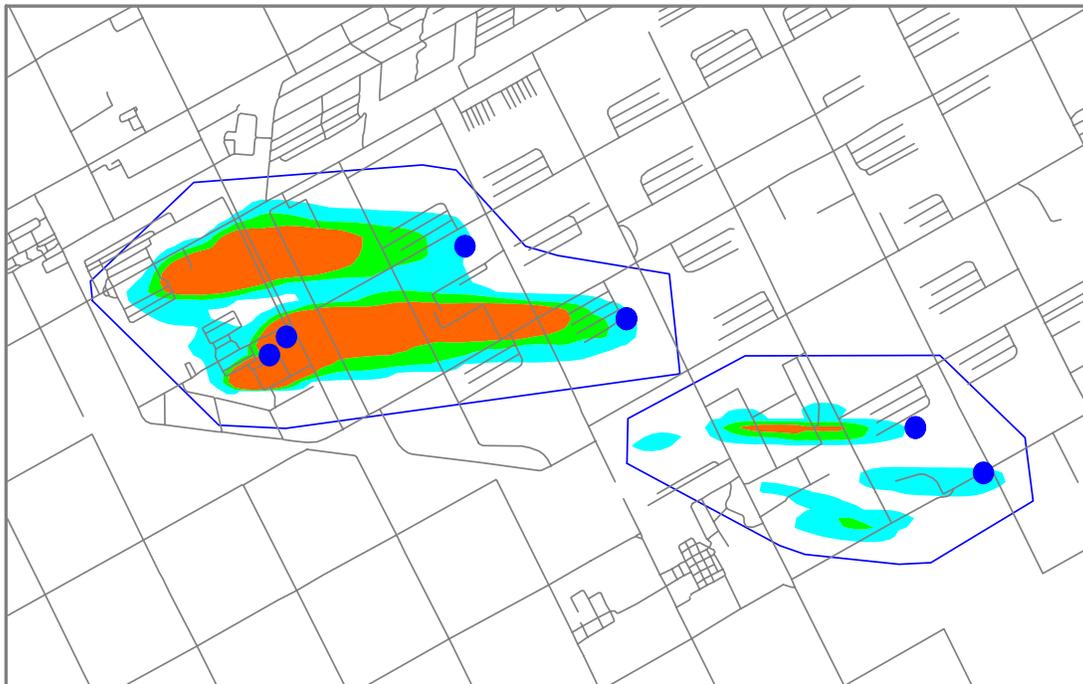


Application of Flow and Transport Optimization Codes to Groundwater Pump-and-Treat Systems: Former Blaine Naval Ammunition Depot, Hastings, Nebraska

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and

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ABSTRACT

This report presents the results of an optimization modeling analysis at the former Blaine Naval Ammunition Depot near Hastings, Nebraska. The study is the third in a series of field-scale optimization modeling demonstrations supported jointly by the U.S. DoD Environmental Security Technology Certification Program (ESTCP) and the U.S. EPA Technology Innovation Office. A general-purpose global optimization code was used to solve three optimization formulations for the Hastings site. For Formulation 1 with both containment and cleanup constraints, an optimal dynamic strategy was developed with a total cost of \$45.28 million in net present value. The optimal solution features a phased approach that emphasizes containment over cleanup and gradually increases the number of pumping wells to achieve cleanup at the end of the 30-year project horizon. The remediation costs are relatively low in early years but increase significantly near the end of the project duration. The optimal solution identified for Formulation 1 was found to be applicable to Formulation 2 as well, which is identical to Formulation 1 except for the assumption that up to 2400 gpm of extracted may be diverted without incurring any treatment or discharge costs. For Formulation 3 with the containment constraint only, the optimization analysis identifies an optimal dynamic strategy requiring 13 pumping wells with a maximum total pumping rate of 2737 gpm in any management period. Again, the optimal strategy features the phased approach that adds new pumping wells as necessary to ensure containment in each management period.

1

Introduction

1.1 PURPOSE AND SCOPE

The purpose of this study is to apply a general-purpose flow and transport optimization code to develop optimal pumping strategies for the former Blaine Naval Ammunition Depot near Hastings, Nebraska. The study is the third in a series of field-scale optimization modeling demonstrations supported jointly by the U.S. DoD Environmental Security Technology Certification Program (ESTCP) and the U.S. EPA Technology Innovation Office. 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 complex hydrogeological conditions. The information obtained from these studies will be useful to future optimization efforts.

1.2 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). The key features of MGO include:

- 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 (Zheng and Wang, 2002). 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.

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 study, including Dave Becker, Rob Greenwald, Karla Harre, Barbara Minsker, Richard Peralta, Kathy Yager, Laura Yeh, and Yan Zhang.

2

Optimal Solution: Formulation 1

2.1 OBJECTIVE FUNCTION

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

$$\text{MINIMIZE}(CCE + CCT + CCD + FCM + FCS + VCE + VCT + VCD) \quad (2.1)$$

where

CCE: Capital costs of new extraction wells (\$400,000 for installing a new extraction well independent of its location)

CCT: Capital costs of treatment plant (proportional to the maximum total pumping rate in any of the management period, \$1,000 per gpm)

CCD: Capital costs of discharge piping (proportional to the maximum total pumping rate in any of the management period, \$1,500 per gpm)

FCM: Fixed costs of management (\$115,000 per year)

FCS: Fixed costs of sampling (\$300,000 per year)

VCE: Variable costs of electricity for operating wells (\$46 per gpm)

VCT: Variable costs of treatment (\$283 per gpm)

VCD: Variable costs of discharge (\$66 per gpm)

More detailed cost information can be found in a companion report on optimization problem formulation by GeoTrans (2002). Note that all cost terms in equation (2.1) are computed in net present value (NPV) with the following discount function:

$$NPV = \frac{cost_{iy}}{(1+r)^{iy-1}} \quad (2.2)$$

where NPV is the net present value of a cost incurred in year iy with a discount rate of r ($r = 3.5\%$ 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 (2.1) must be evaluated at the end of each year to account for annual decrease in net worth when the discount rate $r > 0$.

The total project duration considered for this analysis is 30 years, beginning in January 2003 ($iy = 1$). The modeling period was divided into 6 management periods of 5 years each. The decision variables include the number and locations of new pumping wells, and the flow rates of each pumping well at each management period.

2.2 CONSTRAINTS

Formulation 1 includes the following constraints that must be satisfied while the cost objective function is minimized (see GeoTrans, 2002):

- (1) Modifications to the pump-and-treat system may only occur at the beginning of each management period.
- (2) Cleanup must be achieved in model layers 3-6 within the 30-year project horizon.
- (3) TCE and TNT concentrations must not exceed their cleanup levels of 5 and 2.8 ppb, respectively, beyond the predefined containment zones in model layers 3-6 at the end of the first management period and thereafter.
- (4) The capacities of new pumping wells must not exceed 350 gpm per model layer in which the well is screened.
- (5) No remediation well is allowed in certain pre-selected areas.
- (6) No remediation well is allowed in model cells with irrigation wells to prevent excessive drawdown.
- (7) No model cell can be dewatered (becoming a “dry cell”) due to excessive pumping.
- (8) Pumping rates for irrigation wells must not be altered in any stress period.
- (9) No remediation well is allowed in model layer 6.

2.3 MODELING APPROACH

Based on the cost information described above, a prescreening analysis indicated that the cost objective function for Formulation 1 is controlled by the number of years to cleanup and the total pumping rate. Because a significant amount of TCE remains stuck in low-permeability layer 2, it is likely that pumping in layers 3-5 needs to continue, even after these layers have been cleaned up prior to the end of the 30-year project horizon, to prevent the concentration in layer 3 from rebounding to above the cleanup level. Thus, the most cost-effective pumping strategy is likely the one that minimizes pumping while achieving the cleanup near the end of the 30-year project horizon.

The flow and transport model for the Hastings site takes over 2 hours per simulation on a Pentium III 1-GHz PC. To reduce the computational burden, a sequential approach was used to obtain the optimization solution. The optimization modeling was carried out one management period at a time, sequentially from period 1 (2003-2008), then period 2 (2008-2013), period 3 (2013-2018), period 4 (2018-2023), period 5 (2023-2028), and finally period 6 (2028-2033). In each management period, only those constraints that are applicable to that period were imposed on the optimization solution. If these constraints could not be satisfied in a particular period, the optimal solution obtained in the preceding period was adjusted by adding new wells in the locations where constraints were violated. The initial locations of remediation wells were determined manually. The final locations were optimized through tabu search (TS) or genetic algorithms (GA) by defining a candidate region in which any model cell can be a potential well location.

The theoretical background of TS and GA and the guidelines for their effective applications are provided in Zheng and Wang (2001). In this analysis, the following empirical TS and GA solution options were used with some small variations:

For Tabu Search (TS)

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)

For Genetic Algorithms (GA)

POPSIZE = 50 – 100 (population size)

NPOSIBL = 16 – 32 (number of discretizations for the flow rate decision variable)

PCROSS = 0.5 – 0.6 (crossover probability)

PMUTATE = 0.01 – 0.02 (mutation probability, set equal to the inverse of POPSIZE)

The long runtime of the flow and transport simulation model posed a significant challenge to global optimization techniques such as tabu search and genetic algorithms, which require a large number of flow and transport simulation runs. To reduce the total runtimes, the computationally intense TVD solver used in the transport model was changed to the more efficient implicit finite-difference method (FDM). However, the FDM solver is not sufficiently accurate for an advection-dominated transport problem, thus the optimization solution obtained through the FDM solver is generally not optimal. As a result, further adjustment must be made by switching back to the TVD solver in the transport model.

After the well locations were determined, the pumping rates were usually fine-tuned by applying the response function approach as discussed in Zheng and Wang (2002). With the response function approach, the results of the simulation runs required by TS and GA are saved in a database. These results are then used to fit a response function (or surrogate model) that approximates the flow and transport model. In this analysis, the cost objective function is a linear function of pumping rates, thus it is unnecessary to develop a response function between these two. Instead, a quadratic response function was constructed that relates the concentrations at selected constraint points to the pumping rate decision variables. The response function was then used in lieu of the simulation model to obtain the optimal pumping rates. Because the response function is only an approximation of the true simulation model, the optimal pumping rates obtained using the response function must be verified against the true simulation model. Details on the response function approach used in this study can be found in Zheng and Wang (2002).

2.4 OPTIMAL SOLUTION

The optimal solution obtained for Formulation 1 is presented in Table 2.1. Six wells with a total pumping rate of 1968 gpm are used in management period 1. Nine new wells are added in subsequent management periods. Thus a total of 15 wells are required for

Formulation 1. The total costs in net present value are \$45.28 million, with the cumulative cost for each management period listed in Table 2.1. The breakdown of various cost terms is shown in Figure 2.1 and the percentages of 3 major cost categories are shown in Figure 2.2.

Figures 2.3(a) – (g) show the TCE plumes in model layer 3 and locations of active pumping wells at the start or end of each management period. Figures 2.4(a) – (g) are the same illustrations for TNT plumes. It can be seen that the containment constraints are satisfied at the end of each management period (i.e., the beginning of the subsequent period). At the end of the 30-year project horizon the cleanup is achieved for both TCE and TNT. Both contaminant and cleanup constraints are also satisfied in model layers 5 and 6.

Table 2.1. Optimal dynamic pumping strategy identified for Formulation 1.

Well ID	Location			P1	P2	P3	P4	P5	P6
	(K	I	J)	2003-2008	2013	2018	2023	2028	2033
1	3	27	59	-350	-15	-50	-45	-350	
2	3	35	78	-290	-170	-180	-305		
	4	35	78	-290	-170	-180	-305		
	5	35	78	-290	-170	-180	-305		
3	3	52	120	-295	-240	-275	-240		
4	3	47	112	-120	-330	-310	-155		
	4	47	112	-120	-330	-310	-155		
5	3	37	38	-66	-170	-100	-100	-50	-50
6	3	39	36	-147	-79	-231	-215		
7	3	28	61		-286	-225	-190	-275	-330
	4	28	61		-286	-225	-190	-275	-330
8	3	30	65		-254	-110	-125	-350	-325
	4	30	65		-254	-110	-125	-350	-325
9	3	57	109		-350	-350	-185		
10	3	31	70			-260	-215	-350	
	4	31	70			-260	-215	-350	
11	3	32	62				-315	-200	-350
	4	32	62				-315	-200	-350
12	3	26	55					-300	-345
	4	26	55					-300	-345
13	4	32	75					-200	
	5	32	75					-200	
14	3	27	32						-330
	4	27	32						-330
15	3	27	30						-170
	4	27	30						-170
Total Rate (gpm)				-1968	-3104	-3356	-3700	-3750	-3750
New Wells				6	3	1	1	2	2
Cumulative Costs				17,347	24,814	30,864	36,337	41,193	45,281

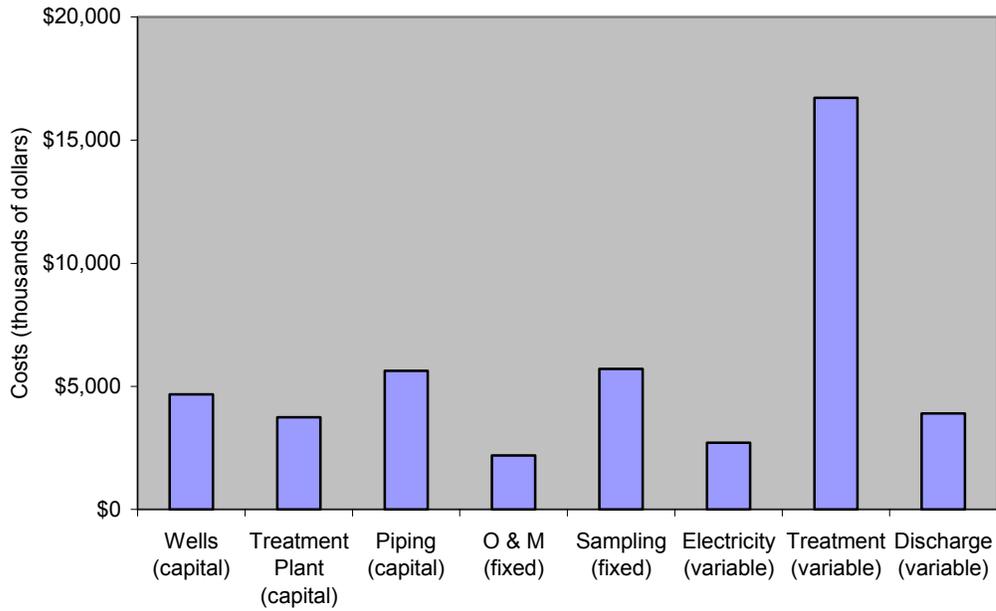


Figure 2.1. Breakdown of cost terms for the pumping strategy developed for Formulation 1.

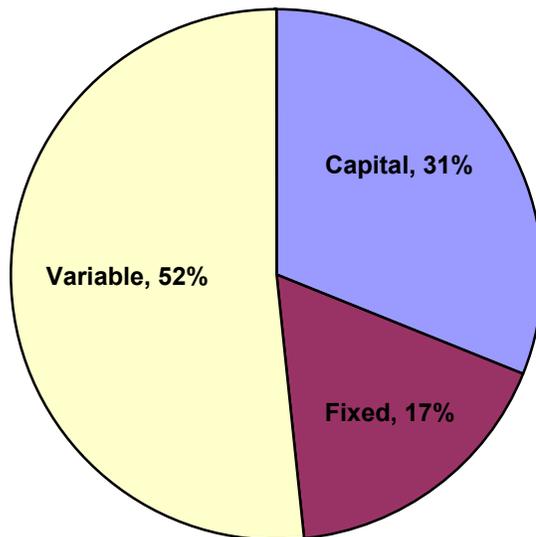
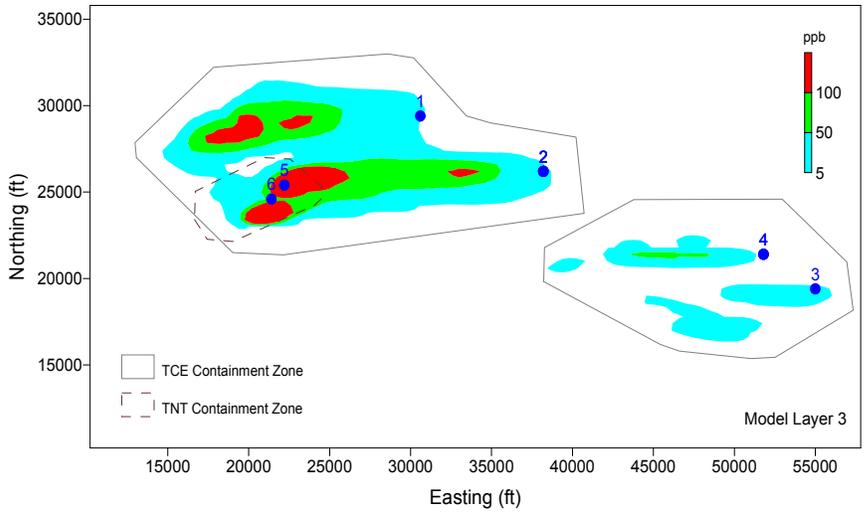
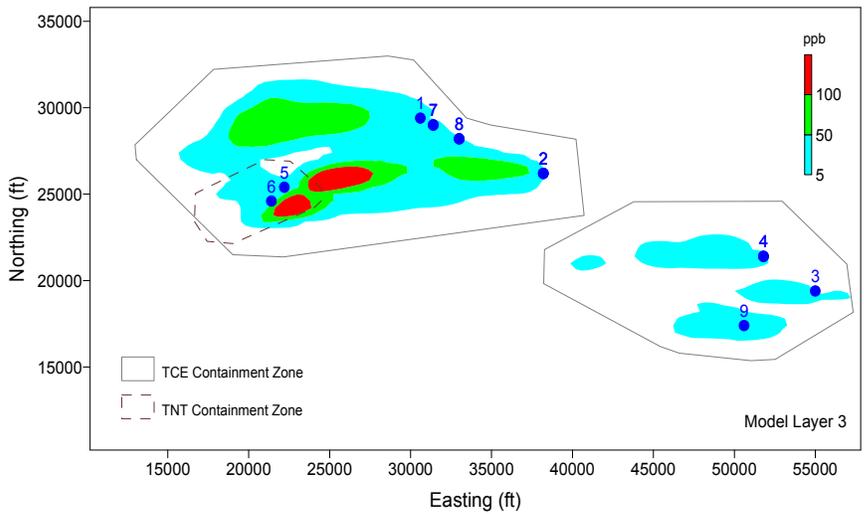


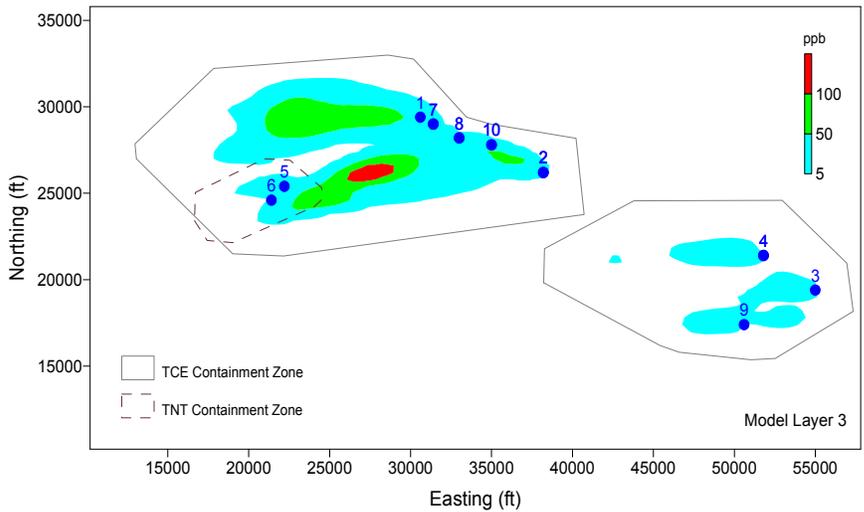
Figure 2.2. Distribution of three major cost categories for the optimal solution of Formulation 1.



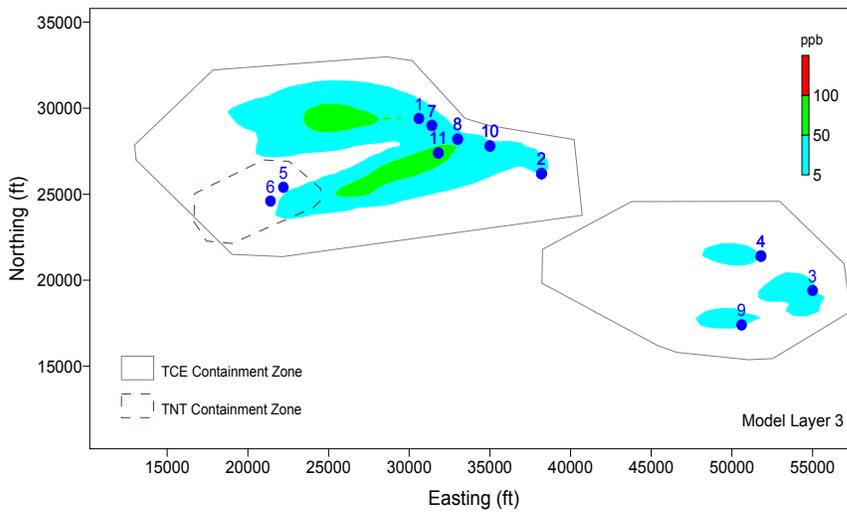
(a) Management period 1 (2003-08)



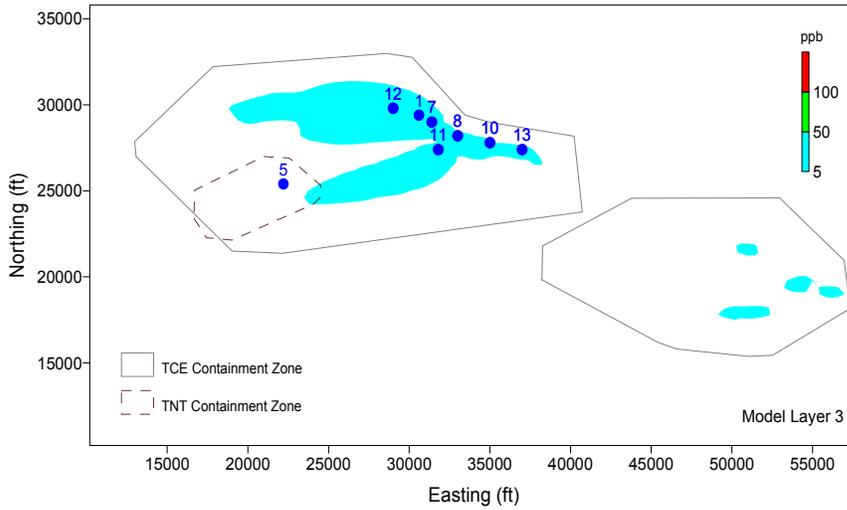
(b) Management period 2 (2008-13)



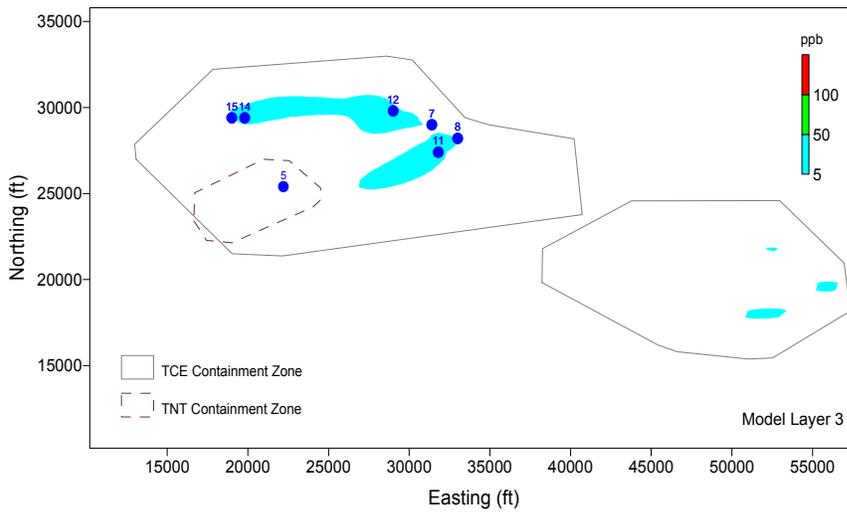
(c) Management period 3 (2013-18)



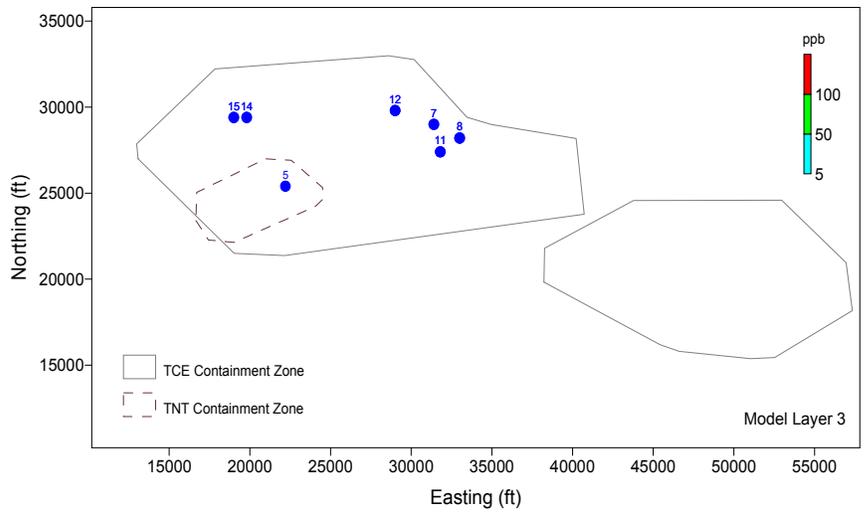
(d) Management period 4 (2018-23)



(e) Management period 5 (2023-28)

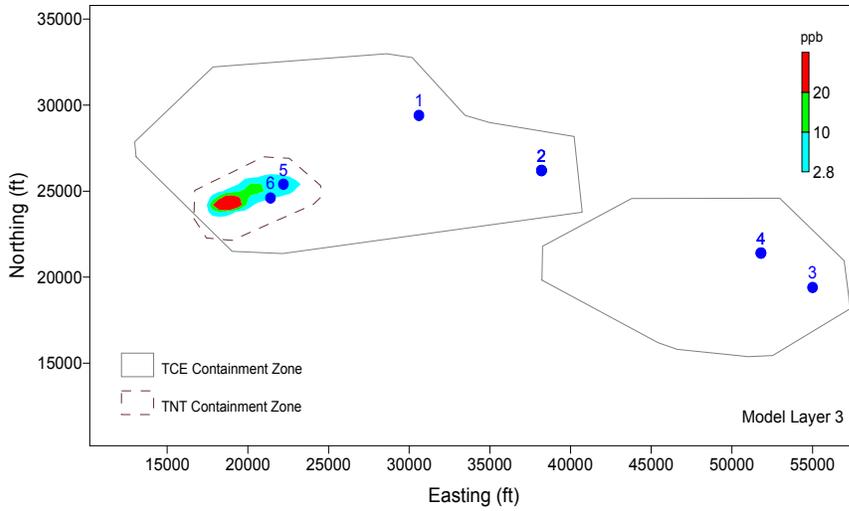


(f) Management period 6 (2028-2033)

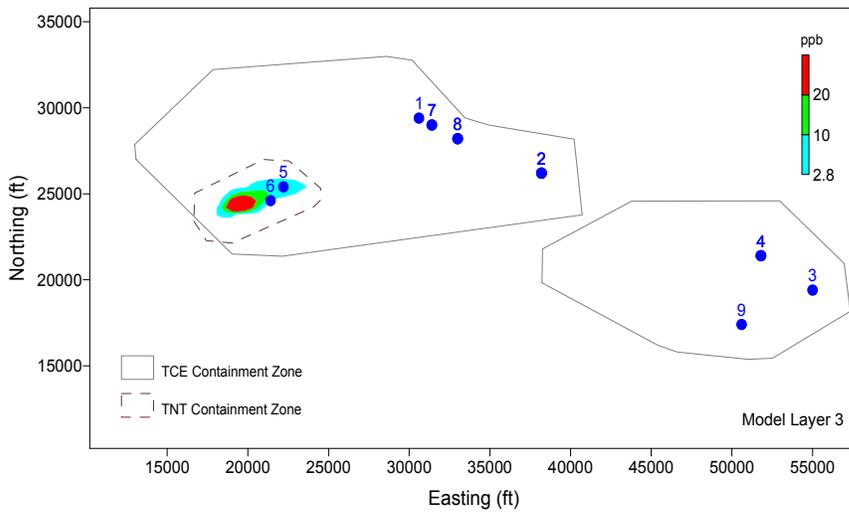


(g) End of the project horizon (2033)

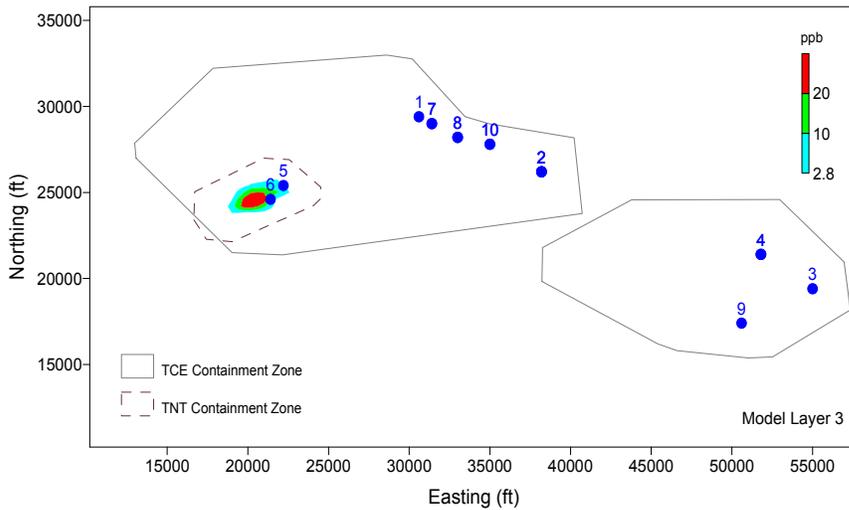
Figure 2.3. Calculated TCE plumes in model layer 3 at the start of six management periods (a)–(f) and at the end of the 30-year project horizon (g). The dots indicate the locations of pumping wells that are active during the management period in which the wells are shown.



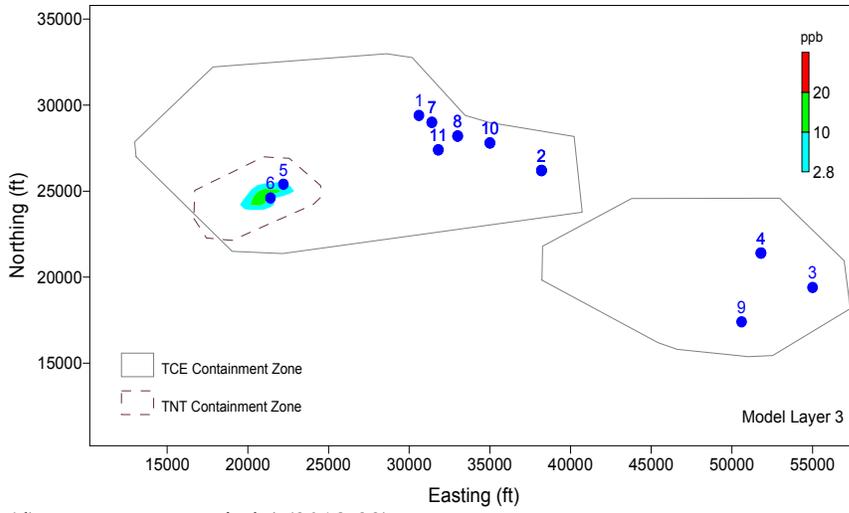
(a) Management period 1 (2003-08)



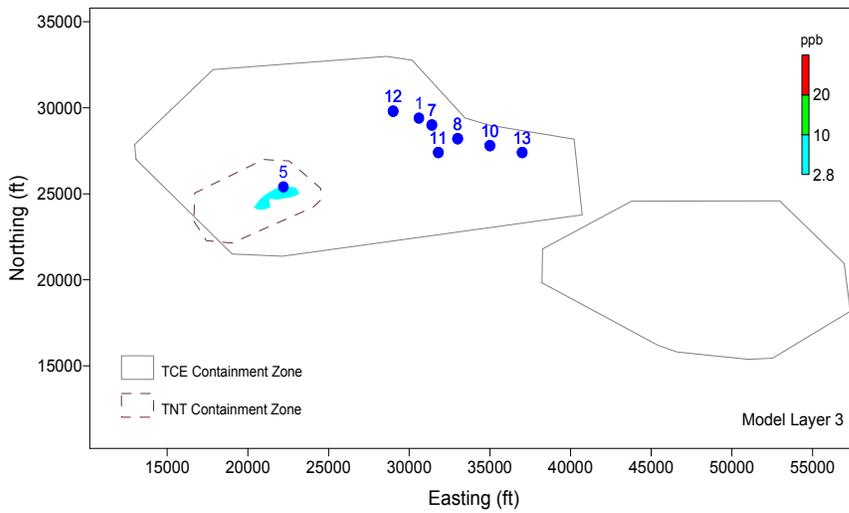
(b) Management period 2 (2008-13)



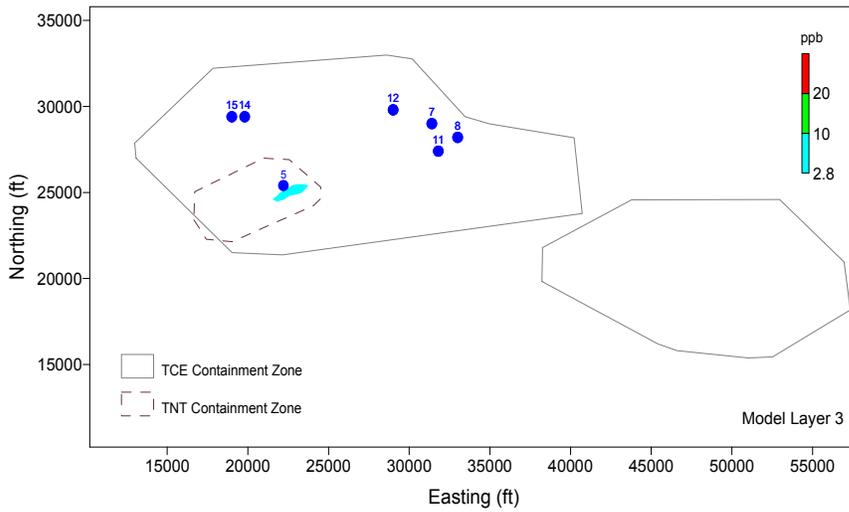
(c) Management period 3 (2013-18)



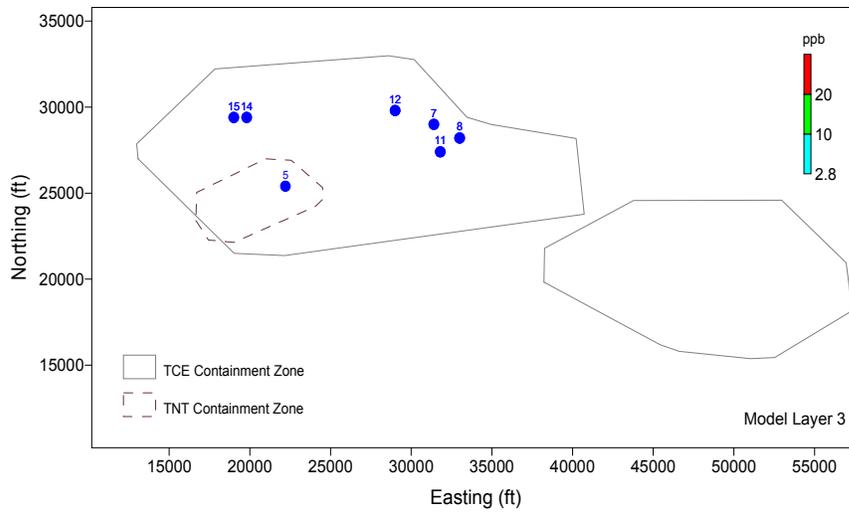
(d) Management period 4 (2018-23)



(e) Management period 5 (2023-28)



(f) Management period 6 (2028-33)



(g) End of the project horizon (2033)

Figure 2.4. Calculated TNT plumes in model layer 3 at the start of six management periods (a)–(f) and at the end of the 30-year project horizon (g). The dots indicate the locations of pumping wells that are active during the management period in which the wells are shown.

3

Optimal Solution: Formulation 2

3.1 OBJECTIVE FUNCTION AND CONSTRAINTS

The objective function for Formulation 2 is identical to that for Formulation 1 as expressed in equation (2.1). However, it is assumed that up to 2400 gpm of extracted water can be disposed of without incurring any treatment or discharge costs. Thus, all cost terms that are a function of the total pumping rate are equal to zero if the total pumping rate is smaller than 2400 gpm. Only the amount above the 2400-gpm limit is used in computing the fixed capital costs of treatment plant and discharge piping as well as and the variable costs of treatment and discharge. The constraints (1) – (9) defined for Formulation 1 also apply to Formulation 2.

3.2 OPTIMAL SOLUTION

The same modeling approach used for Formulation 1 is applicable to Formulation 2. In fact, because the objective function is of the same form and the constraints are identical between the two formulations, the optimal pumping strategy developed for Formulation 1 (see Table 2.1) applies to Formulation 2 as well. The value of cost objective function for Formulation 2, however, is much lower than that of Formulation 1 because of the diversion of up to 2400 gpm of extracted water. The total costs for the 30-year project are \$24.04 million in net present value. In addition, because the total pumping rate required for the first 5 years (management period 1) is only 1968 gpm, below the diversion cutoff amount of 2400 gpm, the construction of the treatment plant and associated discharge piping can be postponed to the second management period. This translates into cost savings of \$0.53 million because of the 3.5% discount rate.

4

Optimal Solution: Formulation 3

4.1 OBJECTIVE FUNCTION AND CONSTRAINTS

The objective function for Formulation 3 is to minimize the maximum total remediation pumping rate in any management period over the entire project horizon, i.e.,

$$\text{MINIMIZE } (Q_{\max})$$

where Q_{\max} is the maximum total pumping rate from all remediation wells. The constraints for Formulation 3 are identical to those for Formulation 1 except that the cleanup constraint is removed (i.e., cleanup need not be achieved within 30 years) and the total number of new remediation wells cannot exceed 25 over the entire project horizon.

4.2 MODELING APPROACH

The same sequential optimization approach used to solve Formulation 1 is used to obtain the optimization solution for Formulation 3. The optimization modeling was carried out one management period at a time, sequentially from period 1, then period 2, period 3, period 4, period 5, and finally period 6. In each management period, only those constraints that are applicable to that period were imposed on the optimization solution. If these constraints could not be satisfied in a particular period, the optimal solution obtained in the preceding period was adjusted by adding new wells in the locations where constraints were violated. The initial locations of remediation wells were determined manually. The final locations were optimized through tabu search (TS) or genetic algorithms (GA) by defining a candidate region in which any model cell can be a potential well location. Typical values of TS and GA solution options used in the current analysis are given in Section 2.2.

As mentioned previously, the long runtime of the simulation model posed a significant challenge to global optimization techniques such as tabu search and genetic algorithms, which require a large number of simulation runs. To reduce the computational burden, two runtime-reduction techniques were adopted. The first technique was to replace the computationally intense TVD solver used in the transport model with the more efficient implicit finite-difference method (FDM). The second was to construct a response function for use as a surrogate model for the flow and transport simulation model. The first technique proved ineffective because the transport problem at the Hastings site is dominated by advection so that the pumping strategy obtained using the FDM solver would be far apart from the optimal solution. The response function approach, however, generally worked quite well. Details on the response function approach used in this study can be found in Zheng and Wang (2002).

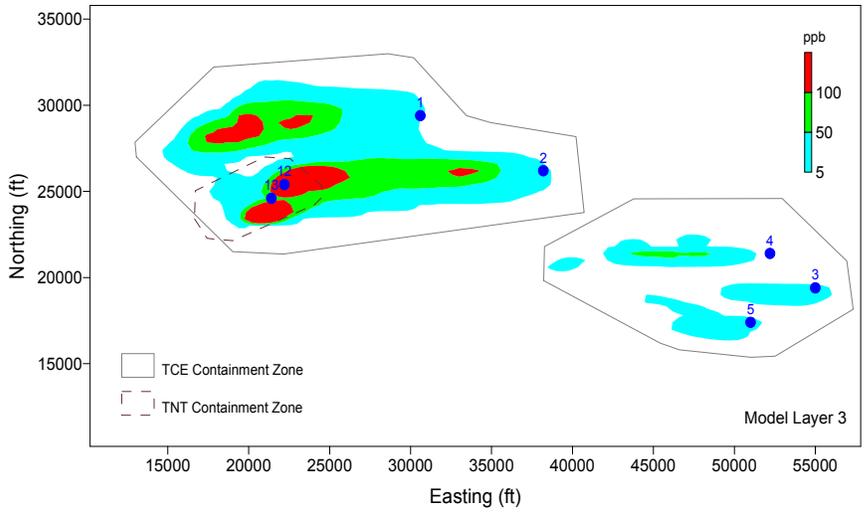
4.3 OPTIMAL SOLUTION

The optimal solution obtained for Formulation 1 is presented in Table 4.1. A total of 6 wells with a total pumping rate of 1968 gpm are used in management period 1. Seven new wells are needed for management period 1 and more wells are added in subsequent management periods. A total of 13 wells are used for Formulation 1 with the maximum total pumping rate in any period (objective function) equal to 2737 gpm.

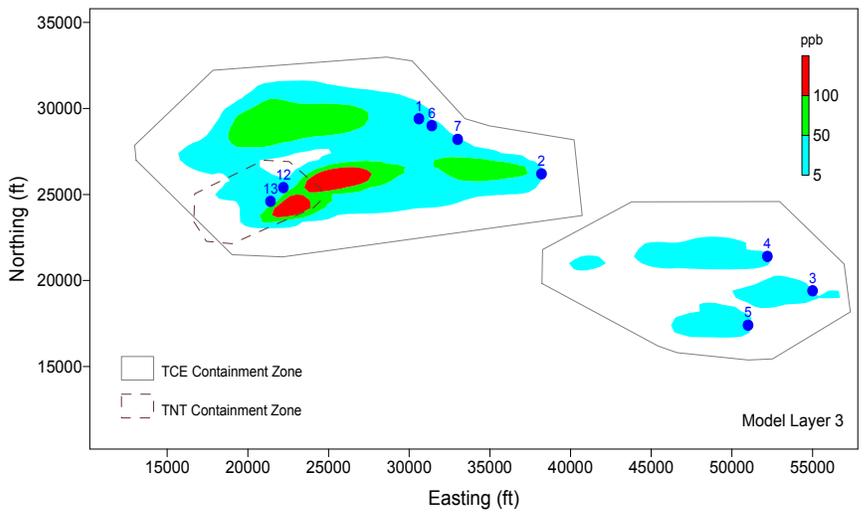
Figures 4.1(a) – (g) show the TCE plumes in model layer 3 and locations of active pumping wells at the start or end of each management period. Figures 4.2(a) – (g) show the same illustrations for TNT plumes. It can be seen that the containment constraints are satisfied at the end of each management period (i.e., the beginning of the following management period). At the end of the 30-year project horizon the cleanup is achieved for TNT but not TCE (not required). All required constraints are also satisfied in model layers 4 and 5 (not shown).

Table 4.1. Optimal dynamic pumping strategy identified for Formulation 3.

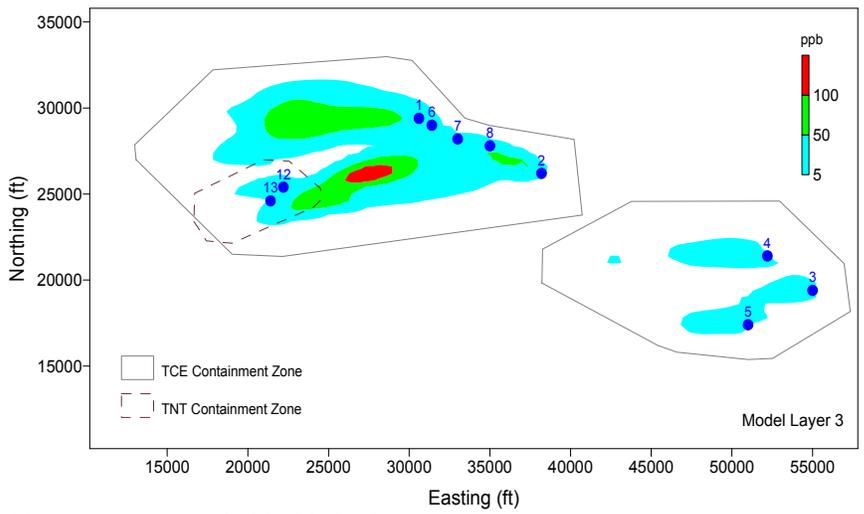
Well ID	Location (K I J)			P1	P2	P3	P4	P5	P6
				2003-2008	2013	2018	2023	2028	2033
1	3	27	59	-350	-15	-50			-95
2	3	35	78	-290	-170	-180	-200	-310	-120
	4	35	78	-290	-170	-180	-200	-310	-120
	5	35	78	-290	-170	-180	-200	-310	-120
3	3	52	120	-290	-240	-265	-350		
4	3	47	113	-320	-195	-165	-230		
	4	47	113	-320	-195	-165	-230		
5	3	57	110	-350	-240	-100	-100		
6	3	28	61		-286	-225	-270	-350	
	4	28	61		-286	-225	-270	-350	
7	3	30	65		-254	-110	-180		-240
	4	30	65		-254	-110	-180		-240
8	3	31	70			-260	-30		
	4	31	70			-260	-30		
9	3	32	62					-350	-350
	4	32	62					-350	-350
10	3	26	58						-50
	4	26	58						-50
11	3	32	75						-200
	4	32	75						-200
12	3	37	38	-120	-152	-152	-152	-152	-152
13	3	39	36	-110	-110	-110	-110	-110	-110
Total Rate (gpm)				-2730	-2737	-2737	-2732	-2592	-2397
New Wells				7	2	1	0	1	2



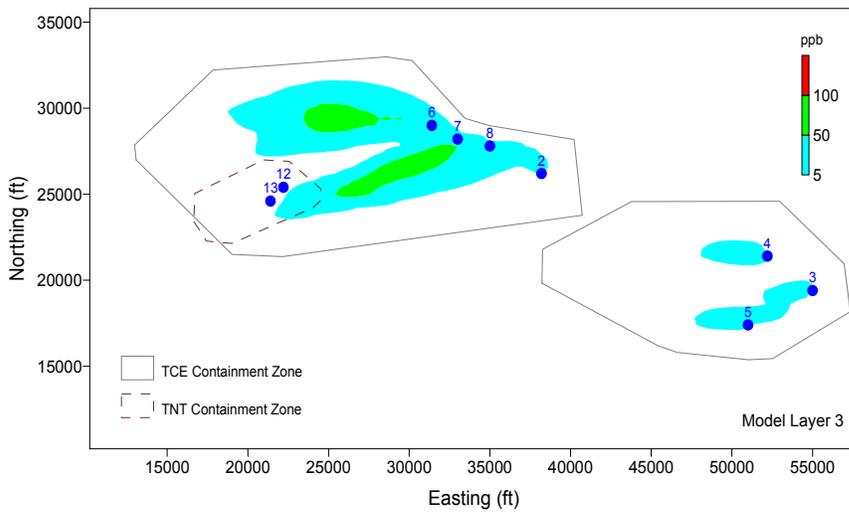
(a) Management period 1 (2003-08)



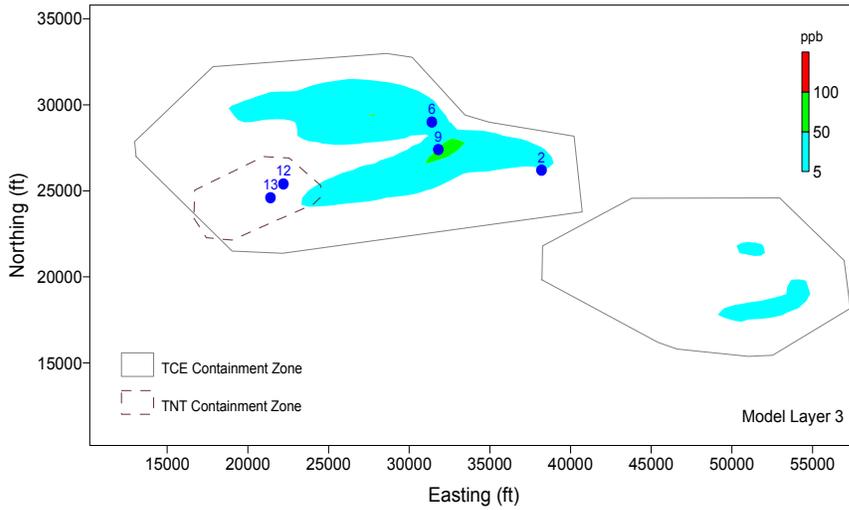
(b) Management period 2 (2008-13)



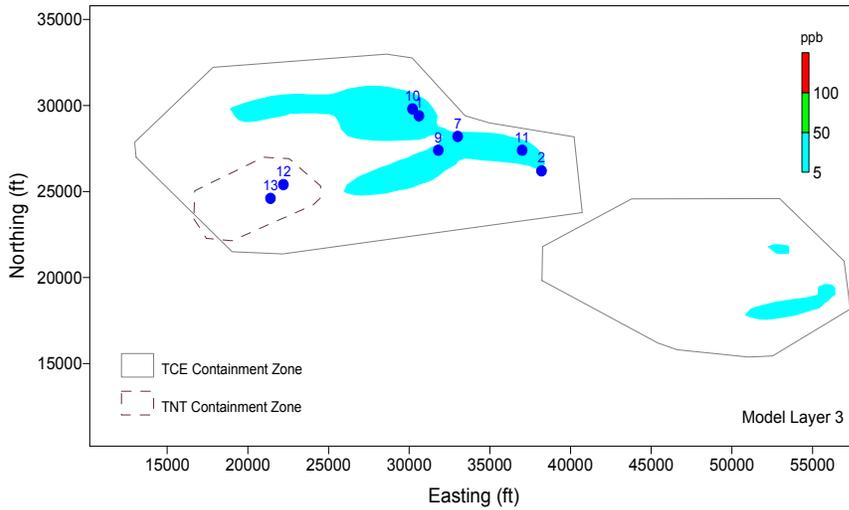
(c) Management period 3 (2013-18)



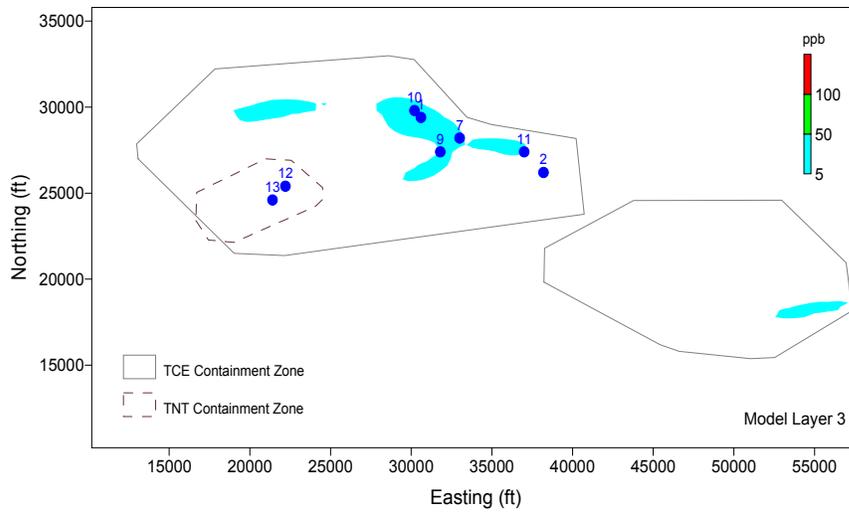
(d) Management period 4 (2018-23)



(e) Management period 5 (2023-28)

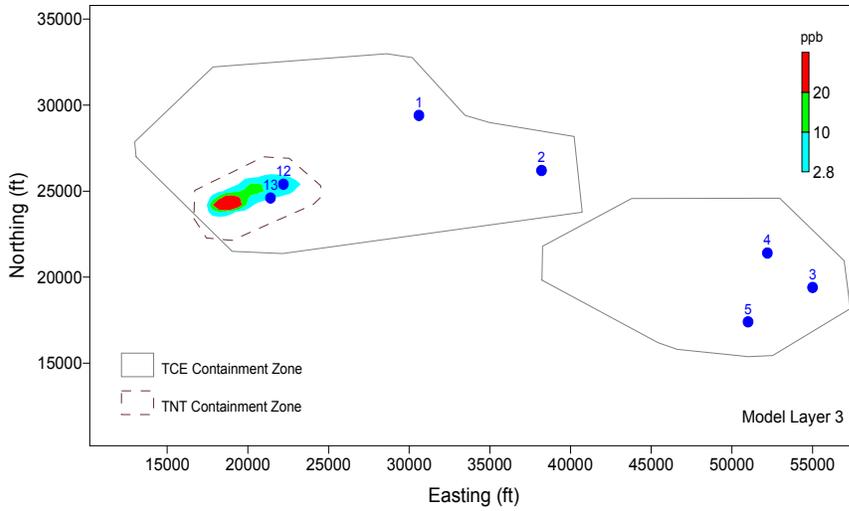


(f) Management period 6 (2028-2033)

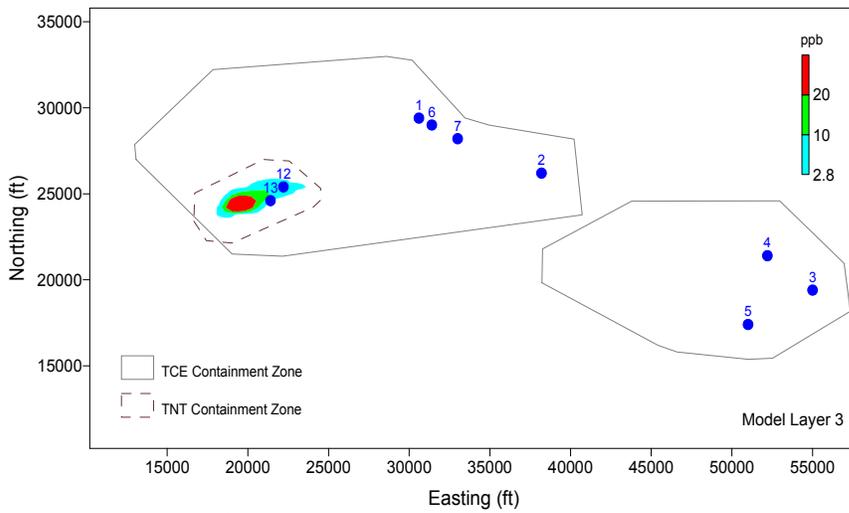


(g) End of the project horizon (2033)

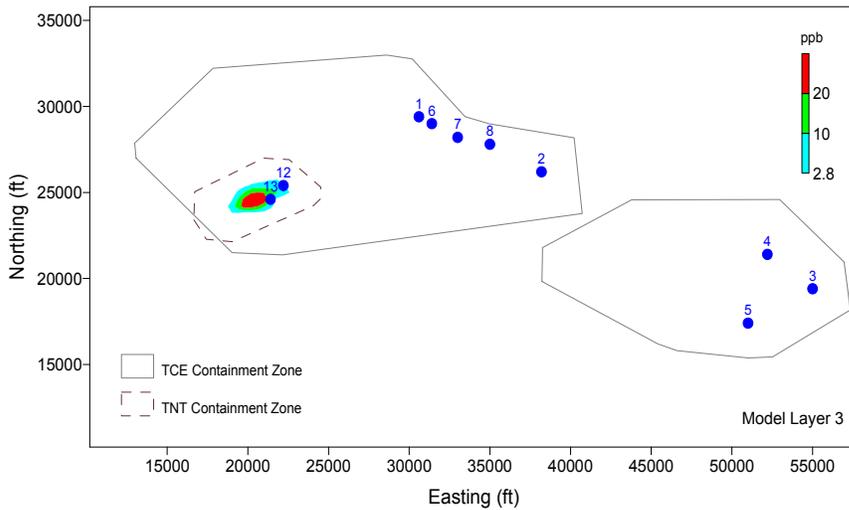
Figure 4.1. Calculated TCE plumes in model layer 3 at the start of six management periods (a)–(f) and at the end of the 30-year project horizon (g). The dots indicate the locations of pumping wells that are active during the management period in which the wells are shown.



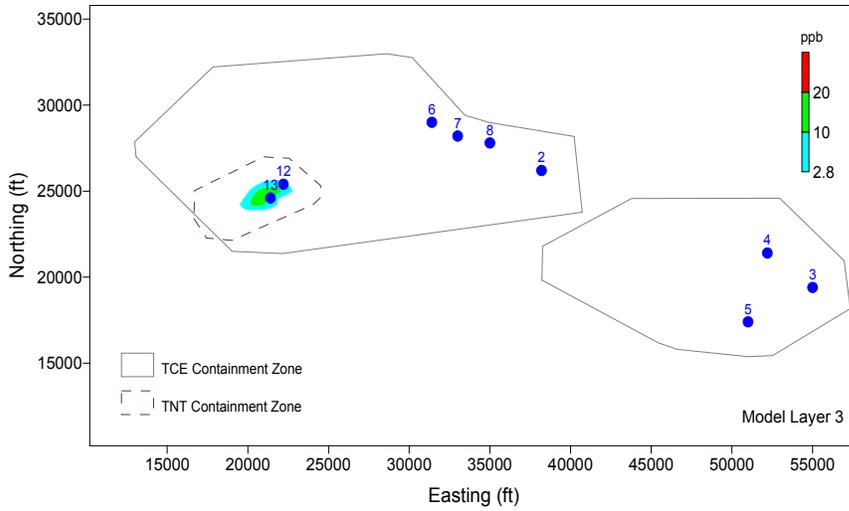
(a) Management period 1 (2003-08)



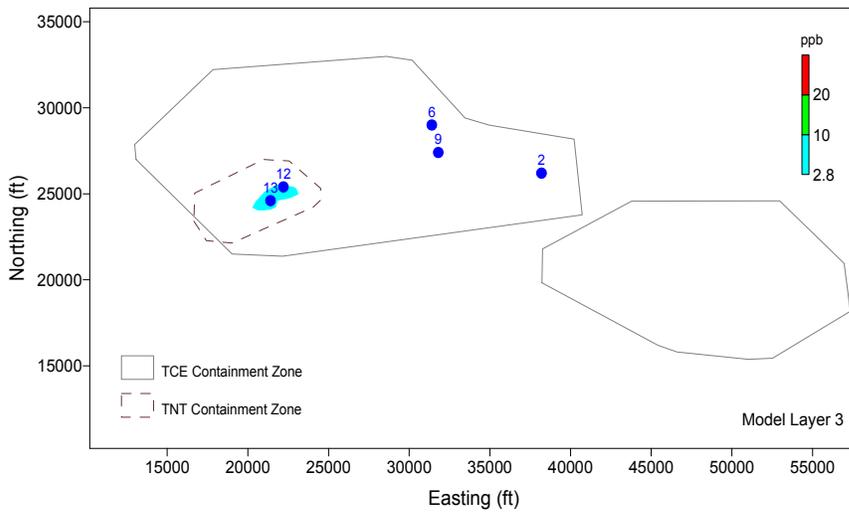
(b) Management period 2 (2008-13)



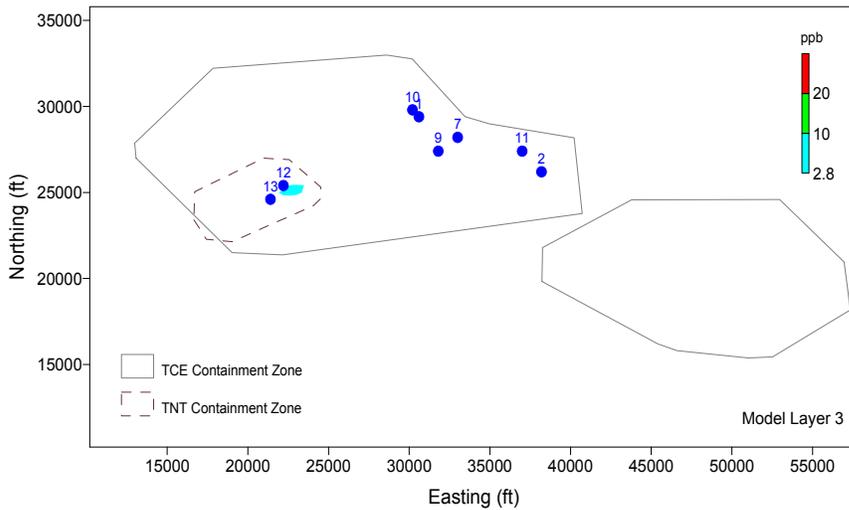
(c) Management period 3 (2013-2018)



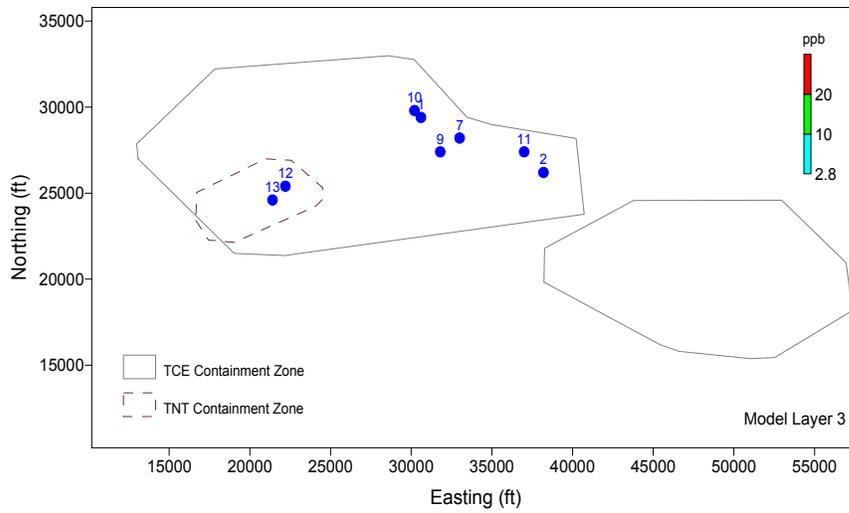
(d) Management period 4 (2018-23)



(e) Management period 5 (2023-28)



(f) Management period 6 (2028-2033)



(g) End of the project horizon (2033)

Figure 4.2. Calculated TNT plumes in model layer 3 at the start of six management periods (a)–(f) and at the end of the 30-year project horizon (g). The dots indicate the locations of pumping wells that are active during the management period in which the wells are shown.

5

Summary and Discussions

5.1 SUMMARY OF STRATEGIES

Table 5.1 summarizes the optimal management solutions developed for the Hastings site with a cost objective function value of \$45.28 million, \$24.04 million, and 2737 gpm, for Formulations 1, 2, and 3, respectively. Note that the actual cost function value for Formulation 2 should be 23.51 to reflect the cost savings of 0.53 resulting from the fact that the treatment plant and discharge piping is not necessary for management period 1 (the first 5 years). The optimal pumping strategies for Formulations 1 and 2 are identical with a total of 15 new wells. Formulation 3 requires a total of 13 new wells. The optimal management solutions developed for Formulations 1 and 2 are based on a sequential or phased approach that emphasizes containment over cleanup and gradually increases the number of pumping wells to achieve cleanup at the end of the 30-year project horizon. As a result, the total costs are relatively low in early years but increase significantly near the end of the project duration. The objective function of Formulation 3 may be reduced by using more wells.

Figure 5.1. Optimal solutions developed for the Hastings site under different formulations.

Formulation	1	2	3
Feasible Solution?	Y	Y	Y
Objective Function Value	\$45.28 m	\$24.04 m*	2737 gpm
Number of New Pumping Wells	15	15	13

*Note: the actual value for the cost function should be \$23.51 m to reflect the cost savings of 0.53 m due to a 5-year delay in construction of treatment plant and discharge piping.

5.2 COMPUTATIONAL PERFORMANCE

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. Instead of one large all-encompassing optimization run, the optimization problem was usually broken into several 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 empirical solution options. Furthermore, it provided the modeler the 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 often advantageous to optimize these two different types of decision variables iteratively, particularly when a large number of candidate well locations are involved.

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. Some labor time was spent on improving the optimization code to make it more general and more computationally efficient.

The flow and transport model for the Hastings site takes over 2 hours per simulation on a Pentium III 1-Ghz PC. This very long runtime poses a formidable challenge for global optimization methods such as tabu search and genetic algorithms. To reduce the computational burden, a sequential approach was used to obtain the optimization solution. The optimization modeling was carried out one management period at a time, sequentially from period 1 to period 6. In each management period, only those constraints that are applicable to that period were imposed on the optimization solution. If these constraints could not be satisfied in a particular period, the optimal solution obtained in the preceding period was adjusted by adding new wells in the locations where constraints were violated. While the sequential approach is computationally efficient, it can lead to larger objective

function values compared to those obtained from a simultaneous approach in which the decision variables for all six management periods are considered together. The simultaneous approach would be computationally prohibitive for the Hastings site considering that several thousand forward simulation runs are usually needed for each optimization run.

Two computational techniques were used to further reduce the long runtimes. The first technique was to replace the computationally intense TVD solver used in the transport model with the more efficient implicit finite-difference method (FDM). The second was to construct a response function for use as a surrogate model for the flow and transport simulation model. The first technique proved ineffective because the transport problem at the Hastings site is dominated by advection so that the FDM solver is not sufficiently accurate. As a result, the pumping strategy obtained using the FDM solver would be far apart from the final optimal solution. The response function approach, however, generally worked quite well.

6

References

- GeoTrans Inc., 2002, Transport Optimization Hastings Naval Ammunition Depot Draft Mathematical Formulations, GeoTrans Inc., Freehold, NJ.
- McDonald, M.G. and A.W., Harbaugh, 1988, *A Modular Three-Dimensional Finite-Difference Groundwater Flow Model*, Techniques of Water Resources Investigations, Book 6, U.S. Geological Survey, Reston, VA.
- Harbaugh, A.W. and M.G. McDonald, 1996, *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.
- 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 U.S. Environmental Protection Agency, 170 pp.
- Zheng, C. and P.P. Wang, 1999, *MT3DMS: Documentation and User's Guide*, Report to the US Army Corps of Engineers Waterways Experiment Station (available at <http://hydro.geo.ua.edu/mt3d>).
- Zheng, C. and P.P. Wang, 2001, *MGO – Modular Groundwater Optimizer, Documentation and User's Guide*, University of Alabama and Groundwater Systems Research Ltd., Tuscaloosa, AL.
- Zheng, C. and P.P. Wang, 2002, A field demonstration of the simulation-optimization approach for remediation system design, *Ground Water*, 40(3), 258-265.