Application of Flow and Transport Optimization Codes to Groundwater Pump-and-Treat Systems: Umatilla Army Depot, Oregon

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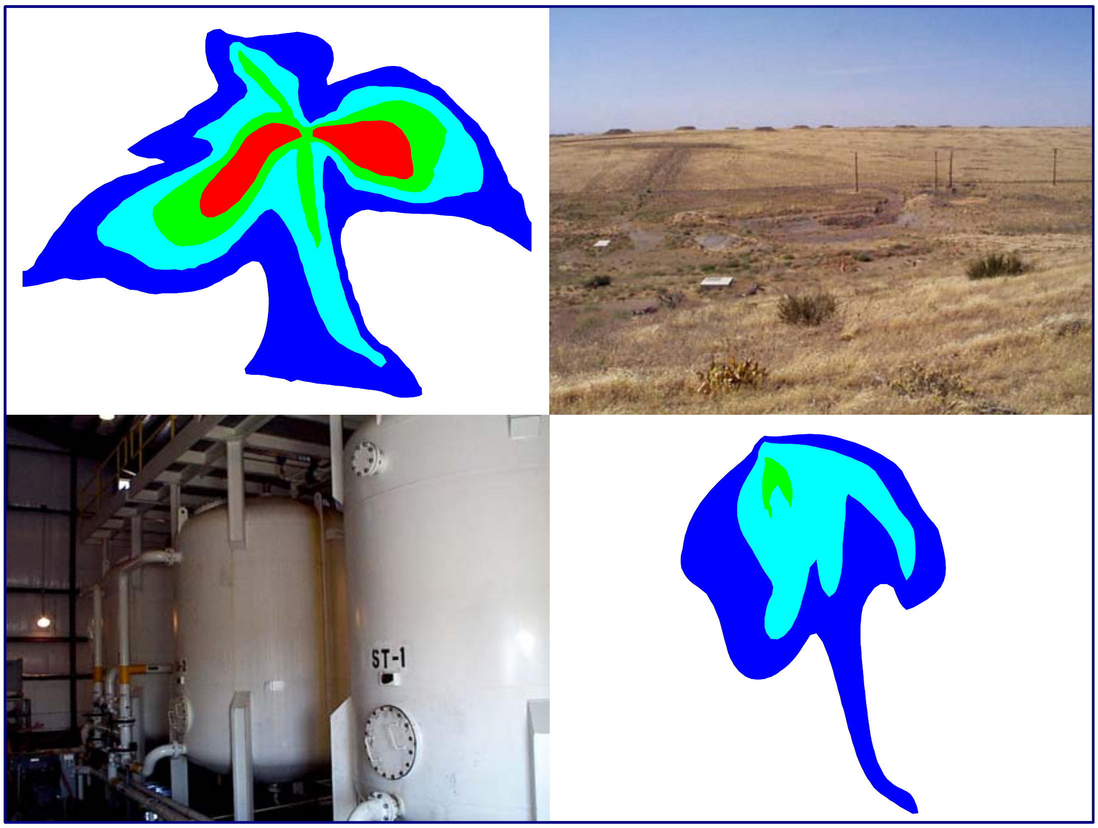

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Contents

ABSTRACT

Since the early 1980s, many researchers have shown that the simulation-optimization (S/O) approach is superior to the traditional trial-and-error method for designing cost-effective groundwater pump-and-treat systems. However, application of the S/O approach to real field problems has remained limited. This report describes the application of a new general-purpose simulation-optimization code referred to *Modular Groundwater Optimizer (MGO)* to optimize an existing pump-and-treat system at the Umatilla Army Depot in Oregon. Two optimization formulations were developed to minimize the total capital and operational costs under the current and possibly expanded treatment plant capacities. Another formulation was developed to minimize the total contaminant mass of RDX and TNT remaining in the shallow aquifer by the end of the project duration. For the first two formulations, this study produced an optimal pumping strategy that would achieve the cleanup goal in 4 years with a total cost of $1.66 million in net present value. For comparison, the existing design in operation was calculated to require 17 years for cleanup with a total cost of $3.83 million in net present value. Thus, the optimal pumping strategy represents a reduction of 13 years in cleanup time and a reduction of 56.6% in the expected total expenditure. For the third formulation, this study identified an optimal dynamic pumping strategy that would reduce the total mass remaining in the shallow aquifer by 89.5% compared with that calculated for the existing design. In spite of their intensive computational requirements, this study shows that the global optimization techniques such as tabu search and genetic algorithms can be applied successfully to large-scale field problems involving multiple contaminants and general hydrogeological conditions.

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Introduction

1.1 PURPOSE AND SCOPE

Groundwater remediation is associated with enormous costs. According to a recent study by the U.S. Environmental Protection Agency (USEPA, 1997), the remaining remediation costs for contaminated soil and groundwater in the United States are estimated at $187 billion in 1996 U.S. dollars. A great portion of the costs is tied to pump-and-treat remedies. Through 1996, 93% of the 605 sites remaining on the EPA National Priority List (Superfund sites) had pump-and-treat remedies only while additional 6% had a combination of pump-and-treat and *in situ* remedies. Recent studies completed by the Department of Defense and the U.S. Environmental Protection Agency indicate that the majority of pump-and-treat systems are not operating as designed, have unachievable or undefined goals, and have not been improved since installation. Nevertheless, to comply with existing regulations, numerous pump-and-treat systems will continue to operate for years to come.

Since the early 1980s, many researchers have shown that optimization techniques can be used in conjunction with aquifer simulation models to design more cost-effective pump-and-treat systems than traditional trial-and-error methods. However, although significant progress has been made in the theoretical development of the simulation-optimization (S/O) approach, the application of the S/O approach to large, field-scale problems has remained limited. Several factors may have contributed to this lack of practical applications. First, the use of the S/O approach requires intensive computing capabilities, thus making many complex three-dimensional field problems intractable. Second, there are currently few general-purpose and easy-to-use S/O codes available to practitioners at the field project level. Finally, the advantages of the S/O approach over the traditional trial-and-error approach in solving real-world problems have not been adequately demonstrated since most studies presented in the literature use simple hypothetical examples.

The purpose of this work is to apply a general-purpose simulation-optimization software tool referred to *Modular Groundwater Optimizer* (*MGO*) (Zheng and Wang, 2001) to optimize an existing pump-and-treat system at the Umatilla Army Depot in Oregon. The work is part of a field demonstration project funded by the Environmental Security Technology Certification Program (ESTCP) to demonstrate the practical applicability of selected simulation-optimization modeling codes at several field sites. The field demonstration project is intended to serve as well-controlled case studies to demonstrate the key steps involved in remediation system optimization at real field sites with general hydrogeological conditions. The information obtained from this project will be useful to future optimization efforts.

1.2 ORGANIZATION OF THE REPORT

Following this introduction, Section 2 provides a brief overview of the simulation-optimization approach and the modeling software used in this work. Section 3 describes various assumptions and formulations of the optimization problem for the Umatilla site and presents the optimal pumping strategies for different formulations. Section 4 summarizes the key findings and lessons learned from this work.

1.3 ACKNOWLEDGMENTS

The funding for this study was provided by the Naval Facilities Engineering Service Center (NFESC) and the U.S. Environmental Protection Agency through the DoD ESTCP Program. We are grateful to many individuals who contributed to the success of this project, including Kathy Yager, USEPA; Dave Becker, Army Corps of Engineers; Karla Harre, Paul Lefebvre, Nick Ta, Laura Yeh, and Doug Zillmer, NFESC; Rob Greenwald and Yan Zhang, GeoTrans Inc.; Richard Peralta, Utah State University; and Barbara Minsker, University of Illinois.

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The Simulation-Optimization Approach and Software

2.1 OPTIMIZATION PROBLEM FORMULATION

There are two sets of variables associated with a groundwater management problem, decision variables and state variables. The variables that can be used to define and differentiate alternative decisions are known as decision variables. One primary decision variable is the pumping or injection rate of wells. Other possible decision variables include well locations and the “on/off” status of a well. These decision variables can be specified or managed in the calculation process to identify their best combination, also referred to as the optimal management policy or strategy. The variables that describe the flow and transport conditions of an aquifer are known as state variables. Common state variables are hydraulic head, which is the dependent variable in the groundwater flow equation, and concentration, which is the dependent variable in the transport equation. In a coupled simulation-optimization model, the simulation component updates the state variables, and the optimization component determines the optimal values of all decision variables.

An optimization problem is defined in terms of an objective function and a set of constraints. The objective function can be formulated, for example, as the net present value of the management costs, taken over an engineering planning horizon. The costs can include the capital costs associated with well drilling and installation, and operational costs associated with pumping and/or treatment over the lifetime of the project. Other forms of the objective function are also possible. For example, for a long-term contamination containment system, the objective function could be defined simply in terms of the total pumping rate, if the one-time drilling and installation costs are negligible compared to the cumulative pumping and treatment costs. For a remediation design problem, alternative objective functions include maximization of contaminant mass removal by a remediation system or minimization of the contaminant mass remaining in the aquifer. Some remediation or monitoring network design problems could be formulated as multi-objective problems. The exact form of the objective function is determined by the nature of the individual problem.

In all cases, management objectives must be achieved within a set of constraints, which can be derived from technical, economic, legal, or political conditions associated with the project. These constraints may apply to both decision variables and state variables. They may take the form of either equalities or inequalities. Constraints on the decision variables might include the number and locations of candidate wells, and the upper and lower bounds of pumping/injection rates at each candidate well. Constraints on the state variables might include the requirement that hydraulic heads be maintained above or below a certain level, or that contaminant concentrations not exceed regulatory standards at specified compliance points.

2.2 OPTIMIZATION SOLUTION TECHNIQUES

The optimization problem as defined above can be solved through manual trial-and-error adjustment or through a formal optimization technique. While the trial-and-error method is simple and thus widely used, testing and checking hundreds to thousands of trial solutions is tedious and cannot guarantee that the optimal solution has been identified. In contrast, an optimization technique can be used to identify the optimal solution, and equally important, to prove whether a particular management scenario or remedial alternative is feasible in terms of meeting the management objective and satisfying all the constraints.

Mathematical programming techniques have been commonly used for groundwater management optimization, including, 1) linear programming (LP) (e.g., Lefkoff and Gorelick, 1987); 2) nonlinear programming (NLP) (e.g., Ahlfeld et al., 1988); 3) mixed integer linear programming (MILP) (e.g., Willis, 1976 and 1979); 4) mixed integer nonlinear programming (MINLP) (e.g., McKinney and Lin, 1995); and 5) differential dynamic programming (DDP) (e.g., Culver and Shoemaker, 1992; Sun and Zheng, 1999). LP is applicable only when the aquifer simulation model and the objective function are both linear. When neither of them can be treated as linear, NLP must be applied. In optimization problems where discrete decision variables such as well locations and fixed capital costs are involved, MILP or MINLP must be used. DDP is particularly efficient for optimization problems with a large number of management periods.

Linear programming is computationally efficient and has been implemented in a number of practical simulation-optimization codes such as AQMAN (Lefkoff and Gorelick, 1987), MODMAN (Greenwald, 1994 and 1999), and MODOFC (Ahlfeld and Riefler, 1999), all of which involve flow-related constraints only. The major limitation of linear programming is that the method is restricted to confined aquifers and generally cannot deal with solute transport problems effectively. Nonlinear programming and dynamic programming have much wider applicability. However, it is necessary in these methods to evaluate the derivatives (or gradients) of the objective function with respect to the decision variables (and also the state variables for DDP); this is the reason that these methods are often referred to as "gradient" methods. While the gradient methods can be advantageous in terms of computational efficiency, they have some significant limitations as well. First, if the objective function is highly complex and nonlinear, there may exist multiple local optimal points in the solution space. As a result, a gradient method may be trapped in one of the local optima, thus failing to identify the globally optimal solution. Second, gradient calculation is a major source of numerical difficulty, which can lead to instability and convergence problems.

More recently, a class of optimization methods based on heuristic search techniques have been applied to groundwater management problems, including simulated annealing, genetic algorithms, tabu search, artificial neural networks, and outer approximation. These optimization techniques have been collectively referred to as global optimization methods because of their ability to identify the global or near-global optimum. They have also been called "gradient-free" methods because of the fact that they mimic certain natural systems, such as biological evolution in the case of genetic algorithms, to identify the optimal solution, instead of being guided by the gradients of the objective function. Even so, some elements of gradient-based search can be incorporated into a global optimization framework.

Global optimization methods generally require intensive computational efforts. In spite of this, however, they are being used increasingly to solve groundwater management problems to take advantage of their ability to identify the global optimum, their efficiency in handling discrete decision variables such as well locations, and the ease and generality with which they can be linked with any flow and transport simulation model. Examples of the application of simulated annealing to remediation design optimization problems include Dougherty and Marryott (1991), Rizzo and Dougherty (1996), and Wang and Zheng (1998). Examples of the application of genetic algorithms include McKinney and Lin (1994), Wang and Zheng (1997), and Reed et al. (2000). Examples of the application of artificial neural networks include Ranjithan et al. (1993), Rogers and Dowla (1994), and Aly and Peralta (1999). The first applications of outer approximation and tabu search to groundwater remediation problems are presented by Karatzas and Pinder (1993) and Zheng and Wang (1999b), respectively.

The intensive computational requirements of global optimization methods may be mitigated in a number of ways. For example, Zheng and Wang (1999b) present an integrated approach in which a global optimization algorithm, tabu search, is used to find the optimal well locations, while linear programming is used to find the optimal pumping rates. In essence, the large mixed integer problem is decomposed into smaller sub-problems, each of which has a much smaller number of decision variables so that the optimal solution can be reached much faster. Aly and Peralta (1999) combine artificial neural networks with a genetic algorithm to reduce the number of forward simulations required. The idea is to use artificial neural networks to construct a response function after a certain number of forward simulations have been performed, and then use the response function in lieu of the simulation model thereafter. Zheng and Wang (2002) demonstrate the application of a coupled GA and response function approach to the optimization of a large pump-and-treat system at the Massachusetts Military Reservation.

A prerequisite for the application of the S/O approach is the existence of a calibrated flow and/or transport simulation model. The uncertainties inherent in simulation models will obviously affect the identification of optimal solutions. To account for such uncertainties and associated risks, a number of stochastic approaches have been developed (e.g., Wagner and Gorelick, 1987; Tiedeman and Gorelick, 1993; Minsker and Shoemaker, 1998; Freeze and Gorelick, 1999). One approach is to translate the uncertainties into probabilistic constraints. For example, one can specify that constraints be satisfied within a specified, say 95%, reliability. Another approach is to express an uncertain aquifer parameter such as hydraulic conductivity in terms of multiple realizations. One can then specify constraints that satisfy all realizations, rather than one single realization in the deterministic approach.

2.3 SOFTWARE PACKAGE USED IN THIS STUDY

The simulation-optimization software used in this project is a recently developed general-purpose simulation-optimization code referred to as *Modular Groundwater Optimizer* (*MGO*) (Zheng and Wang, 2001). MGO represents one of the most advanced optimization tools currently available for field scale applications and has the following key features:

- Multiple solution algorithms. The MGO code is implemented with three global optimization methods, namely, simulated annealing, genetic algorithms, and tabu search. In addition, MGO also includes options for integrating the response function approach with a global optimization method for greater computational efficiency. Since no one single optimization technique is effective under all circumstances, the availability of multiple solution algorithms in a single software system makes MGO well suited for a wide range of field problems.
- Flexible objective function. The objective function of the MGO code can be highly nonlinear and complex. It can accommodate multiple cost terms such as fixed capital costs, drilling costs, pumping costs, and treatment costs. The optimization problem can be formulated as minimization, maximization or multi-objective.
- Dual discrete and continuous decision variables. The MGO code can be used to simultaneously optimize both discrete decision variables such as well locations and continuous decision variables such as injection/pumping rates.
- Multiple management periods. The MGO code can provide optimized solutions for multiple management periods, further reducing the remediation costs for problems where groundwater flow and solute transport conditions vary significantly with time.

- Multiple constraint types. The MGO code can accommodate many types of constraints that are commonly used in remediation designs, such as, maximum well capacities, minimum inward and upward hydraulic gradients for a capture zone, maximum drawdowns at pumping wells, and maximum concentration levels at compliance points. In addition, MGO can accommodate various balance constraints that relate one constraint to another.
- Full compatibility with MODFLOW and MT3DMS. The MGO code is fully compatible with the various versions of MODFLOW (McDonald and Harbaugh, 1988; Harbaugh and McDonald, 1996) and MT3DMS (Zheng and Wang, 1999a), which is the latest multi-species version of MT3D (Zheng, 1990). The flow and transport model input files that are set up for MODFLOW and MT3DMS before the optimization run can be used exactly without any modification. Thus, all commercially available pre- and post-processors for MODFLOW and MT3DMS can be used for pre- and post-processing purposes.

3

Development of Optimal Pumping Strategies

3.1 SITE HISTORY AND REMEDIAL ACTION

Umatilla Chemical Depot is a 19,728 acre military reservation established in 1941 as an ordnance depot for storage and handling of munitions. The facility is located in northeastern Oregon straddling the border of the Umatilla and Morrow counties, three miles south of the Columbia River and six miles west of Hermiston, Oregon. Originally Umatilla's mission included the storage, renovation and demilitarizing of conventional munitions and storage of chemical munitions. In 1994, as a result of the Base Realignment and Closure (BRAC) Act, the depot's mission was changed to storing chemical munitions until their destruction under the Chemical Stockpile Disposal Program and site remediation.

From the 1950s until 1965, the depot operated an onsite explosives washout plant. The plant processed munitions to remove and recover explosives using a pressurized hot water system. The wash water from the plant was disposed in two unlined lagoons, where wash water infiltrated into the soil. During the 15 years of operation of the washout plant, an estimated 85 million gallons of wash water were discharged to the lagoons. Although lagoon sludge was removed regularly during operation of the plant, explosives contained in the wash water migrated into the soil and groundwater at the site. Because of the soil and groundwater contamination, the site was placed on USEPA's National Priorities List (NPL) in 1984.

Two of the most common contaminants at the Umatilla site are 2,4,6 Trinitrotoluene (TNT) and Hexahydro-1,3,5-trinitro-1,3,5-triazine (commonly referred to as Royal Demolition Explosive or RDX. A pump-and-treat system was designed by the U.S. Army

Corps of Engineers (USACE, 1996 and 2000) to contain and remove the RDX and TNT plumes (Figure 3.1). The existing pump-and-treat system consists of three extraction wells (EW1, EW3, and EW4) and three infiltration basins (IF1, IF2, and IF3). The well labeled 'EW2' and the infiltration basin labeled 'IFL' are not in active use. All extraction wells and infiltration basins are located in the shallow aquifer with their respective pumping and injection rates listed in column 3 of Table 3.1. Calculated on the basis of the existing USACE design, the RDX and TNT plumes at the end of year 2002 are shown in Figure 3.1, with the maximum RDX and TNT concentrations at 28.2 and 86.7 ppb, respectively. The RDX/TNT plumes for year 2002 constitute the initial conditions for the optimal pumping strategies developed in this study.

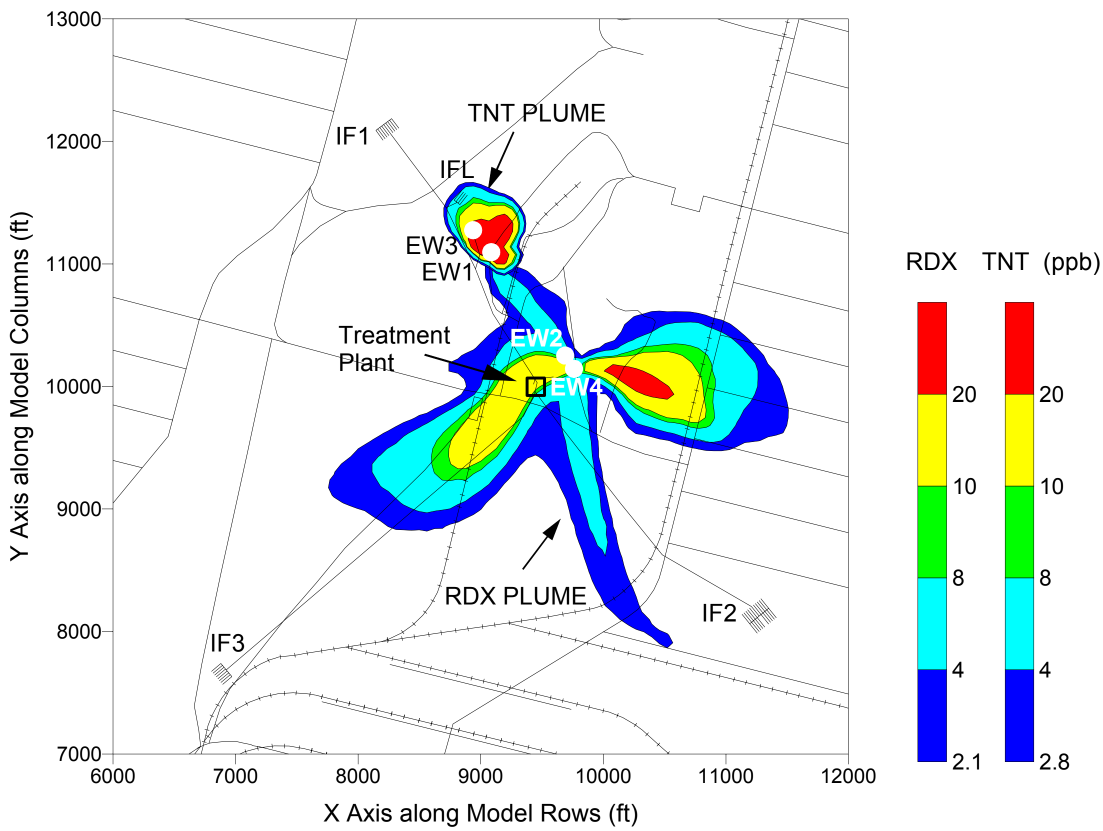


Figure 3.1. Simulated RDX and TNT plumes in the shallow aquifer at the end of year 2002 under the existing pump-and-treat system on Umatilla Army Depot, Oregon. The existing pump-and-treat system consists of three extraction wells (EW1, EW3, and EW4) and three infiltration basins (IF1, IF2, and IF3). The existing well 'EW2' and infiltration basin 'IFL' are not in active use. The extracted water, after treatment by adsorbent units at the on-site treatment plant, is injected back into the aquifer through the infiltration basins.

3.2 MINIMAL-COST STRATEGIES UNDER EXISTING TREATMENT PLANT CAPACITY

3.2.1 Objective Function

The objective of the first formulation for the optimization modeling analysis at the Umatilla site is to minimize the total costs (including both fixed capital costs and operation/maintenance, or O/M, costs) for the entire project duration. Thus the objective function of Formulation 1 can be expressed as follows:

$$\text{Minimize } \left(CCW + CCB + CCG + FCL + FCE + VCE + VCG + VCS\right) \qquad (3.1)$$

where

CCW: Capital costs of new wells ($75,000 for installing a new well, $25,000 for putting an existing unused well into service)

CCB: Capital costs of new recharge basins ($25,000 for installing a new recharge basin independent of its location)

CCG: Capital cost of new GAC unit (no new GAC unit is permitted for Formulation 1)

FCL: Fixed cost of labor ($237,000 is the fixed annual O&M labor cost)

FCE: Fixed costs of electricity ($3,600 is the fixed annual electric cost)

VCE: Variable electrical costs of operating wells (a function of the pumping rate)

VCG: Variable costs of changing GAC units (dependent on the average influent concentrations of RDX and TNT discharged into the treatment plant)

VCS: Variable cost of sampling ($150,000 in the first year, decreasing subsequently proportional to the ratio of the total plume area in any particular year over that in the first year)

More detailed cost information can be found in a companion report on optimization problem formulation (GeoTrans, 2001).

Note that all cost terms in equation (3.1) are computed in net present value (NPV) with the following discount function:

$$NPV = \frac{cost_{iy}}{\left(1+r\right)^{iy-1}} \qquad (3.2)$$

where NPV is the net present value of a cost incurred in year iy with a discount rate of r (r = 5% in this analysis). The value of $iy = 1$ corresponds to the first year of remedial operation. For example, if the remedial system starts in 2003, $iy = 1$ for 2003, $iy = 2$ for 2004, and so on. The cost terms in equation (3.1) must be evaluated at the end of each year to account for annual discounting and to ensure that no costs are incurred after the cleanup is achieved.

3.2.2 Constraints

Formulation 1 includes the following constraints that must be satisfied while the cost objective function is minimized (see GeoTrans, 2001):

(1) The modeling period consists of 4 management periods of 5 years each, beginning in January 2003 ($iy = 1$).

(2) Modifications to the pump-and-treat system may only occur at the beginning of each management period.

(3) Cleanup must be achieved within 20 years. In other words, the maximum concentrations of RDX and TNT in the shallow aquifer (i.e., model layer 1) must be less than their respective cleanup targets by the end of year 20:

$$C_{RDX}^{\max} \le 2.1 \text{ ppb}$$
$$C_{TNT}^{\max} \le 2.8 \text{ ppb}$$

(4) The total pumping rate, after adjustment for the average amount of system uptime, cannot exceed 1300 gpm, i.e., the current maximum capacity of the treatment plant:

$$\tfrac{1}{\alpha} Q_{total} \le 1300$$

where α is a coefficient representing the average amount of system uptime ($\alpha = 0.9$ for this analysis). Note that this constraint prohibits installation of additional GAC units.

(5) The pumping capacity of individual wells must not exceed 400 gpm in the less permeable portion of the aquifer (zone 1) and 1000 gpm in the more permeable portion (zone 2):

$$\tfrac{1}{\alpha} Q_i \le 400 \qquad \text{if well } i \text{ is in zone 1}$$
$$\tfrac{1}{\alpha} Q_i \le 1000 \qquad \text{if well } i \text{ is in zone 2}$$

(6) RDX and TNT concentrations must not exceed their respective cleanup levels beyond a specified area (buffer zone) when evaluated at the end of each management period. This constraint requires the containment of the RDX and TNT plumes within the buffer zone.

(7) The total amount of pumping must equal the total amount of injection through the infiltration basins within an error tolerance (1 gpm for this study).

3.2.3 Optimization Modeling Approach

From the cost information described above, it can be seen that the cost objective function for Formulation 1 are dominated by two terms, i.e., the fixed annual O&M labor cost ($237,000 in net present value) and the variable sampling cost ($150,000 in the first year and proportionally decreasing afterwards). Since these two cost terms depend directly on the number of years for which the pump-and-treat system must be operated, a simple and effective surrogate to minimizing the cost objective function is to achieve the cleanup goals as quickly as possible with the full pumping capability allowed under the existing treatment plant. This can be accomplished by minimizing the maximum concentrations (C_{max}) of RDX and TNT in the shallow aquifer (represented as layer 1 in the simulation model). Thus, the optimization modeling approach adopted for Formulation 1 is to identify a pumping strategy that lowers the C_{max} values of RDX/TNT to their respective cleanup targets of 2.1 and 2.8 ppb as quickly as possible while satisfying all the prescribed constraints. This is accomplished in this study by starting with the predetermined project duration of 20 years and sequentially reducing the required length of project duration until no feasible solution can be found.

The existing pump-and-treat system designed by the U.S. Army Corps of Engineers (USACE, 1996 and 2000) was used as the starting point for the optimization modeling analysis. The existing USACE design is shown in Figure 3.1 with three active extraction wells and three active infiltration basins. At the start of optimization modeling, four potential new pumping wells and three potential new infiltration basins were added to the existing design (Figure 3.2). The selection of candidate locations for the potential new pumping wells and infiltration basins was based on the judgment that they would speed up the cleanup of both RDX and TNT plumes. The 'moving well' option as implemented in the

MGO code was used to define the candidate locations for the potential new wells and infiltration basins. This was done by associating each well or infiltration basin with a rectangular region of the model grid within which the well or infiltration basin can move freely in search of the optimal location. Each pumping well was represented by a single model node while each infiltration basin by four nodes with the total injection rate partitioned equally among them. All wells and infiltration basins were required to be in model layer 1, as other model layers beneath layer 1 were only intended to approximate the mass storage effect of the bedrocks underlying the shallow aquifer.

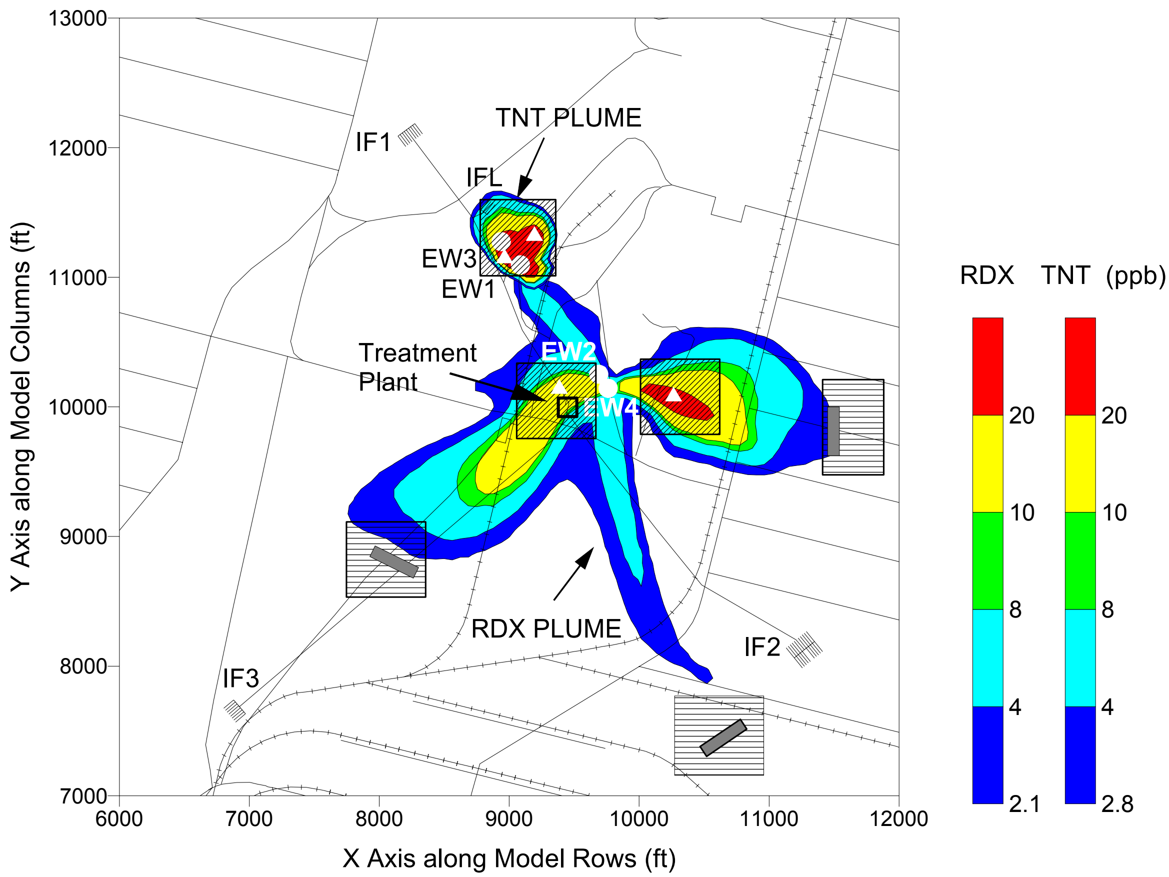


Figure 3.2. Potential new wells (shown as triangles) and new infiltration basins (shown as solid blocks) along with their respective candidate locations defined by the rectangles with line patterns.

Tabu search (TS), one of the three global optimization solvers available in the MGO code, was used to obtain the optimal strategy. The theoretical background of the TS technique and guidelines for its effective application are provided in Zheng and Wang (1999b and 2001). In this analysis, the following empirical solution options were selected after some initial experiments:

NSIZE0 = 5 (tabu size)

INC = 5 (increment of tabu size)

MAXCYCLE = 100 (the maximum number of TS iterations allowed to cycle)

NSAMPLE = 10 (the number of TS iterations between cycling checks)

NRESTART = 50 (the number of TS iterations allowed without improvement)

NSTEPSIZE = 2 (the search step-size, reduced to 1 for refined local search)

TOL = 0.0 (the stopping criterion)

3.2.4 Optimal Solution

The optimal pumping strategy obtained for Formulation 1 is illustrated in Figure 3.3. Of the most interest to note is that no well is selected by the new strategy in the RDX plume area. Neither the existing pumping well 'EW2' nor 'EW4' is utilized. Furthermore, the two potential new wells added to the RDX plume area are not used either. Instead, two new pumping wells 'NEW1' and 'NEW2' are selected in the TNT plume area, in addition to the two existing pumping wells 'EW1' and 'EW3'. Existing infiltration basins 'IF1' and 'IFL' are not utilized by the new strategy. None of the three new candidate infiltration basins is selected either. All extracted water is injected into the existing infiltration basins 'IF2' and 'IF3'.

The logic behind the new pumping strategy is apparently to concentrate the pumping on the TNT plume, which is strongly sorptive and more difficult to remove than the RDX plume. Turning off the existing infiltration basins 'IF1' and 'IFL' and injecting all extracted water into 'IF2' and 'IF3' also help push the RDX plume toward the TNT plume, both of which will be eventually removed by the four pumping wells located in the TNT plume area (Figure 3.3).

The pumping and injection rates for the optimal strategy are listed in column 4 of Table 3.1. Because the cleanup targets are achieved within five years, the optimal pumping strategy was developed for only one management period. The maximum concentrations of RDX and TNT in the shallow aquifer (model layer 1) calculated under the optimal pumping strategy are plotted in Figures 3.4. Also shown in Figure 3.4 are the maximum concentrations calculated for the existing USACE design prior to the optimization modeling analysis. The cleanup targets for RDX and TNT are both achieved in 4 years. In contrast, the existing design requires 8 and 17 years, respectively, to clean up the RDX and TNT plumes. The cost objective function for the optimal pumping strategy is $1.66 in net present value, as compared to $3.83 for the existing design. Thus the optimal strategy represents a 56% reduction in the total costs. The detailed cost breakdown is listed in Table 3.2.

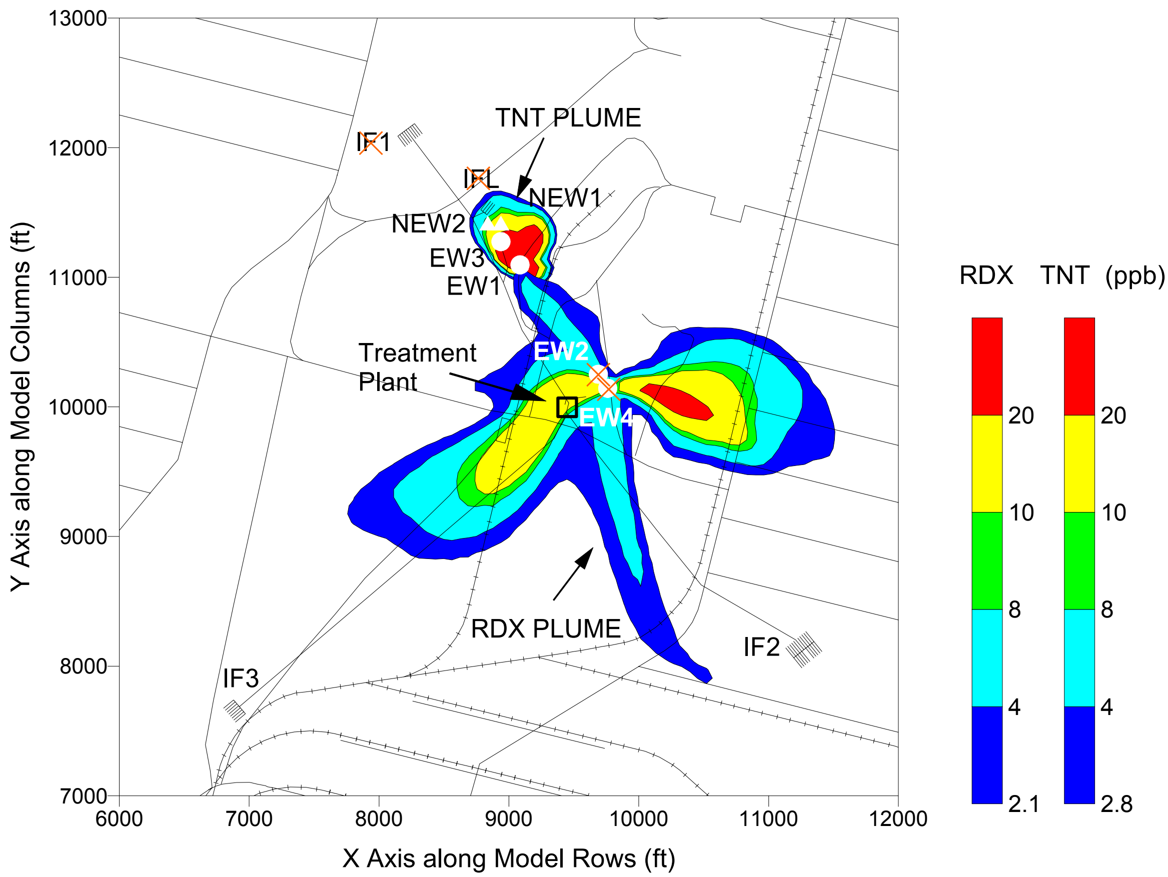


Figure 3.3. Locations of extraction wells and infiltration basins for the optimal strategy identified under Formulation 1. It consists of two existing wells (EW1 and EW3, marked as cycles) and two new wells (NEW1 and NEW2, marked as triangles), all of which are located in the TNT plume area. The existing wells labeled 'EW2' and 'EW4' and infiltration basins labeled 'IF1' and 'IFL' are not used in the optimal strategy, as indicated by the cross symbols.

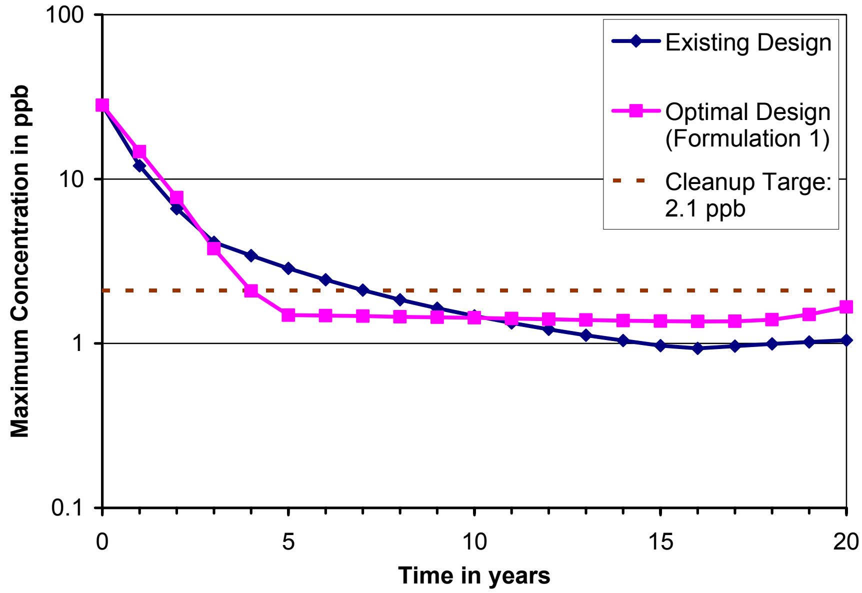
Table 3.1. Optimal pumping strategy for Formulation 1 as compared with the existing design (a negative flow rate for pumping and positive for injection).

Name	Location (Layer, Row, Column)	Pumping/Injection Rate (GPM)	
		Existing Design	Formulation 1
EW-1	(1,60,65)	-128	-307.5
EW-2	(1,83,84)	0	0
EW-3	(1,53,59)	-105	-219.5
EW-4	(1,85,86)	-887	0
New-1	(1,48,59)	0	-360
New-2	(1,48,55)	0	-283
IF-1	*	233	0
IF-2	*	405	380
IF-3	*	483	790
IF-L	*	0	0
Total costs in net present value (dollars)		*$3,836,285*	*$1,664,395*

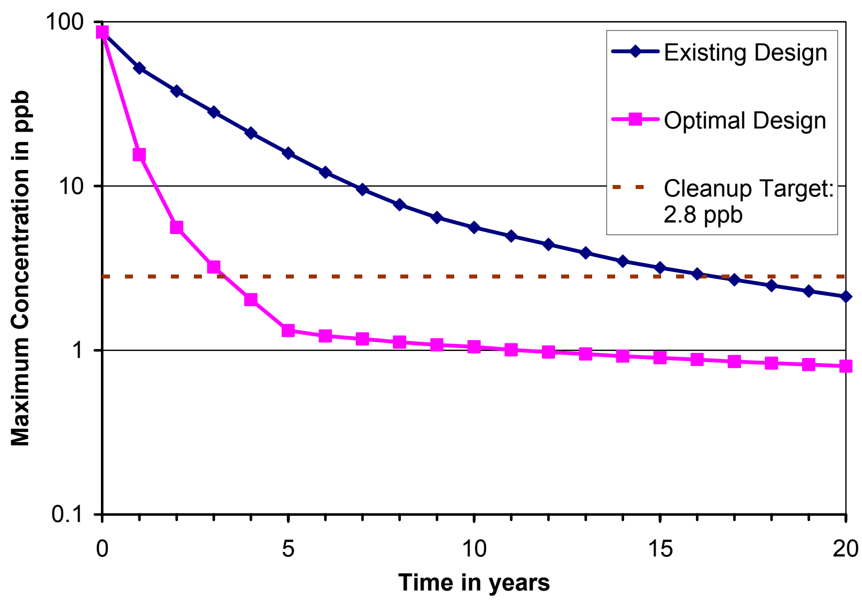
*Note: Each infiltration basin occupies more than one model cell. The exact location is indicated in the MODFLOW Well Package input file named 'Formuln1.WEL' (see Attachment A).

Table 3.2. Breakdown of the capital and O/M costs.

Cost Components	Existing Design	Optimal Strategy
Capital Costs of New Wells	0	$150,000
Capital Costs of New Recharge Basins	0	0
Capital Costs of New GAC Units	0	0
Fixed Costs of Labor	$2,805,552	$882,410
Fixed Costs of Electricity	$42,616	$13,404
Variable Costs of Electricity for Operating Wells	$251,405	$48,394
Variable Costs of Changing GAC Units	$16,338	$11,700
Variable Costs of Sampling	$720,374	$558,487
Objective Function Value	*$3,836,285*	*$1,664,395*



(a) RDX



(b) TNT

Figure 3.4. Calculated maximum concentrations of the two contaminants (RDX and TNT) in the shallow aquifer (model layer 1) starting at the end of 2002 (year 0). The line with diamond symbols indicates the existing pumping strategy while the line with square symbols indicates the new optimal strategy. The dashed line indicates the cleanup target.

3.3 MINIMAL-COST STRATEGIES UNDER THE EXPANDED TREATMENT PLANT CAPACITY

The optimization problem defined under Formulation 1 requires the total pumping, after adjustment for system uptime, not to exceed 1300 gpm, i.e., the maximum capacity of the existing on-site treatment plant. A logical question to ask is whether the total costs can be further reduced if the treatment plant capacity is allowed to increase. Thus, a second formulation was developed to address this question. The objective function for Formulation 2 is identical to that of Formulation 1, i.e., to minimize the total costs as expressed in equation (3.1). The constraints are also the same as those defined for Formulation 1 except that the total pumping rate, after adjustment for the average amount of system uptime, cannot exceed 1950 gpm, i.e.,

$$\frac{1}{\alpha} Q_{total} \leq 1950$$

where as defined previously α is a coefficient representing the average amount of system uptime ($\alpha = 0.9$ for this study). The modified total pumping capacity allows the installation of up to two additional GAC units each with a capacity of 325 gpm. The cost for adding a new GAC unit is $150,000 (by converting a GAC changeout unit in the current system into an adsorption unit).

The same computational procedure as described in the previous section for Formulation 1 was applied to obtain an optimal strategy for Formulation 2. The optimal strategy of Formulation 1 was used as the initial solution for Formulation 2. Interestingly, no better strategy was found for the new formulation than that obtained for Formulation 1, after approximately 2000 flow and transport simulation runs (i.e., objective function evaluations). This suggests that any cost savings that might be derived from the expanded treatment plant capacity could not offset the significant startup capital costs required for installation of any new GAC units. Thus the optimal strategy identified for Formulation 1 also applies to Formulation 2. In other words, although the treatment plant is allowed to expand from the current capacity of 1300 gpm to a higher capacity of 1950 gpm, it is more cost effective to keep the total pumping within the current capacity.

3.4 OPTIMAL PUMPING STRATEGIES FOR MINMIZING THE TOTAL CONTAMINANT MASS REMAINING

3.4.1 Objective Function

The objective of the third formulation for development of optimal pumping strategies at the Umatilla site is to minimize the total contaminant mass remaining in the shallow aquifer (model layer 1) within 20 years. Thus the objective function of Formulation 3 can be expressed as follows:

$$\text{Minimize } \left(M_{RDX} + M_{TNT}\right) \tag{3.3}$$

where M_{RDX} and M_{TNT} are the total RDX and TNT mass remaining in model layer 1 at the end of the 20-year project duration. Both dissolved and sorbed phases must be included in the computation of total mass.

3.4.2 Constraints

All constraints previously defined for Formulation 1 were applied directly to Formulation 3. In addition, two new constraints were considered for Formulation 3:

- The maximum number of new wells installed over the project duration must not exceed four.
- The maximum number of new recharge basins added over the project duration must not exceed three.

These new constraints were intended to keep the total costs of Formulation 3 comparable with those of Formulation 1. This allows a qualitative comparison of Formulations 1 and 3 under different objective functions.

3.4.3 Optimization Modeling Approach

The modeling approach adopted for this analysis is to determine the optimal pumping strategy for the management period one (year 0 – 5) first, followed by the second management period (year 6 – 10), the third management period (year 11 – 15), and finally the last management period (year 16 – 20). The RDX/TNT plumes calculated at the end of the first management period under the optimal strategy constitute the initial conditions for the simulation model used in the second management period. The same procedure was repeated for the subsequent management periods. This sequential modeling approach is more efficient computationally than the alternative approach in which all decision variables are optimized simultaneously in all management periods. Other studies have shown that the difference between the two approaches is small in the quality of the obtained optimal solutions.

As in the analysis of Formulation 1, the pumping wells and infiltration basins in the existing design were used as the starting point. In addition, the same candidate wells and infiltration basins as defined for Formulation 1 (Figure 3.2) were considered for Formulation 3. Both tabu search (TS) and genetic algorithms (GA) were used in the optimization modeling. The solution options for tabu search have been described previously in Section 3.2.3. For GA, various combinations of solution options were experimented. In general, the following options were found to be effective:

NPOPSIZ = 100 – 200 (population size)

PCROSS = 0.5 – 0.6 (crossover probability)

PMUTATE= $1/\text{NPOPSIZ}$ (mutation probability)

NPOSSIBL = 64 or 128 (number of possibilities for discretization of flow rate variables)

3.4.4 Optimal Solution

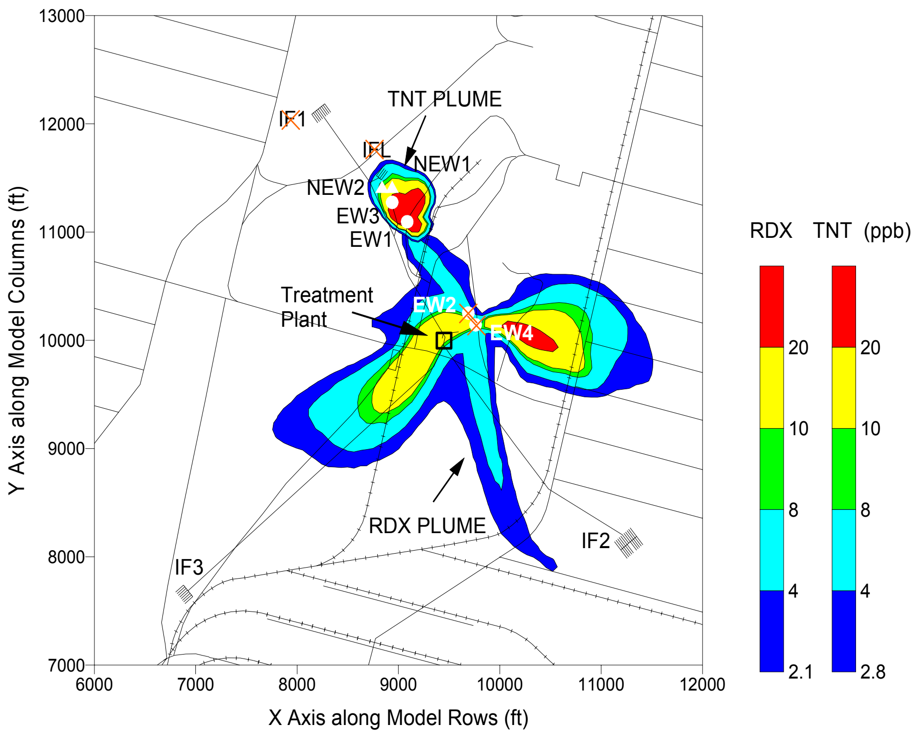
The dynamic optimal pumping strategies for the four management periods of Formulation 3 are shown in Figure 3.5(a)-(d). The optimal pumping and injection rates are listed in Table 3.3. The RDX and TNT plumes shown in each figure represent the conditions at the beginning of each management period. Moreover, it should be noted that the color contour scales are different in Figure 3.5(a)-(d). This becomes necessary for visualization purposes because the concentrations are reduced to very low levels after the initial management period.

For Management Period 1 [see Figure 3.5(a)], two existing wells (EW1 and EW3) and two new wells (NEW1 and NEW2) are selected in the TNT plume area, as in Formulation 1. No pumping well is used in the RDX plume area. Nor is any new infiltration basin needed. Moreover, the existing infiltration basins ‘IF1’ and ‘IFL’ are not used. All extracted water is discharged into the existing infiltration basins ‘IF2’ and ‘IF3’, which helps push the RDX plume toward the TNT plume. The calculated total RDX/TNT mass remaining in the shallow aquifer at the end of the first management period (year 5) is 3.14 kg. Compared with 12.95 kg calculated for the existing USACE design, the optimal strategy represents a mass reduction of 76.3%. Moreover, both RDX/TNT cleanup targets are achieved within the first 5 years.

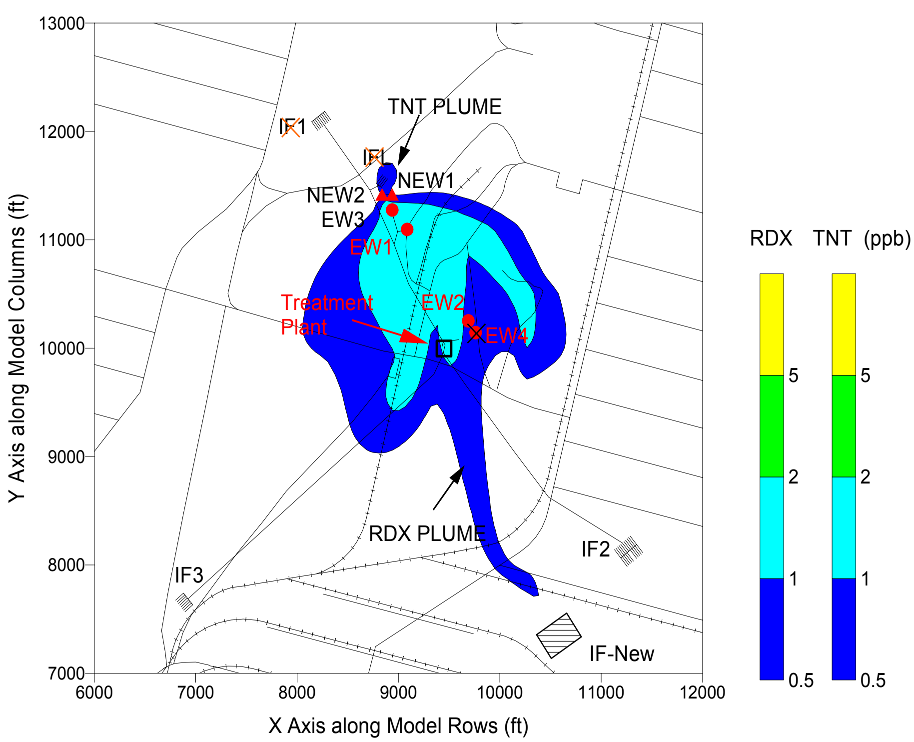
For Management Period 2 [see Figure 3.5(b)], the existing well labeled 'EW2' is utilized. This shifts more pumping back to the RDX plume as the TNT plume has been nearly all removed. Furthermore, a new infiltration basin labeled 'IF-NEW' is added to push the residual mass along a zone of low hydraulic conductivity toward the pumping well near the center of the RDX plume. The total RDX/TNT mass remaining in the shallow aquifer at the end of the second management period (year 10) is 0.85 kg. Compared with 5.184 kg calculated for the existing USACE design, the optimal strategy represents a mass reduction of 83.5%.

Management Period 3 continues the trend started in Management Period 2 by utilizing both existing wells 'EW2' and 'EW4' [see Figure 3.5(c)]. A new well added in Management Period 1 (NEW2) is no longer required. The new infiltration basin added in Management Period 2 (IF-NEW) continues to be active, along with the existing infiltration basins 'IF2' and 'IF3'. The total RDX/TNT mass remaining in the shallow aquifer at the end of the third management (year 15) is 0.30 kg. Compared with 2.85 kg calculated for the existing USACE design, the optimal strategy represents a mass reduction of 89.4%.

The optimal solution for Management Period 4 is similar to that for Management Period 3 except that the existing well 'EW2' is no longer used [see Figure 3.5(d)]. Note that the maximum concentration of either RDX or TNT at the start of Management Period 4 is less than 0.5 ppb, indicating very little mass still left in the aquifer. The total RDX/TNT mass remaining in the shallow aquifer at the end of the fourth management (year 20) is 0.185 kg. Compared with 1.765 kg calculated for the existing USACE design, the optimal strategy represents a mass reduction of 89.5%.

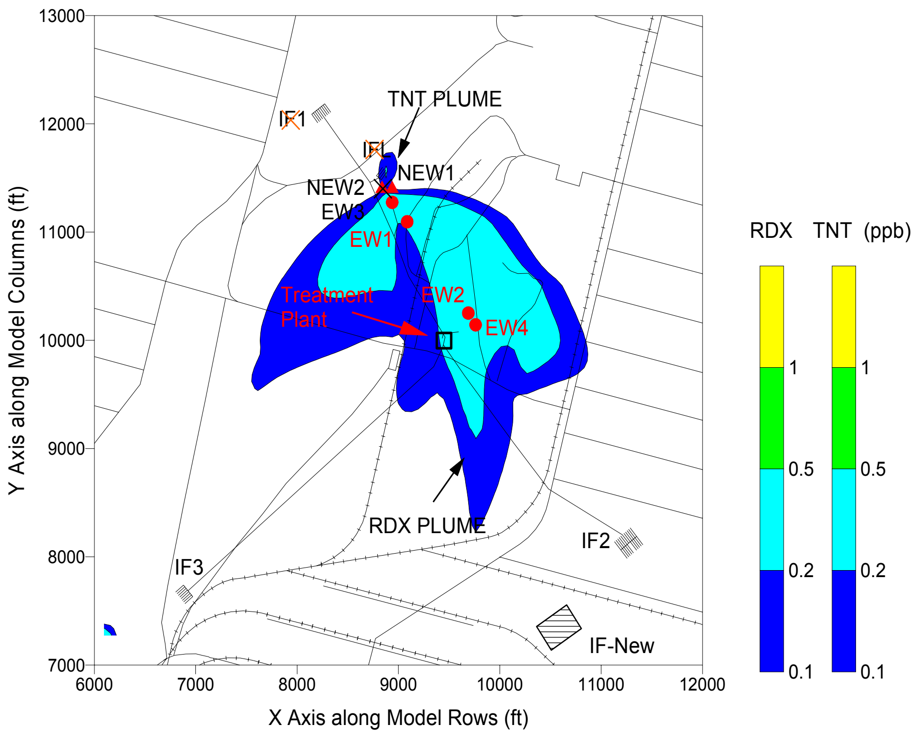


(a) Management Period 1 (Year 0-5)

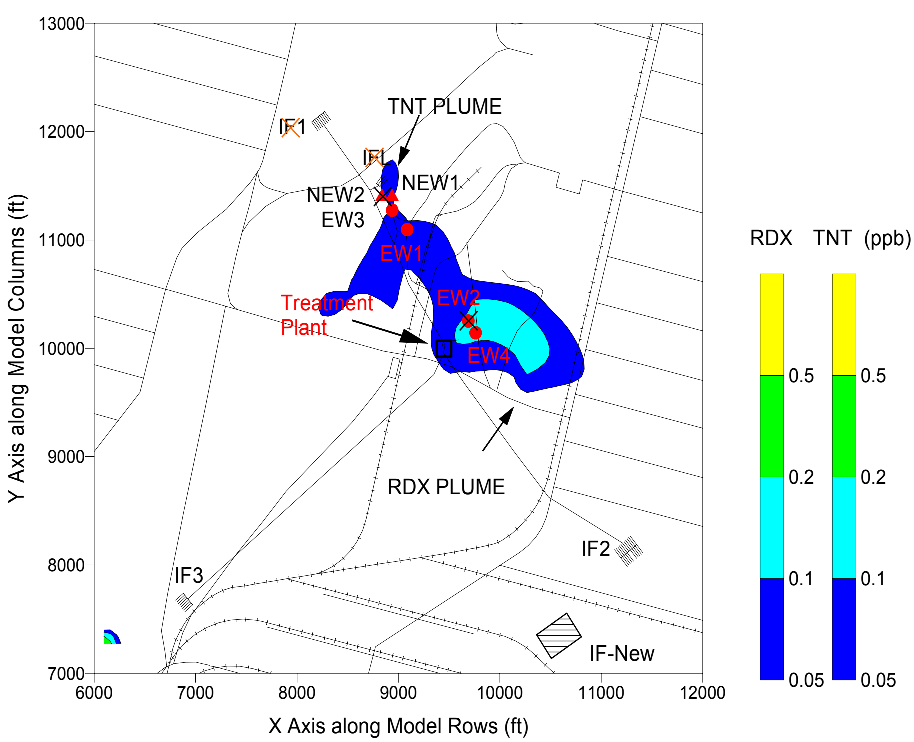


(b) Management Period 2 (Year 6-10)

Figure 3.5. (continued)



(c) Management Period 3 (Year 11-15)



(d) Management Period 4 (Year 16-20)

Figure 3.5. Locations of extraction wells and infiltration basins for the dynamic optimal pumping strategy identified under Formulation 3.

Table 3.3. Optimal solution and objective function value for Formulations 3 (a negative flow rate for pumping and positive for injection).

Name	Location (Layer, Row, Column)	Pumping/Injection Rate (GPM)			
		1st 5 years	2nd 5 years	3rd 5 years	4th 5 years
EW-1	(1,60,65)	-90	-118	-110	-215
EW-2	(1,83,84)	0	-276	-360	0
EW-3	(1,53,59)	-360	-286	-80	-70
EW-4	(1,85,86)	0	0	-360	-690
New-1	(1,48,59)	-360	-286	-145	-150
New-2	(1,48,55)	-360	-204	0	0
New-3	(1,78,45)	0	0	-115	-45
IF-1	*	0	0	0	0
IF-2	*	626	234	50	936
IF-3	*	544	585	440	117
IF-L	*	0	0	0	0
IF-New	*	0	351	680	117
Total mass (RDX and TNT) remaining in model layer 1 (kg)		*3.415*	*0.851*	*0.301*	*0.185*

*Note: Each infiltration basin occupies more than one model cell. The exact location of each infiltration basin is indicated in the MODFLOW Well Package input file named 'Formuln3.WEL' (see Attachment B).

Figure 3.6 shows the objective function value for the optimal strategy of Formulation 3, in comparison with that for the existing design. It can be seen that the rate of mass reduction is substantially faster under the optimal strategy than under the existing design. For comparison, the optimal strategy results in a 89.5% less mass remaining in the shallow aquifer by the end of the project duration (year 20). Because there is very little mass still remaining in the shallow aquifer at the Umatilla site after the first few years, the benefits of the optimal strategy are not significant in terms of the absolute amount of mass remaining. However, at a different site with a higher amount of contaminant mass, the benefits would be much more substantial.

Figure 3.7 shows the calculated maximum concentrations in the shallow aquifer under Formulation 3. Note that the cleanup targets of RDX = 2.1 ppb and TNT = 2.8 ppb are achieved in year 5 and year 3, respectively. These cleanup times are similar to those under Formulation 1 where the cleanup targets are both achieved in 4 years. The total costs for the first management period of Formulation 3 is approximately $2 million. This suggests that the optimal strategy obtained under Formulation 1 is more cost-effective and preferred over that under Formulation 3. Thus, it is more advantageous to formulate a remediation design problem in the context of a cost objective. On the other hand, considering the amount of time and efforts that would be needed to develop a detailed and accurate cost objective function, a simpler objective function such as minimizing mass remaining can be used effectively as a reasonable surrogate for more complex and detailed objective functions. This is particularly true for pump-and-treat systems whose costs are dominated by those components dependent on cleanup times, as the case at the Umatilla site.

Figure 3.8 presents a graphical illustration of the dynamic nature of the optimal pumping strategy developed for Formulation 3. This indicates that the optimization modeling code used in this analysis is sensitive to the changes in flow and transport conditions. It also demonstrates the need to consider multiple contaminant species simultaneously as the pattern of pumping and injection is clearly affected by the physical distributions and chemical properties of different species.

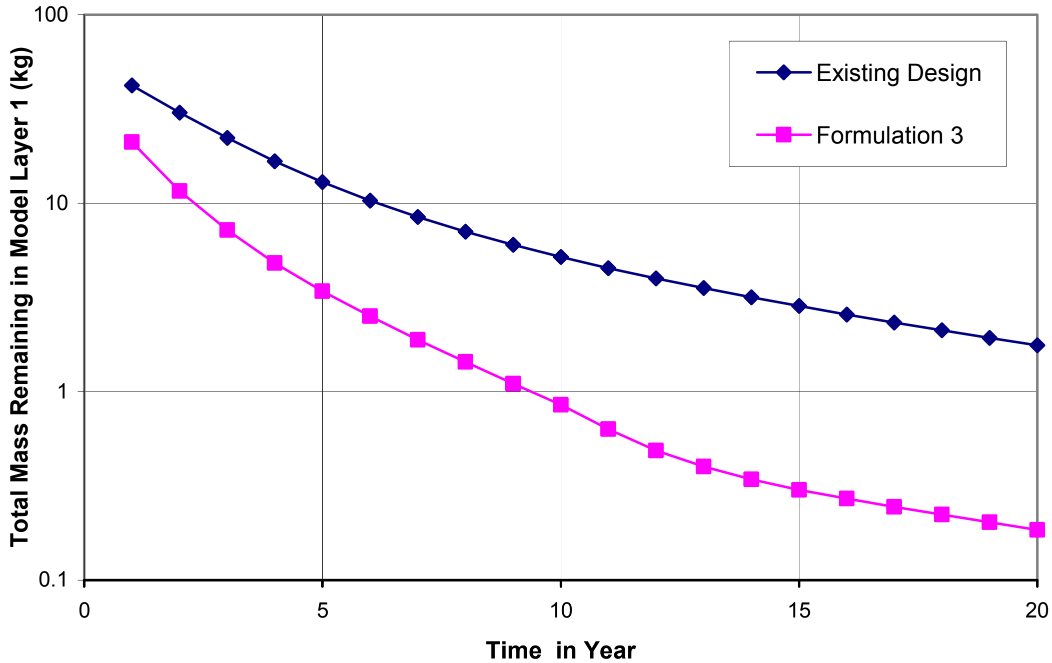


Figure 3.6. Total RDX/TNT mass remaining in the shallow aquifer under the optimal pumping strategy (Formulation 3) and under the existing design.

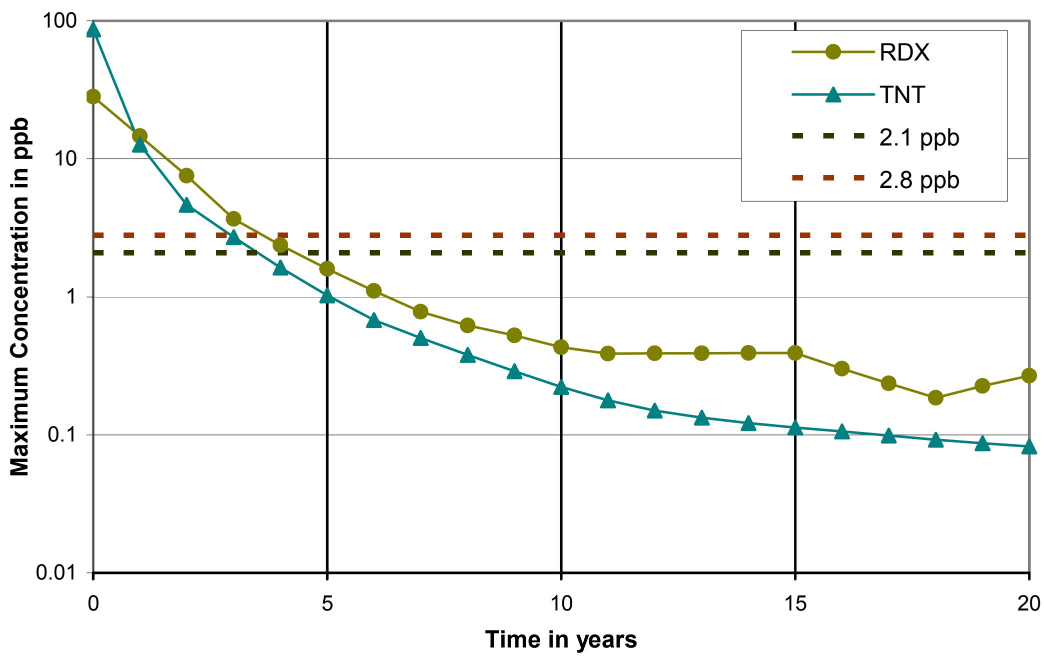
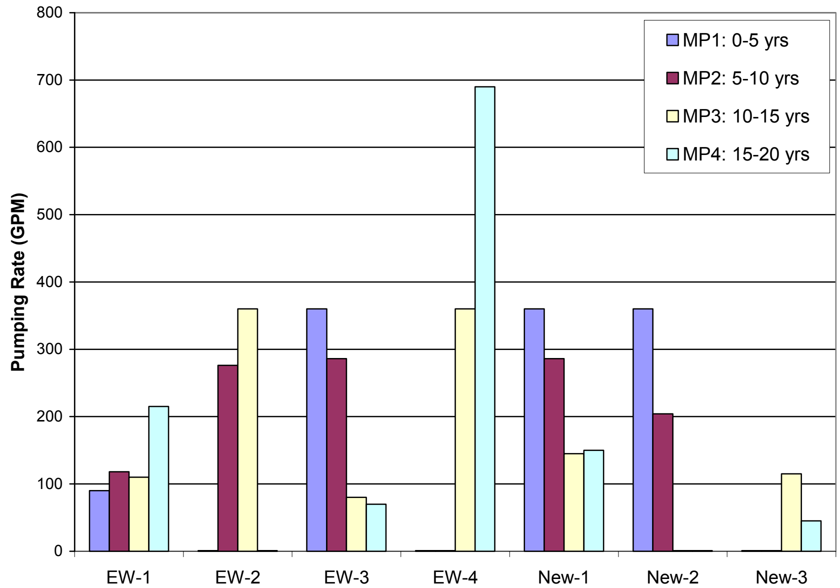
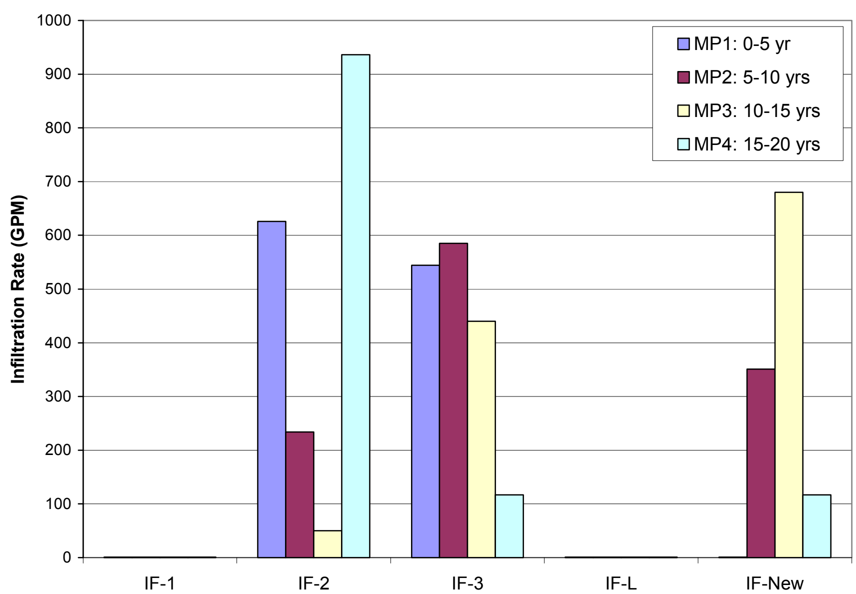


Figure 3.7. Calculated maximum concentrations under the optimal pumping strategy (Formulation 3). The cleanup targets of RDX = 2.1 ppb and TNT = 2.8 ppb are achieved in year 5 and year 3, respectively.



(a) Distribution of optimal pumping rates



(b) Distribution of optimal injection rates

Figure 3.8. Comparison of (a) optimal pumping rates and (b) optimal injection rates for the four management periods of Formulation 3.

3.5 COMPUTATIONAL ASPECTS

Global optimization techniques such as tabu search and genetic algorithms require a large number of flow and transport simulation runs before an optimal strategy can be identified. As mentioned previously, the tabu search solver implemented in the MGO code was used to solve Formulation 1. Instead of one large all-encompassing optimization run, the optimization problem was broken into many smaller runs, each of which consisted of several dozens to several hundreds of flow and transport simulations. This allowed the modeler to examine the intermediate results and determine whether to adjust the tabu search solution options. Furthermore, it provided the modeler an opportunity to optimize the well locations while keeping the pumping/injection rates fixed, and vice versa. Although the MGO code has the capability to optimize the well locations and pumping/injection rates simultaneously, it is sometimes advantageous to optimize these two different types of decision variables iteratively, particularly when a large number of candidate well locations are involved.

Many optimization runs were aborted or were intended for experimental purposes at the beginning of the project as the optimization code was modified and improved. Thus it is difficult to provide a precise estimate of the total number of simulation runs conducted and the actual amount of labor time spent on the analysis. Roughly, a total of 5000 flow and transport simulations were executed by the optimization code. These simulation runs were for only one management period (5 years) and each took an average of about 2.5 minutes on a PC equipped with a Pentium III 1 Ghz CPU, 256 MB RAM, and 5 GB hard drive space. Some simulation runs performed for Formulation 3 also contributed to the solution of Formulation 1.

The set-up of an optimization run was simple as all input files for MODFLOW and MT3DMS were used directly without modification. A simple optimization file was prepared to define the objective function, decision variables, constraints, and optimization solver options. Definition of candidate well locations was straightforward using the 'moving well' option by associating a rectangular block of the model grid with a potential new well within which it can move freely in search of its optimal location. Little labor time was required for postprocessing after each optimization run. More labor time was spent on improving the optimization code to make it more general and more computationally efficient.

For the solution of Formulation 3, approximately 8000 flow and transport simulations were executed by the optimization code. These simulation runs were all for 5 years (per management period) and each took an average of 2.5 minutes on a PC with a Pentium III 1-Ghz CPU. Again, very little labor time was required for postprocessing of optimization runs. Instead, more labor time was spent on improving the optimization code to make it more general and more computationally efficient.

4

Summary and Discussions

4.1 SUMMARY OF STRATEGIES

Formulation 1: minimize the total costs while satisfying the prescribed containment and cleanup constraints, under the existing treatment plant capacity.

This study identified an optimal solution which achieves the cleanup goal for both RDX and TNT in 4 years with a total cost of $1.66 million in net present value. The optimal solution uses two new wells but no new recharge basins (see Table 4.1). For comparison, the existing design requires a cleanup time of 17 years with a total cost of $3.83 million in net present value. Thus, the optimal solution represents a reduction of 13 years in cleanup time and a reduction of 56.6% in the expected total expenditure.

Formulation 2: minimize the total costs while satisfying the prescribed containment and cleanup constraints, given an increased treatment plant capacity.

This study found that the installation of up to two additional GAC units to the current treatment plant could offer no benefit for the objective of reducing the total costs under the same containment and cleanup constraints as set for Formulation 1. Thus, the optimal solution for Formulation 2 is identical to that for Formulation 1.

Formulation 3: minimize the total mass (RDX and TNT) remaining in the shallow aquifer while satisfying the prescribed containment and cleanup constraints, under the current treatment plant capacity.

This study identified an optimal dynamic pumping strategy that uses three new wells and one new recharge basin (Table 4.1). It achieves the cleanup goal for RDX in 5 years and TNT in 3 years. The mass remaining in the shallow aquifer (model layer 1) at the end of each 5-year management period is 3.415, 0.851, 0.301, and 0.185 kg, respectively. For comparison, the mass remaining calculated from the current design is 12.953, 5.184, 2.846, and 1.765 kg, respectively. Thus, the optimal strategy represents a mass reduction of 73.6%, 83.5%, 89.4%, and 89.5%, respectively.

Figure 4.1. Comparison of three formulations for development of optimal pumping strategies at the Umatilla site.

Formulation No.	1	2	3
Objective Function Value	$1,664,395	$1,664,395	0.185 kg
Number of New Extraction Wells Installed	2	2	3
Number of New Recharge Basins Installed	0	0	1
Number of New GAC Units Installed	N/A	0	N/A
Cleanup Time for RDX	4	4	5
Cleanup Time for TNT	4	4	3

4.2 OVERALL OBSERVATIONS

1. In spite of their intensive computational requirements, global optimization techniques including tabu search and genetic algorithms were applied successfully to the Umatilla site. All modeling work was carried out on desktop PCs equipped with Pentium II or III CPUs and 256 MB RAM.
2. For pump-and-treat systems where the total costs are dominated by the time required to achieve cleanup, a simple objective function such as the total mass remaining in the aquifer (Formulation 3) could be used as a reasonable approximation for a much more complex cost objective function (Formulation 1).
3. The advantage of a dynamic pumping strategy is significant. For example, in Formulation 3, if the well locations and flow rates optimized for Management Period 1 were held constant throughout the project duration, the reduction of mass remaining

in the aquifer at the end of year 20 would have been 71.3% relative to that calculated for the existing design, rather than 89.5% under the dynamic strategy.

4. This study demonstrates the need to consider multiple contaminant species simultaneously as the pattern of pumping and injection is clearly affected by the physical distributions and chemical properties of different species.
5. The 'moving well' option as implemented in the MGO code was found to be very efficient in dealing with a large number of candidate well locations. With this option, each candidate well is associated with a region (or cube in 3-D) representing a large number of model cells within which the candidate well can move freely in search of its optimal location. If the well is screened in more than one model layer, the total flow rate is partitioned among all layers according to their transmissivity values. A flow rate in any arbitrary layer is defined as the decision variable while the flow rates in other layers depend on the selected decision variable.

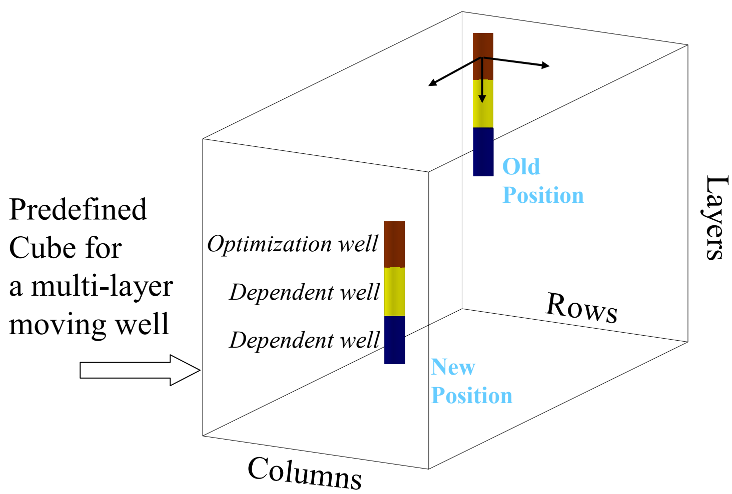


Figure 4.1. Illustration of the moving well option for defining well locations.

5

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ATTACHMENT A

MODFLOW WELL PACKAGE INPUT FILE
FOR OPTIMIZATION FORMULATION 1

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         1        85        86         0
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         1        60        65 -21605718
         1        83        84         0
         1        48        59 -25294500
         1        48        55 -19884288
         1        86        93         0
         1        86        74         0
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         1        30        40         0
         1        31        39         0
         1        31        40         0
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         1       105       102  13349875     1
         1       109        23  13876844     2
         1       109        24  13876844     2
         1       110        23  13876844     2
         1       110        24  13876844     2
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         1        98        41         0
         0  /sp2
         0  /sp3
         0  /sp4
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ATTACHMENT B

MODFLOW WELL PACKAGE INPUT FILE
FOR OPTIMIZATION FORMULATION 3

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        1       109        24   9555700     2
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        1        42        54         0
        1        42        55         0
        1        42        56         0
        1        42        57         0
        1        43        53         0
        1        43        54         0
        1        43        55         0
        1        43        56         0
        1        44        54         0
        1        44        55         0
        1        88       104         0
        1        89       104         0
        1        90       104         0
        1        91       104         0
        1        92       104         0
        1        97        38         0
        1        97        39         0
        1        98        40         0
        1        98        41         0
       34  /Stress Period:  2                   (year 6-10)
        1        85        86         0
        1        53        59 -20095076
        1        60        65  -8290975
        1        83        84 -19392450
        1        48        59 -20095076
        1        48        55 -14333550
        1        78        60         0
        1        60        85         0
        1        30        39         0
        1        30        40         0
        1        31        39         0
```

```
 1       31       40         0
 1      104      102   8220713     1
 1      105      102   8220713     1
 1      109       23  10275891     2
 1      109       24  10275891     2
 1      110       23  10275891     2
 1      110       24  10275891     2
 1       41       55         0
 1       41       56         0
 1       42       54         0
 1       42       55         0
 1       42       56         0
 1       42       57         0
 1       43       53         0
 1       43       54         0
 1       43       55         0
 1       43       56         0
 1       44       54         0
 1       44       55         0
 1      112       96   6165535     4
 1      112       97   6165535     4
 1      113       96   6165535     4
 1      113       97   6165535     4
34  /Stress Period:  3                       (year 11-15)
 1       85       86 -25294500
 1       53       59  -5621000
 1       60       65  -7728875
 1       83       84 -25294500
 1       48       59 -10188062
 1       48       55         0
 1       78       45  -8080188
 1       60       85         0
 1       30       39         0
 1       30       40         0
 1       31       39         0
 1       31       40         0
 1      104      102   1756563     1
 1      105      102   1756563     1
 1      109       23   7728875     2
 1      109       24   7728875     2
 1      110       23   7728875     2
 1      110       24   7728875     2
 1       41       55         0
 1       41       56         0
 1       42       54         0
 1       42       55         0
 1       42       56         0
 1       42       57         0
 1       43       53         0
 1       43       54         0
 1       43       55         0
 1       43       56         0
 1       44       54         0
 1       44       55         0
 1      112       96  11944625     4
 1      112       97  11944625     4
 1      113       96  11944625     4
 1      113       97  11944625     4
34  /Stress Period:  4                       (year 16-20)
 1       85       86 -48481124
```

1	53	59	-4918375	
1	60	65	-15106438	
1	83	84	0	
1	48	59	-10539375	
1	48	55	0	
1	78	45	-3161813	
1	60	85	0	
1	30	39	0	
1	30	40	0	
1	31	39	0	
1	31	40	0	
1	104	102	32882850	1
1	105	102	32882850	1
1	109	23	2055178	2
1	109	24	2055178	2
1	110	23	2055178	2
1	110	24	2055178	2
1	41	55	0	
1	41	56	0	
1	42	54	0	
1	42	55	0	
1	42	56	0	
1	42	57	0	
1	43	53	0	
1	43	54	0	
1	43	55	0	
1	43	56	0	
1	44	54	0	
1	44	55	0	
1	112	96	2055178	4
1	112	97	2055178	4
1	113	96	2055178	4
1	113	97	2055178	4