
43	1	60	48	
44	1	61	47	
45	1	65	49	
46	1	64	49	
47	1	65	48	
48	1	68	50	
49	1	67	50	
50	1	68	49	
51	1	71	51	
52	1	70	51	
53	1	71	50	
54	1	75	52	
55	1	74	52	
56	1	75	51	
57	1	79	52	
58	1	78	52	
59	1	79	51	
60	1	82	53	
61	1	82	52	
62	1	85	53	
63	1	85	52	
64	2	90	15	/*deep 5-ppb
65	2	89	15	
66	2	90	16	
67	2	84	17	
68	2	83	17	
69	2	84	18	
70	2	79	20	
71	2	78	20	
72	2	79	21	
73	2	75	24	
74	2	74	24	
75	2	75	25	
76	2	72	28	
77	2	71	28	
78	2	72	29	
79	2	70	31	
80	2	69	31	
81	2	70	32	
82	2	69	35	
83	2	68	35	
84	2	69	36	
85	2	69	39	
86	2	70	39	

```
        87          2          69          41
        88          2          70          41
        89          2          69          43
        90          2          70          43
        91          2          69          45
        92          2          70          45
        93          2          71          49
        94          2          70          49
        95          2          71          48
        96          2          74          52
        97          2          73          52
        98          2          74          51
        99          2          76          54
       100          2          75          54
       101          2          76          53
       102          2          79          55
       103          2          78          55
       104          2          79          54
       105          2          82          55
       106          2          82          54
       107          2          84          55
       108          2          84          54
       109          2          86          55
       110          2          86          54
       111          2          88          55
       112          2          88          54
       113          2          91          54
       114          2          91          53
SET4: Head Limits
   0
SET5: Head Difference Limits
  12
         1          1          28          29         .02      1.E+20     /*first 3 are shallow
         2          1          60          61         .02      1.E+20
         3          1          62          63         .02      1.E+20
         4          1          85          86         .02      1.E+20     /*next 9 are deep
         5          1          87          88         .02      1.E+20
         6          1          89          90         .02      1.E+20
         7          1          91          92         .02      1.E+20
         8          1         105         106         .02      1.E+20
         9          1         107         108         .02      1.E+20
        10          1         109         110         .02      1.E+20
        11          1         111         112         .02      1.E+20
        12          1         113         114         .02      1.E+20
SET6: Drawdown Limits
   0
SET7A: Gradient Limits
  60
         1          1           1           2     -10.00      1.E+20     /*first 38 are shallow
         2          1           1           3     1.E-04      1.E+20
         3          1           4           5     -10.00      1.E+20
         4          1           4           6     1.E-04      1.E+20
         5          1           7           8     -10.00      1.E+20
         6          1           7           9     1.E-04      1.E+20
         7          1          10          11     -10.00      1.E+20
         8          1          10          12     1.E-04      1.E+20
         9          1          13          14     -10.00      1.E+20
        10          1          13          15     1.E-04      1.E+20
        11          1          16          17     -10.00      1.E+20
        12          1          16          18     1.E-04      1.E+20
        13          1          19          20     -10.00      1.E+20
        14          1          19          21     1.E-04      1.E+20
        15          1          22          23     -10.00      1.E+20
        16          1          22          24     1.E-04      1.E+20
        17          1          25          26     -10.00      1.E+20
        18          1          25          27     1.E-04      1.E+20
```

19	1	30	31	-10.00	1.E+20	
20	1	30	32	1.E-04	1.E+20	
21	1	33	34	-10.00	1.E+20	
22	1	33	35	1.E-04	1.E+20	
23	1	36	37	-10.00	1.E+20	
24	1	36	38	1.E-04	1.E+20	
25	1	39	40	-10.00	1.E+20	
26	1	39	41	1.E-04	1.E+20	
27	1	42	43	-10.00	1.E+20	
28	1	42	44	1.E-04	1.E+20	
29	1	45	46	-10.00	1.E+20	
30	1	45	47	1.E-04	1.E+20	
31	1	48	49	-10.00	1.E+20	
32	1	48	50	1.E-04	1.E+20	
33	1	51	52	-10.00	1.E+20	
34	1	51	53	1.E-04	1.E+20	
35	1	54	55	-10.00	1.E+20	
36	1	54	56	1.E-04	1.E+20	
37	1	57	58	-10.00	1.E+20	
38	1	57	59	1.E-04	1.E+20	/* next 22 are deep
39	1	64	65	-10.00	1.E+20	
40	1	64	66	1.E-04	1.E+20	
41	1	67	68	-10.00	1.E+20	
42	1	67	69	1.E-04	1.E+20	
43	1	70	71	-10.00	1.E+20	
44	1	70	72	1.E-04	1.E+20	
45	1	73	74	-10.00	1.E+20	
46	1	73	75	1.E-04	1.E+20	
47	1	76	77	-10.00	1.E+20	
48	1	76	78	1.E-04	1.E+20	
49	1	79	80	-10.00	1.E+20	
50	1	79	81	1.E-04	1.E+20	
51	1	82	83	-10.00	1.E+20	
52	1	82	84	1.E-04	1.E+20	
53	1	93	94	-10.00	1.E+20	
54	1	93	95	1.E-04	1.E+20	
55	1	96	97	-10.00	1.E+20	
56	1	96	98	1.E-04	1.E+20	
57	1	99	100	-10.00	1.E+20	
58	1	99	101	1.E-04	1.E+20	
59	1	102	103	-10.00	1.E+20	
60	1	102	104	1.E-04	1.E+20	

SET7B: Velocity Limits

0

SET7C: Relative Gradient Limits

30

1	2	1	.36	/*first 19 are shallow
2	4	3	.36	
3	6	5	.36	
4	8	7	.36	
5	10	9	.47	
6	12	11	.70	
7	14	13	.70	
8	16	15	.70	
9	18	17	.84	
10	20	19	.70	
11	22	21	.27	
12	24	23	.27	
13	26	25	.27	
14	28	27	.27	
15	30	29	.27	
16	32	31	.27	
17	34	33	.27	
18	36	35	.27	
19	38	37	.18	
20	40	39	.27	/* next 11 are deep

```
      21        42        41       .70
      22        44        43       .84
      23        46        45      1.19
      24        48        47      1.73
      25        50        49      1.73
      26        52        51      5.67
      27        54        53      1.73
      28        56        55      1.00
      29        58        57      1.00
      30        60        59       .27
SET8: Balance Constraints
 17
       1        A        1        L    0.E+00                  /*pumping = injection
       2        C                 E    0.E+00        2         /*multi-aquifer wells
 1   8        1.00
 1   9       -4.88
       3        C                 E    0.E+00        2
 1  10        1.00
 1  11       -1.50
       4        C                 E    0.E+00        2
 1  12        1.00
 1  13        -.20
       5        C                 E    0.E+00        2
 1  12        1.00
 1  14        -.56
       6        C                 E    0.E+00        2
 1  15        1.00
 1  16        -.15
       7        C                 E    0.E+00        2
 1  20        1.00
 1  21        -.33
       8        C                 E    0.E+00        2
 1  22        1.00
 1  23       -4.00
       9        C                 E    0.E+00        2
 1  25        1.00
 1  26       -3.54
      10        C                 E    0.E+00        2
 1  30        1.00
 1  31       -1.22
      11        C                 E    0.E+00        2
 1  32        1.00
 1  33       -1.22
      12        C                 E    0.E+00        2
 1  35        1.00
 1  36       -1.50
      13        C                 E    0.E+00        2
 1  37        1.00
 1  38       -3.00
      14        C                 E    0.E+00        2
 1  41        1.00
 1  42       -4.00
      15        C                 L    0.E+00       23   /*sums existing extraction wells

 1   1   5.194E-03
 1   2   5.194E-03
 1   3   5.194E-03
 1   4   5.194E-03
 1   5   5.194E-03
 1   6   5.194E-03
 1   7   5.194E-03
 1   8   5.194E-03
 1   9   5.194E-03
 1  10   5.194E-03
 1  11   5.194E-03
 1  12   5.194E-03
```

```
 1  13   5.194E-03
 1  14   5.194E-03
 1  15   5.194E-03
 1  16   5.194E-03
 1  17   5.194E-03
 1  18   5.194E-03
 1  19   5.194E-03
 1  20   5.194E-03
 1  21   5.194E-03
 1  22   5.194E-03
 1  23   5.194E-03
      16          C                    L    0.E+00        20    /*sums new shallow extraction
 1  43   5.194E-03
 1  44   5.194E-03
 1  45   5.194E-03
 1  46   5.194E-03
 1  47   5.194E-03
 1  48   5.194E-03
 1  49   5.194E-03
 1  50   5.194E-03
 1  51   5.194E-03
 1  52   5.194E-03
 1  53   5.194E-03
 1  54   5.194E-03
 1  55   5.194E-03
 1  56   5.194E-03
 1  57   5.194E-03
 1  58   5.194E-03
 1  59   5.194E-03
 1  60   5.194E-03
 1  61   5.194E-03
 1  62   5.194E-03
      17          C                    L    0.E+00        18    /*sums new deep extraction
 1  63   5.194E-03
 1  64   5.194E-03
 1  65   5.194E-03
 1  66   5.194E-03
 1  67   5.194E-03
 1  68   5.194E-03
 1  69   5.194E-03
 1  70   5.194E-03
 1  71   5.194E-03
 1  72   5.194E-03
 1  73   5.194E-03
 1  74   5.194E-03
 1  75   5.194E-03
 1  76   5.194E-03
 1  77   5.194E-03
 1  78   5.194E-03
 1  79   5.194E-03
 1  80   5.194E-03
SET9: Integer Constraints
 3
      1          B          1          L        20        20    /* places limit on # new shallow wells
43
44
45
46
47
48
49
50
51
52
53
```

54
55
56
57
58
59
60
61
62

2	B	1	L	18	18	/*paces limit on # new deep wells

63
64
65
66
67
68
69
70
71
72
73
74
75
76
77
78
79
80

3	B	1	L	38	38	/*places limit on # new total wells

43
44
45
46
47
48
49
50
51
52
53
54
55
56
57
58
59
60
61
62
63
64
65
66
67
68
69
70
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72
73
74
75
76
77

```
 78
 79
 80
SET10: Objective Function
        1        61
 1   1  -5.194E-03    /*factor converts to gpm, neg allows minimize
 1   2  -5.194E-03    /*factor converts to gpm, neg allows minimize
 1   3  -5.194E-03    /*factor converts to gpm, neg allows minimize
 1   4  -5.194E-03    /*factor converts to gpm, neg allows minimize
 1   5  -5.194E-03    /*factor converts to gpm, neg allows minimize
 1   6  -5.194E-03    /*factor converts to gpm, neg allows minimize
 1   7  -5.194E-03    /*factor converts to gpm, neg allows minimize
 1   8  -5.194E-03    /*factor converts to gpm, neg allows minimize
 1   9  -5.194E-03    /*factor converts to gpm, neg allows minimize
 1  10  -5.194E-03    /*factor converts to gpm, neg allows minimize
 1  11  -5.194E-03    /*factor converts to gpm, neg allows minimize
 1  12  -5.194E-03    /*factor converts to gpm, neg allows minimize
 1  13  -5.194E-03    /*factor converts to gpm, neg allows minimize
 1  14  -5.194E-03    /*factor converts to gpm, neg allows minimize
 1  15  -5.194E-03    /*factor converts to gpm, neg allows minimize
 1  16  -5.194E-03    /*factor converts to gpm, neg allows minimize
 1  17  -5.194E-03    /*factor converts to gpm, neg allows minimize
 1  18  -5.194E-03    /*factor converts to gpm, neg allows minimize
 1  19  -5.194E-03    /*factor converts to gpm, neg allows minimize
 1  20  -5.194E-03    /*factor converts to gpm, neg allows minimize
 1  21  -5.194E-03    /*factor converts to gpm, neg allows minimize
 1  22  -5.194E-03    /*factor converts to gpm, neg allows minimize
 1  23  -5.194E-03    /*factor converts to gpm, neg allows minimize
 1  43  -5.194E-03    /*factor converts to gpm, neg allows minimize
 1  44  -5.194E-03    /*factor converts to gpm, neg allows minimize
 1  45  -5.194E-03    /*factor converts to gpm, neg allows minimize
 1  46  -5.194E-03    /*factor converts to gpm, neg allows minimize
 1  47  -5.194E-03    /*factor converts to gpm, neg allows minimize
 1  48  -5.194E-03    /*factor converts to gpm, neg allows minimize
 1  49  -5.194E-03    /*factor converts to gpm, neg allows minimize
 1  50  -5.194E-03    /*factor converts to gpm, neg allows minimize
 1  51  -5.194E-03    /*factor converts to gpm, neg allows minimize
 1  52  -5.194E-03    /*factor converts to gpm, neg allows minimize
 1  53  -5.194E-03    /*factor converts to gpm, neg allows minimize
 1  54  -5.194E-03    /*factor converts to gpm, neg allows minimize
 1  55  -5.194E-03    /*factor converts to gpm, neg allows minimize
 1  56  -5.194E-03    /*factor converts to gpm, neg allows minimize
 1  57  -5.194E-03    /*factor converts to gpm, neg allows minimize
 1  58  -5.194E-03    /*factor converts to gpm, neg allows minimize
 1  59  -5.194E-03    /*factor converts to gpm, neg allows minimize
 1  60  -5.194E-03    /*factor converts to gpm, neg allows minimize
 1  61  -5.194E-03    /*factor converts to gpm, neg allows minimize
 1  62  -5.194E-03    /*factor converts to gpm, neg allows minimize
 1  63  -5.194E-03    /*factor converts to gpm, neg allows minimize
 1  64  -5.194E-03    /*factor converts to gpm, neg allows minimize
 1  65  -5.194E-03    /*factor converts to gpm, neg allows minimize
 1  66  -5.194E-03    /*factor converts to gpm, neg allows minimize
 1  67  -5.194E-03    /*factor converts to gpm, neg allows minimize
 1  68  -5.194E-03    /*factor converts to gpm, neg allows minimize
 1  69  -5.194E-03    /*factor converts to gpm, neg allows minimize
 1  70  -5.194E-03    /*factor converts to gpm, neg allows minimize
 1  71  -5.194E-03    /*factor converts to gpm, neg allows minimize
 1  72  -5.194E-03    /*factor converts to gpm, neg allows minimize
 1  73  -5.194E-03    /*factor converts to gpm, neg allows minimize
 1  74  -5.194E-03    /*factor converts to gpm, neg allows minimize
 1  75  -5.194E-03    /*factor converts to gpm, neg allows minimize
 1  76  -5.194E-03    /*factor converts to gpm, neg allows minimize
 1  77  -5.194E-03    /*factor converts to gpm, neg allows minimize
 1  78  -5.194E-03    /*factor converts to gpm, neg allows minimize
 1  79  -5.194E-03    /*factor converts to gpm, neg allows minimize
 1  80  -5.194E-03    /*factor converts to gpm, neg allows minimize
```

APPENDIX G:

SAMPLE MODMAN INPUT: OFFUTT

```
OFMM2-1.INP, LF WELLS, CORE WELL, TOE WELL, PLUS 9 NEW WELLS
SET0: General Parameters
   1(MODE)        .01        .01        .01    1.E-03        .01          1
SET1: Time Parameters
         1       1.00          1       1.00
SET2: Well Information
  27   0  27
         1          3         59        127             -2000.00       lf4-pw3
         2          4         59        127             -2000.00       lf4-pw3
         3          3         67        129             -2000.00       lf4-pw4
         4          4         67        129             -2000.00       lf4-pw4
         5          4         61         93             -2000.00       h2c-pw1 (toe)
         6          6         61         93             -2000.00       h2c-pw1 (toe)
         7          3         44         73             -2000.00       h2c-core1
         8          4         44         73             -2000.00       h2c-core1
         9          6         44         73             -2000.00       h2c-core1
        10          4         57        100             -2000.00       toe-new1
        11          6         57        100             -2000.00       toe-new1
        12          4         57        103             -2000.00       toe-new2
        13          6         57        103             -2000.00       toe-new2
        14          4         57        106             -2000.00       toe-new3
        15          6         57        106             -2000.00       toe-new3
        16          4         60        101             -2000.00       toe-new4
        17          6         60        101             -2000.00       toe-new4
        18          4         60        104             -2000.00       toe-new5
        19          6         60        104             -2000.00       toe-new5
        20          4         60        107             -2000.00       toe-new6
        21          6         60        107             -2000.00       toe-new6
        22          4         63        100             -2000.00       toe-new7
        23          6         63        100             -2000.00       toe-new7
        24          4         63        103             -2000.00       toe-new8
        25          6         63        103             -2000.00       toe-new8
        26          4         63        106             -2000.00       toe-new9
        27          6         63        106             -2000.00       toe-new9
    1          1          M              -1.E+04    0.E+00             lf4-pw3
    1          2          M              -1.E+04    0.E+00             lf4-pw3
    1          3          M              -1.E+04    0.E+00             lf4-pw4
    1          4          M              -1.E+04    0.E+00             lf4-pw4
    1          5          M              -1.E+04    0.E+00             h2c-pw1 (toe)
    1          6          M              -1.E+04    0.E+00             h2c-pw1 (toe)
    1          7          M              -1.E+04    0.E+00             h2c-core1
    1          8          M              -1.E+04    0.E+00             h2c-core1
    1          9          M              -1.E+04    0.E+00             h2c-core1
    1         10          M              -1.E+04    0.E+00             toe-new1
    1         11          M              -1.E+04    0.E+00             toe-new1
    1         12          M              -1.E+04    0.E+00             toe-new2
    1         13          M              -1.E+04    0.E+00             toe-new2
    1         14          M              -1.E+04    0.E+00             toe-new3
    1         15          M              -1.E+04    0.E+00             toe-new3
    1         16          M              -1.E+04    0.E+00             toe-new4
    1         17          M              -1.E+04    0.E+00             toe-new4
    1         18          M              -1.E+04    0.E+00             toe-new5
    1         19          M              -1.E+04    0.E+00             toe-new5
    1         20          M              -1.E+04    0.E+00             toe-new6
    1         21          M              -1.E+04    0.E+00             toe-new6
    1         22          M              -1.E+04    0.E+00             toe-new7
    1         23          M              -1.E+04    0.E+00             toe-new7
    1         24          M              -1.E+04    0.E+00             toe-new8
    1         25          M              -1.E+04    0.E+00             toe-new8
    1         26          M              -1.E+04    0.E+00             toe-new9
    1         27          M              -1.E+04    0.E+00             toe-new9
SET3: Control Locations
  59
         1          4         32         79
         2          4         32         80
         3          4         33         79
         4          4         36         83
```

5	4	36	84
6	4	37	83
7	4	40	86
8	4	40	87
9	4	41	86
10	4	43	90
11	4	43	91
12	4	44	90
13	4	46	94
14	4	46	95
15	4	47	94
16	4	49	99
17	4	49	100
18	4	50	99
19	4	52	103
20	4	52	104
21	4	53	103
22	4	54	106
23	4	54	107
24	4	55	106
25	4	56	109
26	4	56	110
27	4	57	109
28	4	58	110
29	4	58	111
30	4	59	110
31	4	61	111
32	4	61	110
33	4	64	110
34	4	65	110
35	4	64	109
36	4	66	108
37	4	67	108
38	4	66	107
39	4	67	104
40	4	68	104
41	4	67	101
42	4	66	101
43	4	67	98
44	4	66	98
45	4	66	92
46	4	65	92
47	4	66	86
48	4	67	86
49	4	65	79
50	4	66	79
51	4	65	80
52	4	64	70
53	4	65	70
54	4	64	71
55	4	63	65
56	4	64	65
57	4	63	66
58	4	67	103
59	4	66	87

SET4: Head Limits

0

SET5: Head Difference Limits

4

1	1	31	32	0.E+00	1.E+20
2	1	41	42	0.E+00	1.E+20
3	1	43	44	0.E+00	1.E+20
4	1	45	46	0.E+00	1.E+20

SET6: Drawdown Limits

0

SET7A: Gradient Limits

34

1	1	1	2	-10.00	1.E+20
2	1	1	3	0.E+00	1.E+20
3	1	4	5	-10.00	1.E+20
4	1	4	6	0.E+00	1.E+20
5	1	7	8	-10.00	1.E+20
6	1	7	9	0.E+00	1.E+20
7	1	10	11	-10.00	1.E+20
8	1	10	12	0.E+00	1.E+20
9	1	13	14	-10.00	1.E+20

```
        10          1          13          15     0.E+00     1.E+20
        11          1          16          17    -10.00      1.E+20
        12          1          16          18     0.E+00     1.E+20
        13          1          19          20    -10.00      1.E+20
        14          1          19          21     0.E+00     1.E+20
        15          1          22          23    -10.00      1.E+20
        16          1          22          24     0.E+00     1.E+20
        17          1          25          26    -10.00      1.E+20
        18          1          25          27     0.E+00     1.E+20
        19          1          28          29    -10.00      1.E+20
        20          1          28          30     0.E+00     1.E+20
        21          1          33          35       0.00     1.E+20
        22          1          33          34    -10.00      1.E+20
        23          1          36          38       0.00     1.E+20
        24          1          36          37    -10.00      1.E+20
        25          1          49          51       0.00     1.E+20
        26          1          49          50    -10.00      1.E+20
        27          1          52          54       0.00     1.E+20
        28          1          52          53    -10.00      1.E+20
        29          1          55          57       0.00     1.E+20
        30          1          55          56    -10.00      1.E+20
        31          1          39          58       0.00     1.E+20
        32          1          39          40    -10.00      1.E+20
        33          1          47          59       0.00     1.E+20
        34          1          47          48    -10.00      1.E+20
SET7B: Velocity Limits
  0
SET7C: Relative Gradient Limits
  17
         1          2          1       1.00
         2          4          3       1.00
         3          6          5       1.00
         4          8          7       1.00
         5         10          9       1.00
         6         12         11       1.00
         7         14         13       1.00
         8         16         15       1.00
         9         18         17       1.20
        10         20         19       1.43
        11         21         22       0.58
        12         23         24       1.00
        13         25         26       2.14
        14         27         28       2.14
        15         29         30       2.14
        16         31         32       5.67
        17         33         34       5.67
SET8: Balance Constraints
  14
         1          C                    E    0.E+00          2    */lf4-pw3
   1     1       1.00
   1     2       -.44
         2          C                    E    0.E+00          2    */lf4-pw4
   1     3       1.00
   1     4       -.49
         3          C                    E    0.E+00          2    */h2c-pw1
   1     5       1.00
   1     6      -1.28
         4          C                    E    0.E+00          2    */h2c-core1
   1     8       1.00
   1     7      -9.03
         5          C                    E    0.E+00          2    */h2c-core1
   1     8       1.00
   1     9      -1.31
         6          C                    E    0.E+00          2    */toe-new1
   1    10       1.00
   1    11      -1.28
         7          C                    E    0.E+00          2    */toe-new2
   1    12       1.00
   1    13      -1.28
         8          C                    E    0.E+00          2    */toe-new3
   1    14       1.00
   1    15      -1.28
         9          C                    E    0.E+00          2    */toe-new4
   1    16       1.00
   1    17      -1.28
```

```
      10          C                    E    0.E+00          2   */toe-new5
  1  18         1.00
  1  19        -1.28
      11          C                    E    0.E+00          2   */toe-new6
  1  20         1.00
  1  21        -1.28
      12          C                    E    0.E+00          2   */toe-new7
  1  22         1.00
  1  23        -1.28
      13          C                    E    0.E+00          2   */toe-new8
  1  24         1.00
  1  25        -1.28
      14          C                    E    0.E+00          2   */toe-new9
  1  26         1.00
  1  27        -1.28
SET9: Integer Constraints
  2
       1          B          1          L          4          4  */limit on # existing wells
  1
  3
  5
  7
       2          B          1          L          9          9  /*limit on # new wells
 10
 12
 14
 16
 18
 20
 22
 24
 26
SET10: Objective Function
      1         27
  1   1     -.005194     /*factor converts to gpm, neg allows minimize
  1   2     -.005194     /*factor converts to gpm, neg allows minimize
  1   3     -.005194     /*factor converts to gpm, neg allows minimize
  1   4     -.005194     /*factor converts to gpm, neg allows minimize
  1   5     -.005194     /*factor converts to gpm, neg allows minimize
  1   6     -.005194     /*factor converts to gpm, neg allows minimize
  1   7     -.005194     /*factor converts to gpm, neg allows minimize
  1   8     -.005194     /*factor converts to gpm, neg allows minimize
  1   9     -.005194     /*factor converts to gpm, neg allows minimize
  1  10     -.005194     /*factor converts to gpm, neg allows minimize
  1  11     -.005194     /*factor converts to gpm, neg allows minimize
  1  12     -.005194     /*factor converts to gpm, neg allows minimize
  1  13     -.005194     /*factor converts to gpm, neg allows minimize
  1  14     -.005194     /*factor converts to gpm, neg allows minimize
  1  15     -.005194     /*factor converts to gpm, neg allows minimize
  1  16     -.005194     /*factor converts to gpm, neg allows minimize
  1  17     -.005194     /*factor converts to gpm, neg allows minimize
  1  18     -.005194     /*factor converts to gpm, neg allows minimize
  1  19     -.005194     /*factor converts to gpm, neg allows minimize
  1  20     -.005194     /*factor converts to gpm, neg allows minimize
  1  21     -.005194     /*factor converts to gpm, neg allows minimize
  1  22     -.005194     /*factor converts to gpm, neg allows minimize
  1  23     -.005194     /*factor converts to gpm, neg allows minimize
  1  24     -.005194     /*factor converts to gpm, neg allows minimize
  1  25     -.005194     /*factor converts to gpm, neg allows minimize
  1  26     -.005194     /*factor converts to gpm, neg allows minimize
  1  27     -.005194     /*factor converts to gpm, neg allows minimize
```

APPENDIX H:

EFFICIENTLY MAKING MODIFICATIONS TO MODMAN FORMULATIONS

Numerous hydraulic optimization formulations were solved with the MODMAN code as part of this demonstration project. However, each formulation did not require a separate execution of the MODMAN code. A MODMAN execution has the following major steps:

(1) execute MODMAN (mode 1) to create an MPS file (a linear or mixed-integer program);

(2) execute LINDO to solve the linear or mixed-integer program; and

(3) execute MODMAN (mode 2) to post-process the LINDO results.

In many cases, it is possible to slightly modify the hydraulic optimization formulation without re-executing MODMAN in mode 1. This can be accomplished by:

(1) modifying the MPS file with a text editor, prior to running LINDO; or

(2) modifying the linear or mixed-integer program directly within LINDO.

In many cases, LINDO results can be extracted manually, and there is no need to execute MODMAN in mode 2 (to post-process LINDO output).

For example, Section 4.4.2 discusses a series of mathematical optimal solutions for Kentucky, where the head limit at cells adjacent to the river is varied. The base formulation has an upper limit of 399.99 ft MSL assigned at 54 cells. To generate the mathematical optimal solutions associated with the other head limits, a text editor was used to modify the upper bounds on the appropriate variables in the MPS file. LINDO then solved the modified MPS file.

Another example is the generation of mathematical optimal solutions for related problems, where integer constraints are used to limit the number of wells selected. There is a specific constraint that has the following general form (see Section 3.1.3):

$$I_1 + I_2 + I_3 + I_4 + I_5 + I_6 \;\; I_7 + I_8 + I_9 \quad \leq \quad 2$$

The "right-hand side" of this constraint sets the limit on the number of active wells. This limit can easily be altered in the MPS file with a text editor, or altered directly within the LINDO software.

A full discussion of the structure of the MPS file, and potential complexities associated with modifying the MPS file (e.g., scaled well rates) is beyond the scope of this report. For more information, refer to the MODMAN User's Guide (Greenwald, 1998a).

APPENDIX I:

SOURCES OF INFORMATION AND REFERENCES FOR OTHER OPTIMIZATION RESEARCH AND APPLICATION

The purpose of this appendix is to guide readers of this report to individuals or organizations that offer additional information on optimizations of groundwater systems. Although this is by no means a comprehensive reference section regarding optimization of groundwater systems, it should provide the reader with sufficient data to pursue additional information on a wide variety of subjects associated with optimization of groundwater systems.

A partial listing of individuals/organizations associated with optimization of groundwater systems is provided below:

Name	Affiliation or Company	Address	Phone/Fax/Email
David Ahlfeld	University of Massachusetts	Dept. of Civil and Env. Engineering 139 Marston Hall University of Massachusetts Amherst, MA 01003	Voice: (413) 545-2681 Fax: (413) 545-2202 ahlfeld@ecs.umass.edu
Paul Barlow	U.S.G.S	28 Lord Road Marlborough, MA 01752	Voice: (508) 490-5070 Fax: pbarlow@usgs.gov
Wes Danskin	USGS Water Resources	5735 Kearney Villa Road, Suite 0 San Diego, CA 92123	Voice: 619-637-6832 Fax: 619-637-9201 wdanskin@usgs.gov
David Dougherty	Subterranean Research, Inc.	P.O. Box 1121 Burlington, VT 05402	Voice: (802)-658-8878 Fax: (802)-658-8878 David.Dougherty@subterra.com
Steve Gorelick	Stanford University	Dept. of Geological and Env. Sciences Stanford University Stanford, CA 94305-2115	Voice: (415) 725-2950 Fax: (415) 723-1445 gorelick@geo.stanford.edu
Rob Greenwald	HSI GeoTrans, Inc.	2 Paragon Way Freehold, NJ 07726	Voice: 732-409-0344 Fax: 732-409-3020 rgreenwald@hsigeotrans.com
George Karatzas	Technical University of Crete	Dept. of Environmental Engineering Polytechneioupolis 73 100 Chania Greece	Phone: (011-30-821) 37473 Fax: (011-30-821) 37474 karatzas@emba.uvm.edu
Ann Mulligan	University of Massachusetts	Dept. of Civil and Env. Engineering 139 Marston Hall University of Massachusetts Amherst, MA 01003	Voice: (413) 545-2681 Fax: (413) 545-2202 mulligan@ecs.umass.edu

Name	Affiliation or Company	Address	Phone/Fax/Email
Daene McKinney	University of Texas	Department of Civil Engineering Austin, TX 78712	Voice: 512-471-8772 Fax: 512-471-0072 Daene@AOL.com
Tracy Nishikawa	U.S.G.S.	5735 Kearney Villa Road, Suite 0 San Diego, CA 92123	Voice: 619-637-6848 Fax: 619-637-9201 tnish@usgs.gov
David Watkins	US Army Corps of Eng., Hydrologic Engineering Center	609 Second Street Davis, CA 95616-4587	Voice: 530-756-1104 Fax: 530-756-8250 david.w.watkins@usace.army.mil
Richard C. Peralta	Utah State University	Building EC-216 Utah State University Logan, UT 84322-4105	Voice: 801-797-2786 Fax: 801-797-1248 peralta@cc.usu.edu
George Pinder	University of Vermont	Dept. of Civil and Env. Engineering 371 Votey Building Burlington, VT 05405-0156	Voice: 802-656-8697 Fax: 802-656-8446 George.Pinder@uvm.edu
Eric Reichard	U.S.G.S.	5735 Kearney Villa Road, Suite 0 San Diego, CA 92123	Voice: 619-637-6834 Fax: 619-637-9201 egreich@usgs.gov
Donna Rizzo	Subterranean Research, Inc.	P.O. Box 1121 Burlington, VT 05402	Voice: 802-658-8878 Fax: 802-658-8878 Donna.Rizzo@subterra.com
Christine Shoemaker	Cornell University	Civil Engineering Hollister Hall Ithaca, NY 14853	Voice: 607-255-9233 Fax: 607-255-9004 cas12@cornell.edu
Brian Wagner	U.S.G.S,	Bldg 15, McKelvey Building 345 Middlefield Road, MS 409 Menlo Park, CA 94025	Voice:650-329-4567 Fax: bjwagner@usgs.gov
Chunmiao Zheng	University of Alabama	Department of Geology University of Alabama Tuscaloosa, AL 35487	Voice: 205-348-0579 Fax: 205-348-0818 czheng@wgs.geo.ua.edu

As part of this project, information was solicited from select professionals involved in optimization code development for groundwater problems. The following pages provide brief summaries of codes and/or applications, provided by those professionals who responded:

Code/Method: MODOFC (MODflow Optimal Flow Control)
Description By: David Ahlfeld, University of Massachusetts

Brief Description: MODOFC (MODflow Optimal Flow Control) is a FORTRAN computer program which determines optimal pumping solutions for groundwater flow control problems. MODOFC couples the USGS MODFLOW simulation program with optimization algorithms. The code can accommodate linear pumping costs, well installation costs, bounds on head and head difference, bounds on individual and net well pumping rates and bounds on total number of wells. MODFLOW features that can be accommodated include three-dimensional heterogeneous aquifers, confined or unconfined units, wells screened in single or multiple layers and single or multiple stress periods. MODOFC is designed to utilize existing MODFLOW96 input files along with a user-created file describing the hydraulic control problem. MODOFC converts the groundwater flow control problem into an optimization problem by the response matrix method. MODOFC contains a full implementation of the simplex algorithm. The simplex and branch and bound algorithms are used for mixed binary problems. Sequential linear programming is used for unconfined problems.

Application(s): An early version of MODOFC was used to design a groundwater pump and treat remediation system in coastal New Jersey. The aquifer was contaminated with a plume extending over several hundred acres and nearly 100 feet vertically. The site consisted of approximately 50 extraction wells, several recharge basins and pumped approximately 3 million gallons per day. The site was modeled with MODFLOW with five numerical layers and 35,000 grid cells. The results are presented in Ahlfeld et. al. (1995) and Pinder et. al. (1995).

References:

Ahlfeld, D. P., R. H. Page, and G. F. Pinder.1995. Optimal Ground-water remediation methods applied to a superfund site: From formulation to implementation. Groundwater, 33(1):58-70.

G.F. Pinder, D.P. Ahlfeld, and R.H. Page, 1995. "Conflict Resolution in Groundwater Remediation using Management Models: A Case Study", Civil Engineering, Vol. 65, No. 3, March 1995, pgs. 59-61.

Riefler, R.G. and D.P. Ahlfeld, 1996. "The Impact of Numerical Precision on the Solution of Confined and Unconfined Optimal Hydraulic Control Problems", Hazardous Waste and Hazardous Materials, Vol 13, No. 2, 1996, pgs 167-176.

Availability: MODOFC is available free of charge on the world wide web at "http://www.ecs.umass.edu/modofc/"

Point(s) of Contact: David Ahlfeld (see table at beginning of this Appendix).

Code/Method: MODFLIP

Description By: David Dougherty, Subterranean Research, Inc.

Brief Description: MODFLIP couples the popular *MODF*LOW groundwater simulation program with *l*inear and mixed *i*nteger *p*rogramming optimization [*Fourer et al.*, 1993]. MODFLIP can be used to compute the optimal pumping strategies for groundwater management problem for which a reliable MODFLOW model exists, like other optimization programs described in this Appendix. Linear programming (LP) is limited in applicability to problems having linear (that is, proportionality) relations among cost, pumping rates, and all constraints. This approach can be applied, therefore, to groundwater flow in confined aquifers. If approximations are introduced, it can be applied in other cases that are weakly nonlinear, such as unconfined aquifers with small drawdowns. Mixed integer programming provides for fixed or one-time costs. The design of MODFLIPs mathematical optimization relies on a two-part objective function. The first is proportional to the amounts of pumping out of or into (extraction or injection) candidate wells. Through a linearization method, the energy costs (lift) can be included. The second part of the objective function is proportional to a binary (on-off, or one-zero) variable, which indicates whether a particular candidate well is selected or not. This term allows for costs including drilling, casing, and screen. Constraints on heads, head differences, and pumping rates are possible. In addition, the ratio of total injection to extraction can be constrained (e.g., to ensure that all extracted water is reinjected). *Gorelick et al.* [1989] provide a large number of two-dimensional examples to which linear programming is applicable; this software expands on their list by allowing fully 3-D flow conditions.

Application(s): MODFLIP is applicable to steady flow optimization, linear programming, and linear mixed-binary programming problems.

References:

Fourer, R., D. M. Gay, B. W. Kernighan, *Ampl: A Modeling Language for Mathematical Programming*, Duxbury Press, Pacific Grove, CA, 1993.

Gorelick, S., R. A. Freeze, D. Donahue, and J. F. Keely, *Groundwater Contamination: Optimal Capture and Containment*, Lewis Publishers, 385 pp., 1989.

Subterranean Research, Inc., *MODFLIP, A MODFLOW-based Program for Flow Optimization*, http://www.subterra.com/publications/MODFLIP.pdf, 1999.

Availability: Contact points of contact listed below.

Code/Method: REMAX
Description By: Richard Peralta, Utah State University

Brief Description: REMAX can compute optimal pumping strategies for any ground-water system for which you have a reliable simulation model. For simple dynamic stream-aquifer problems REMAX can also compute optimal conjunctive use strategies. Such a strategy includes optimal surface water diversion and ground-water pumping rates. REMAX can assure that implementing the optimal water management strategy will not cause unacceptable physical system responses. To do this the modeler specifies limits on acceptable responses. REMAX can constrain aquifer hydraulic heads, gradients, and flows. It can constrain streamflow in simple stream-aquifer management problems. For special situations REMAX has been adapted to constrain contaminant concentrations in ground water or surface water, or volumes of nonaqueous phase liquids (free product, residual, extracted). REMAX can address a wide range of volumetric, economic or environmental problems involving ground-water management. To do this it solves optimization problems having objective functions and constraints that are linear, nonlinear, integer or mixed integer. REMAX performs deterministic or stochastic, single- or multi-objective optimization. REMAX simulates using either standard numerical simulation models such as MODFLOW or response matrix (superposition) models that use influence coefficients derived via simulation models. REMAX employs response matrix methods adapted to accurately address nonlinear systems (unconfined aquifers). For special situations (often involving contaminant management), linear and nonlinear response surface methods are also used.

Application(s): 1. Optimal Pumping Strategy to Capture TCE Plume at Southwest Base Boundary, Norton AFB (NAFB), California.TCE Plume was about 4 miles long and 1 mile wide. Site modeled using 3-layer MODFLOW model. Top layer was up to about 300 feet thick.Used REMAX Simulation/Optimization (S/O) model to optimize steady pumping. Initially assumed over 20 candidate wells, 40 gradient constraints in optimization problem. It was challenging because base boundary was irregular and all wells had to be on base. This was <u>steady flow (hydraulic) optimization.</u> Optimal pumping system design and strategy was built and implemented. It involved a total extraction of 2250 gpm; total of 3 extraction wells and 8 injection wells. It saved about 20% ($5.8M in present value) when compared with a design provided by a consulting firm that did not use S/O modelling. Sensitivity analysis demonstrated the strategy should be valid even if hydraulic conductivity differed widely from assumed mean value (ie 60% underestimation .through 80% overestimation).

2. Multiobjective Optimization: Maximizing Pumping for Water Supply versus Minimizing Pumping Needed for Plume Containment Subject to Lower Bound on Seepage from Aquifer to River (an anonymous site in the Northeast US). A contaminant plume existed under an industrial facility that had 3 wells and used some of the pumped water in industrial processes. Pumping from 3 upgradient public supply wells causes plume to be captured by those supply wells. MODFLOW was used to model the three-layer system. An anonymous contractor developed a steady pumping strategy using simulation model alone. REMAX was used for <u>multiobjective linear steady flow (hydraulic) optimization</u>. All scenarios involved Linear Programming. The first scenario was single objective: minimize total pumping needed to prevent the plume from moving to public wells, subject to constraints. The optimal pumping strategy required 40 percent less pumping than that developed by other contractor using only a simulation model. Later the municipality wanted to increase total pumping for water supply. This would require that the industry increase their total pumping to retain plume containment. However, the state water resources agency was concerned that the increases in pumping would dewater the nearby river too much. REMAX was used to develop the pareto optima solutions for this multiobjective problem.

3. Calibration of a Flow Model and Optimal Pumping Strategies to Capture a TCE Plume at Travis AFB (TAFB), California. TCE plume had migrated under a runway and emerged on the other side. It was moving toward a stream that flowed toward and important wetland. Site modeled using 4-layer MODFLOW model, 5040 cells per layer. Plume exists in top three layers. REMAX was used to develop the minimum steady pumping needed from many candidate wells. It used many gradient

constraints. This was steady flow optimization. Optimal pumping system design and strategy involved 5 extraction wells with pumping rates between 5 and 11 gpm. Total extraction is about 40 gpm.

4. Optimal Pumping Strategy to Contain a TCE Plume at March AFB (MAFB), California. TCE plume had crossed base boundaries and was under an urbanized area and was moving toward water supply wells. Site was modeled using a 4-layer SWIFT model. Contamination existed in multiple layers. REMAX was used to develop the minimum steady pumping needed from many candidate wells. It used many gradient constraints. This was steady flow (hydraulic) optimization.

5. Optimal Pumping Strategies to Maximize Dissolved TCE Extraction at Central Base Area, Norton AFB, California. TCE plume at a source area was to be remediated. MODFLOW and MT3D were used for a single layer system. Wells were already installed. Transient (two stress periods) transport optimization was used to develop maximum mass removal transient pumping strategies a specific planning horizon. Strategies were developed for a range of scenarios...differing in the maximum total pumping rate (200-400 gpm) and the wells that could be used. Enhanced REMAX was used. This showed the importance of applying optimization as early in the design process as possible. If one had to use existing wells and the same upper limit on total pumping, the optimal strategy was not much better than the existing strategy. If one could use different wells locations and the same total pumping, the amount of TCE mass removed could increase by about 20%. Increasing total pumping permits increased mass removal.

6. Optimal Pumping Strategies to Maximize Dissolved TCE Extraction at Mather AFB, California. TCE plume at a source area was to be remediated. MODFLOW and MT3D were used to simulate flow and transport in a two layer system having 2184 cells in each layer. Wells were already installed. Transient (two stress periods) transport optimization was used to develop maximum mass removal for a specific planning horizon. Strategies were developed for a range of scenarios.. differing in the maximum total pumping rate and the wells that could be used. Enhanced REMAX was used. Using the existing wells and the same total pumping, over twenty percent increase in total mass removal is possible. Using alternative wells can increase mass removal. Raising upper limit on total pumping increases TCE mass removal.

7. Optimal Pumping Strategies for Cleanup and Containment of TCE and DCE Plumes Near Mission Drive, Wurtsmith Air Force Base (WAFM), Michigan. TCE and DCE plumes were projected to reach a stream. The goal is plume containment and cleanup (to specified concentration) within a planning horizon. MODFLOW and MT3D were the models used to represent this 3-layer system. First, genetic algorithm was used in nonlinear programming transport optimization to maximize mass removal subject to constraints. Strategies were developed for a range of total pumping rates being processed by the treatment plant. Objective was to maximize TCE mass removed subject to: (1) upper limit on final TCE and DCE aquifer concentrations; (2)upper limit on TCE concentration entering the treatment facility during any time step.; and (3)upper limit on total flow. Then the additional minimal pumping needed to achieve containment was determined using REMAX. Additional wells were added as needed. This was linear steady flow (hydraulic) optimization. Objective was to minimize total pumping subject to: (1) using the cleanup wells to the extent possible; and (2)containing the plume using hydraulic gradient constraints. Finally, optimal pumping strategies were developed for a range of treatment facility capacities.

References: Contact Richard Peralta

Availability: For sale (contact Richard Peralta)

Point(s) of Contact: Richard Peralta (see table at beginning of this Appendix).

Code/Method: Global Optimization Methods (Genetic Algorithms, Simulated Annealing, and Tabu Search)
Description By: Chunmiao Zheng, University of Alabama

Brief Description: As part of our research efforts in the area of groundwater remediation design optimization in the last several years, we have developed a number of general-purpose flow and transport simulation-optimization software tools. These software tools combine the MODFLOW (McDonald and Harbaugh, 1988) and MT3D/MT3DMS (Zheng, 1990; Zheng and Wang, 1998) codes for flow and transport simulation with a general optimization package for formulating the most cost-effective groundwater management and remedial strategies under various physical, environmental and budgetary constraints. The optimization package is implemented with three global optimization methods, namely, genetic algorithms, simulated annealing and tabu search. The global optimization methods have the ability to identify the global or near-global optimum, are efficient in handling discrete decision variables such as well locations, and can be easily linked to any flow and transport simulation models for solving a wide range of field problems. They are also very easy to understand and simple to use.

Our global optimization based management tools are capable of determining time-varying pumping/injection rates and well locations for three-dimensional field-scale problems under very general conditions. The objective function of the optimization model can be highly nonlinear and complex.. Most types of constraints that are commonly encountered in the field, such as prescribed hydraulic gradients, minimum drawdowns, and maximum concentration limits, can be readily incorporated. To account for the uncertainties in the groundwater flow and contaminant transport models, our software has a dual formulation to allow the user to perform automated parameter estimation given observed head and concentration data. Since our software does not require any changes to the input files prepared for MODFLOW and MT3D/MT3DMS, it can be used with any graphical user interfaces developed for MODFLOW and MT3D/MT3DMS, including *Visual MODFLOW*, *DoD GMS*, and *Groundwater Vista*.

The most significant limitation of the global optimization based management tools is their intensive computational requirements. To mitigate this problem, global optimization methods may be integrated with linear or nonlinear programming as we have recently demonstrated (Zheng and Wang, 1999). This integrated approach takes advantage of the fact that global optimization methods are most effective for dealing with discrete decision variables such as well locations while traditional programming methods may be more efficient for dealing with continuous decision variables such as pumping rates. Our preliminary work shows that it is possible to achieve dramatic reductions in runtime with the integrated approach.

Application(s): Our simulation-optimization tools have been successfully applied to remediation design optimization problems at several field sites with complex hydrogeologic conditions. A typical example is presented by Wang and Zheng (1997) involving optimization of an existing pump-and-treat system at a gasoline terminal site in Granger, Indiana. Groundwater beneath and down-gradient of the site was found to contain dissolved compounds associated with petroleum hydrocarbons in extensive field investigations. Groundwater flow and solute transport models were developed in previous remedial investigations and feasibility studies to evaluate the various remedial alternatives at the site. A pump-and-treat system was already designed through the trial-and-error approach and implemented at the site.

The optimization approach was applied to the same remediation design problem for comparison with the trial-and-error approach. Because the flow field was considered steady-state, and the fixed capital costs were negligible relative to the pumping and treatment costs, the objective function was simplified as minimizing the total pumping at eight existing wells subject to the constraint that the maximum concentration level in the entire model must not exceed a specified value at a specific time. For comparison with the trial-and-error solution, the concentration limit for the optimization problem was set equal to the calculated maximum concentration at the end of the comparison period based on the

pumping rates from the trial-and-error solution. The optimization solution reduces the total extraction of the trial-and-error solution by approximately 64 percent, demonstrating the significant economic benefits that may be derived from the use of the simulation-optimization models in remediation system designs.

References:

Glover, F. 1986. Future paths for integer programming and links to artificial intelligence. *Comp. and Operations Res.*, 5, p. 533-549.

McDonald, M.G. and A.W., Harbaugh. 1988. *A Modular Three-Dimensional Finite-Difference Groundwater Flow Model.* Techniques of Water Resources Investigations, Book 6, USGS.

McKinney, D.C. and M.-D. Lin. 1994. Genetic algorithms solution of groundwater management models, *Water Resour. Res.*, 30(6), p. 1897-1906.

Rizzo, D.M., and D.E. Dougherty. 1996. Design optimization for multiple management period groundwater remediation, *Water Resour. Res.*, 32(8), p. 2549-2561.

Wang, M. and C. Zheng. 1997. Optimal remediation policy selection under general conditions, *Ground Water*, 35(5), p. 757-764.

Wang, M. and C. Zheng. 1998. Application of genetic algorithms and simulated annealing in groundwater management: formulation and comparison, *Journal of American Water Resources Association*, vol. 34, no. 3, p. 519-530.

Zheng, C. 1990. *MT3D, A Modular Three-Dimensional Transport Model for Simulation of Advection, Dispersion and Chemical Reactions of Contaminants in Groundwater Systems.* Report to the USEPA, 170 pp.

Zheng, C. and P.P. Wang. 1998. *MT3DMS, A Modular Three-Dimensional Multispecies Transport Model*, Technical Report, U.S. Army Engineer Waterways Experiment Station.

Zheng, C. and P.P. Wang. 1999. An integrated global and local optimization approach for remediation system design, *Water Resour. Res.*, 35(1), p. 137-146.

Availability: Contact "points of contact" listed below.

Point(s) of Contact: Chunmiao Zheng (see table at beginning of this Appendix).

Code/Method: Simulated Annealing

Description By: David Dougherty, Subterranean Research, Inc.

Brief Description: Simulated annealing (*SA*) is an optimization method that can be applied to *any* setting. It has been applied to confined aquifers, unconfined aquifers, soil vapor extraction, flow-only control, and solute transport-driven control with constraints ranging from simple to exceedingly complex. It is structured to make discrete decisions (e.g., select from discrete pumping rates at remediation wells), although this can be modified. It can handle multiple management periods (sequences of operating schedules). SA is very well suited to difficult and large optimization problems, and performs poorly on small linear problems; it is therefore a perfect companion to LP. Like the outer approximation method, SA does not require a feasible initial problem to start, unlike many nonlinear (and linear) optimization methods. If there is no feasible solution to the problem, SA will provide "good" (though infeasible) solutions. When naively applied, SA can require enormous computing resources and time, while in experienced hands and when applied to appropriate problems the method is competitive with any other.

Application(s): Simulated annealing (SA) and related methods (e.g., elements of tabu search) were introduced into the groundwater literature by Dougherty and Marryott [1991]. At a central California site, the method was applied in a *post mortem* approach to determine if cleanup could have been accomplished with less expense. Marryott, Dougherty, and Stollar [1991] report that a 40% reduction in pumping rates could have been achieved. Groundwater simulations used an engineering model developed by LLNL that was not modified for the optimization process. The method has been applied to a solvent plume at Lawrence Livermore National Laboratory during the design phase; SA selected clever locations and operating schedules, and cost reductions in the tens of millions of dollars were identified [Rizzo and Dougherty, 1996]. SA has also been applied to a soil vapor extraction application [Sacks, Dougherty, and Guarnaccia, 1994]. To our knowledge, Subterranean Research, Inc. personnel have conducted the only applications of SA to field-scale problems.

References:

Dougherty, D. E., and R. A. Marrott, "Optimal groundwater management, 1. Simulated annealing", *Water Resources Research*, **27**(10), 2493-2508, 1991.

Marryott, R. A., D. E. Dougherty, and R. L. Stollar, "Optimal groundwater management, 2 Application of simulated annealing to a field-scale contamination site", *Water Resources Research*, **29**(4), 847-860, 1993.

Rizzo, D. M., and D. E. Dougherty, "Design optimization for multiple management period groundwater remediation", *Water Resources Research*, **32**(8), 2549-2561, 1996.

Sacks, R. L., D. E. Dougherty, and J. F. Guarnaccia, "The design of SVE remediation systems using simulated annealing", 1994 Groundwater Modeling Conference, Fort Collins, CO, August 10-12, 1994.

Availability: Contact "points of contact" listed below.

Point(s) of Contact: David Dougherty or Donna Rizzo (see table at beginning of this Appendix).

Code/Method: Augmented Outer Approximation

Description By: David Dougherty, Subterranean Research, Inc.

Brief Description: Augmented Outer Approximation can be applied to containment and cleanup groundwater quality problems, as well as other water resources problems. Like the other methods described in this Appendix, a suitable and reliable aquifer simulation model is available. Outer approximation has been combined with the MODFLOW, MT3DMS, and SUTRA simulation models, for example.

The outer approximation method is a cutting plane optimization method designed originally for concave objectives (minimization) and convex constraints. Karatzas (see listing in this Appendix or the Karatzas and Pinder [1996] paper) describes extensions that accommodate nonconvex constraints, which occur in transport and other nonlinear optimization problems.

To solve larger problems faster and more effectively, Subterranean Research, Inc. has augmented outer approximation algorithms for groundwater problems in several ways. Among these are the following:

- A completely new data structure has been implemented, resulting in substantial speedups.
- New nonlinear algorithms adapt to nonconvex problems and a new "cutting depth" strategy.
- Completely new pivoting method for generating hyperplanes and associated data structures.
- Innovative method for subspace projection of optimization problem, resulting in substantially improved efficiency.

Application(s): Karatzas (see listing in this Appendix) cites several applications of the outer approximation method.

Subterranean Research, Inc. has conducted a range of test applications involving both synthetic and real sites.

References:

Karatzas, G. P., and G. F. Pinder, "The solution of groundwater quality management problems have non-convex feasible region using a cutting plane optimization technique", *Water Resources Research*, vol. 32, no.4, 1091-1100, 1996.

Availability: Contact "points of contact" listed below.

Point(s) of Contact: David Dougherty or Donna Rizzo (see table at beginning of this Appendix).

Code/Method: The Outer Approximation Method

Description By: George Karatzas, Technical University of Crete

Brief Description: The Outer Approximation method is a cutting plane technique for the minimization of a concave function over a compact set of constraints that can have a convex or non-convex behavior. The basic concept of the method is that the minimum of a concave function occurs at one of the most "outer" points of the feasible region. The concept of the methodology is describe as follows: Initially, the feasible region is approximated by an enclosing polytope, which is defined by a set of vertices. Then, the vertex that minimizes the objective function is determined. If the vertex belongs to the feasible region this is the optimal solution, if not a cutting plane is introduced to eliminate part of the infeasible region and create a new enclosing polytope that is a "better" approximation of the feasible region. A new set of vertices is determined and the process is repeated until the optimal Solution is obtained. Depending on the behavior of the feasible region, convex or concave, a different approach is applied to determine the equation of the cutting plane. The method guarantees a global optimal solution. The Outer Approximation Method has the potential to solve groundwater management problems related to hydraulic gradient control and/or mass transport optimization problems. Additional features of the method are:

- It incorporates the well installation cost.
- It can incorporate treatment plant design (under development).
- It can handle combination of hydraulic gradient and concentration constraints.
- For small to average problems it can handle multi-period design problems.
- It can incorporate uncertainty (under development).

Application(s):

(1) The Woburn aquifer in Massachusetts. A remediation scheme using the developed Outer Approximation algorithm in combination with the 2-D numerical simulator, GW2SEN.

(2) The Lawrence Livermore National Laboratory Site in California. An optimal design using the Outer Approximation Algorithm in combination with a 2-D numerical simulation, SUTRA, and a 3-D numerical simulator, PTC (Princeton Transport Code).

(3) The U.S. Air Force Plant number 44, Tuscon, Arizona. Preliminary studies on the site, testing the existing pump-and-treat remediation scheme and propose and optimal remediation scheme using the Outer Approximation algorithm and a 3-D numerical simulator, PTC.

References:

Karatzas, G. P., and G. F. Pinder, "Groundwater Management Using Numerical Simulation and the Outer Approximation Method for Global Optimization", Water Resources Research, vol. 29, no. 10, 3371-3378, 1993.

Karatzas, G. P., and G. F. Pinder, "The Solution of Groundwater Quality Management Problems with a Non-convex Feasible Region Using a Cutting Plane Optimization Technique", Water Resources Research, vol. 32, no. 4, 1091-1100, 1996.

Karatzas, G. P., A. A. Spiliotopoulos, and G. F. Pinder, "A Multi-period Approach for the Solution of Groundwater Management Problems using the Outer Approximation Method", Proceedings of the North American Water and Environment Congress '96, American Society of Civil Engineers, CD-ROM, 1996.

Availability: Code not in public domain, not for sale.

Point(s) of Contact: George Karatzas (see table at beginning of this Appendix).