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

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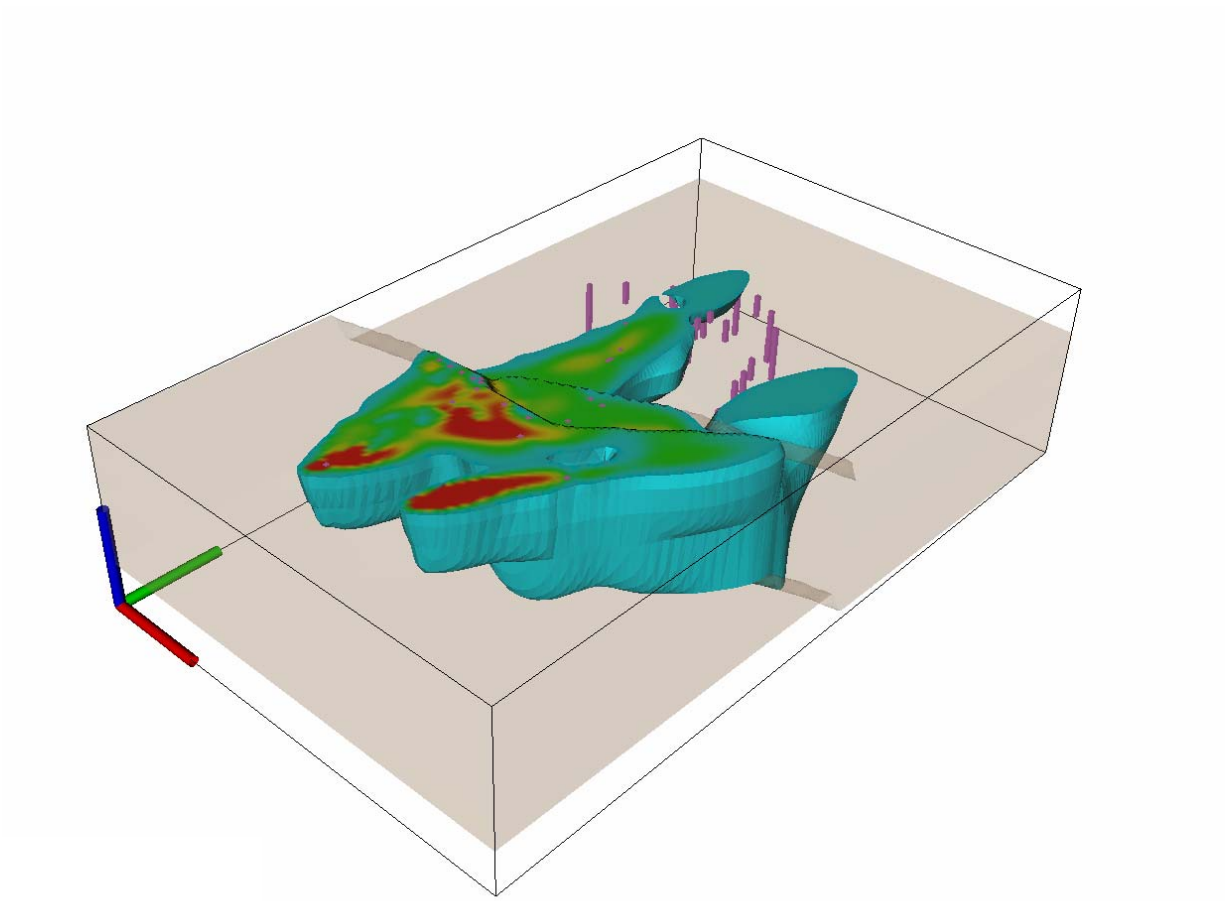

The Hydrogeology Group
The University of Alabama

Technical Report
March 2002
Revised 2/2003

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Prepared for
Naval Facilities Engineering Service Center
Port Hueneme, California
and
U.S. Environmental Protection Agency
Washington, DC

Contents

ABSTRACT

This report presents the results of an optimization modeling analysis at the Tooele Army Depot in Utah. The study is the second 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 Tooele site. For Formulation 1, an optimal dynamic strategy was developed with a total cost of $12.67 million in net present value. The optimization results indicate that all except two of the 15 pumping wells can be shut down, replaced by four new injection wells. This modification to the current system can potentially lead to cost savings of several million dollars while satisfying the newly imposed "point of exposure" constraints . For Formulation 2, an optimal dynamic strategy was developed with a total cost of $14.45 million in net present value. The optimal strategy consists of 1 new pumping well, 7 new injection wells, and 2 existing wells, and satisfies both "point-of-exposure" and "point-of-compliance" constraints. For Formulation 3, the optimization analysis identifies no feasible solution that could satisfy a set of cleanup constraints with only 4 injection and 4 pumping wells. Further analysis suggests alternative formulations that would achieve cleanup either with a minimum number of 4 pumping and 6 injection wells, or with a minimum cost of $18.62 million in net present value.

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Introduction

1.1 PURPOSE AND SCOPE

The purpose of this study is to apply a general-purpose flow and transport optimization code to optimize an existing pump-and-treat system at the Tooele Army Depot in Utah. The study is the second 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 and 2002). 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. 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, Bryton Johnson, Barbara Minsker, Richard Peralta, Kathy Yager, Laura Yeh, and Yan Zhang.

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Optimal Solution: Formulation 1

2.1 OBJECTIVE FUNCTION

The objective of Formulation 1 for the optimization modeling analysis at the Tooele 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:

$$\text{Minimize } \left(CCE + CCI + FCO + VCE + VCS + VCC\right) \tag{2.1}$$

where

CCE: Capital costs of new extraction wells ($307,000 for installing a new extraction well independent of its location)

CCI: Capital costs of new injection wells ($223,000 for installing a new injection well independent of its location)

FCO: Fixed costs of O&M ($525,000 per year)

VCE: Variable costs of electricity for pumping ($34,500/well per year)

VCS: Variable costs of sampling ($208,000 in the first year, decreasing subsequently proportional to the ratio of the total plume area in any particular year over the initial plume area)

VCC: Variable costs of chemicals used for treatment ($20 per gpm of pumping per year)

More detailed cost information can be found in a companion report on optimization problem formulation by GeoTrans (2001). Note that all cost terms in equation (2.1) are computed in net present value (NPV) with the following discount function:

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

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 (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 21 years, beginning in January 2003 ($iy = 1$). The modeling period is divided into 7 management periods of 3 years each. The decision variables include the number and locations of new pumping/injection wells, and the flow rates of both existing and new pumping/injection wells 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, 2001):

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

(2) The total pumping rate, after adjustment for the average amount of system uptime, cannot exceed 8000 gpm, i.e., the current maximum capacity of the treatment plant:

$$\tfrac{1}{\alpha} Q_{total} \le 8000$$

where α is a coefficient representing the average amount of system uptime ($\alpha = 0.95$ for this analysis).

(3) The TCE concentration cannot exceed 5 ppb at a set of prescribed "points of exposure" for the main plume (POE-MP) in all model layers at the end of the first management period and thereafter:

$$C^{\max} \le 5 \text{ ppb at all POE-MP locations for } t \ge 3 \text{ years}$$

The locations of POE-MP are shown in Figure 3-1 as triangles in red color.

(4) The capacities of new pumping and injection wells must not exceed 400 and 600 gpm, respectively:

$\frac{1}{\alpha}|Q_w| \leq 400$ gpm; $\frac{1}{\alpha}|Q_i| \leq 600$ gpm

In addition, if any of existing pumping and injection wells is used, its current capacity as given in GeoTrans (2001) must also be satisfied.

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

In addition to the constraints listed above, it is assumed that a new pumping well is installed to address a separate TCE plume (referred to as the NE Plume) that is still under investigation. This pumping well is considered fixed and not a decision variable in the current optimization analysis. However, the water pumped from this well (fixed at 1500 gpm) must be considered part of the total pumping allowed for the site (8000 gpm).

2.3 MODELING APPROACH

From the cost information described above, it can be seen that the cost objective function for Formulation 1 is dominated by the capital costs of installing new pumping or injection wells, the fixed annual O&M costs, and the electricity costs of pumping on a fixed per well basis. Without the removal of remaining contaminant sources, the current pump-and-treat system is expected to continue operation for the entire project duration of 21 years. Thus, the fixed O&M costs cannot be reduced. The most significant component of the cost savings can be expected to come from minimizing the number of existing pumping wells required and the number of new pumping/injection wells installed.

The existing pump-and-treat system designed by the U.S. Army Corps of Engineers was used as the starting point. The existing design is shown in Figure 2.1, superimposed by the head distributions and TCE plumes as calculated by the calibrated simulation model for January 2003. The current system consists of a total of 16 extractions wells (shown as dots) and 13 injection wells (shown as crossed circles). As indicated in Figure 2.1, most of these wells are screened only in model layer 2 and/or layer 3. There is only one pumping well screened in layers 1 and 4, respectively. The existing design does not satisfy the constraints for Formulation 1 as defined previously.

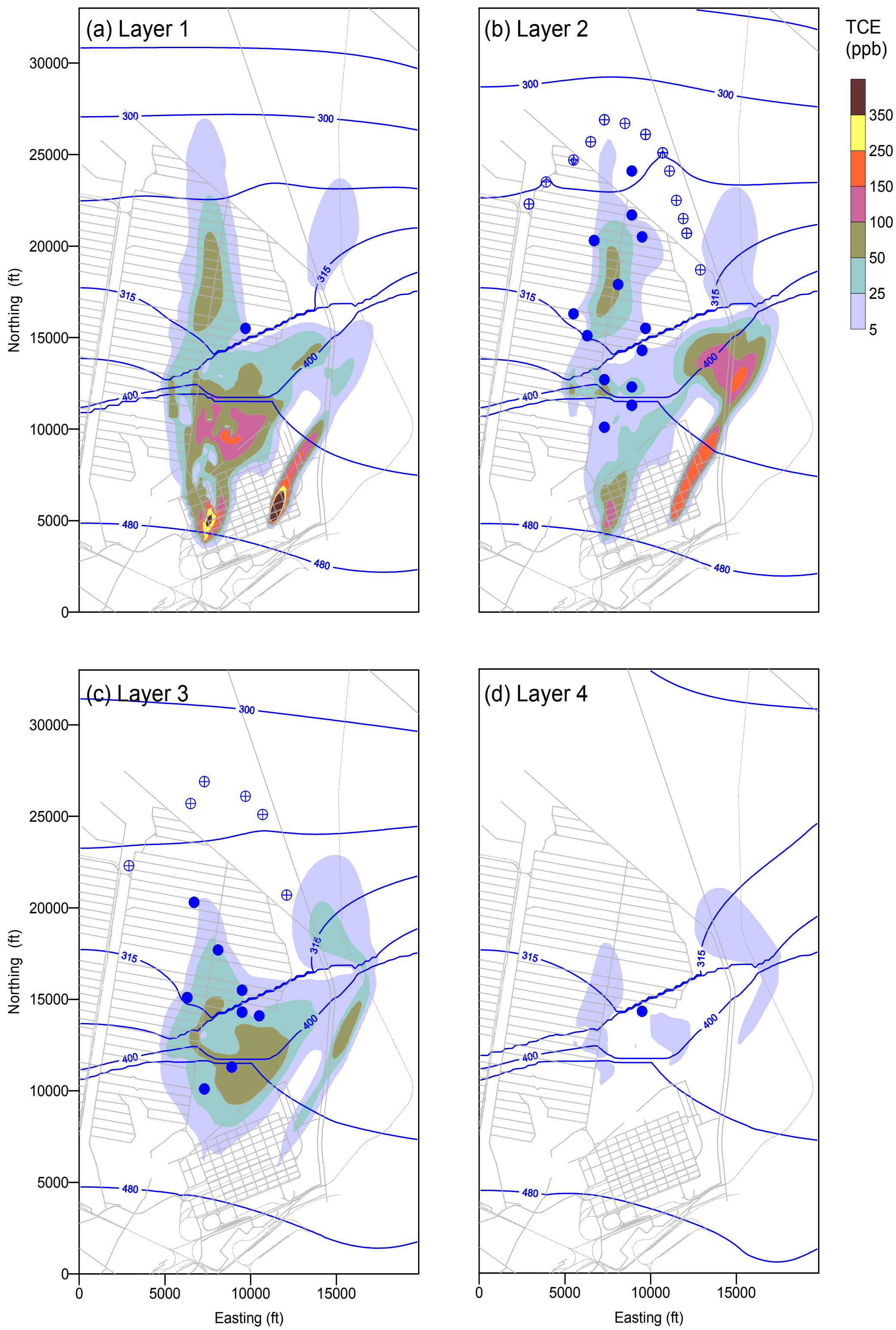


Figure 2.1. Calculated heads and TCE plumes at Tooele Army Depot, Utah for January 2003, the starting date assumed for the optimization analysis: (a) model layer 1; (b) model layer 2; (c) model layer 3; and (d) model layer 4. The existing pump-and-treat system consists of 16 extraction wells (solid dots) and 13 injection wells (crossed circles). Each well may be screened in one or more model layers.

Several optimization runs were attempted during the courses of this analysis. In Run 1, only the flow rates (*Q*) of existing pumping and injection wells were chosen as the decision variables since their locations cannot be changed. Each of the *Q* decision variables was constrained between zero and their respective pumping/injection capacity. The maximum amount of total pumping was required to be equal to that of total injection, at 8000 gpm, i.e., the maximum capacity of the current on-site treatment plant. The genetic algorithm (GA), one of the optimization solvers available in the MGO code, was used to search for an optimal solution that would satisfy all constraints. The theoretical background of GA and guidelines for its effective application are provided in Zheng and Wang (2001). In this analysis, the following GA solution options were used with some small variations:

POPSIZE = 100 – 200 (population size)
NPOSIBL = 16 – 32 (number of discretizations for the flow rate decision variable)
PCROSS = 0.5 – 0.6 (crossover probability)
PMUTATE = 0.005 – 0.01 (mutation probability, set equal to the inverse of POPSIZE)

Run 1 yielded no feasible solution that could satisfy the POE-MP constraints. In other words, the TCE concentration could not be reduced to 5 ppb or lower by the end of year 3 and thereafter at all PCE-MP locations. This is not particularly surprising since a significant amount of TCE mass has already arrived near the POE-MP boundary. Existing wells, operated within their respective capacities, could not possibly reverse the flow direction and prevent the TCE plume from exceeding the concentration limit of 5 ppb at all POE-MP locations. Thus, in subsequent runs, new pumping/injection wells were considered.

In Run 2, a total of 4 new pumping wells were added near the POE-MP boundary. The new pumping wells were initially assumed to be operating at full capacity, leaving only their locations as the integer-valued decision variables. In addition, this run includes the continuous flow rate decision variables of existing pumping/injection wells. The ‘moving well’ option as implemented in the MGO code was used to define a large number of candidate locations for the new pumping wells. This was done by associating each well with a rectangular region of the model grid within which the well could move freely in search of its optimal location (see Figure 2.2). Each pumping well was represented by a single model node. The candidate well region was defined in both layers 1 and 2 so that the final optimal location for each well may be in layer 1 or 2.

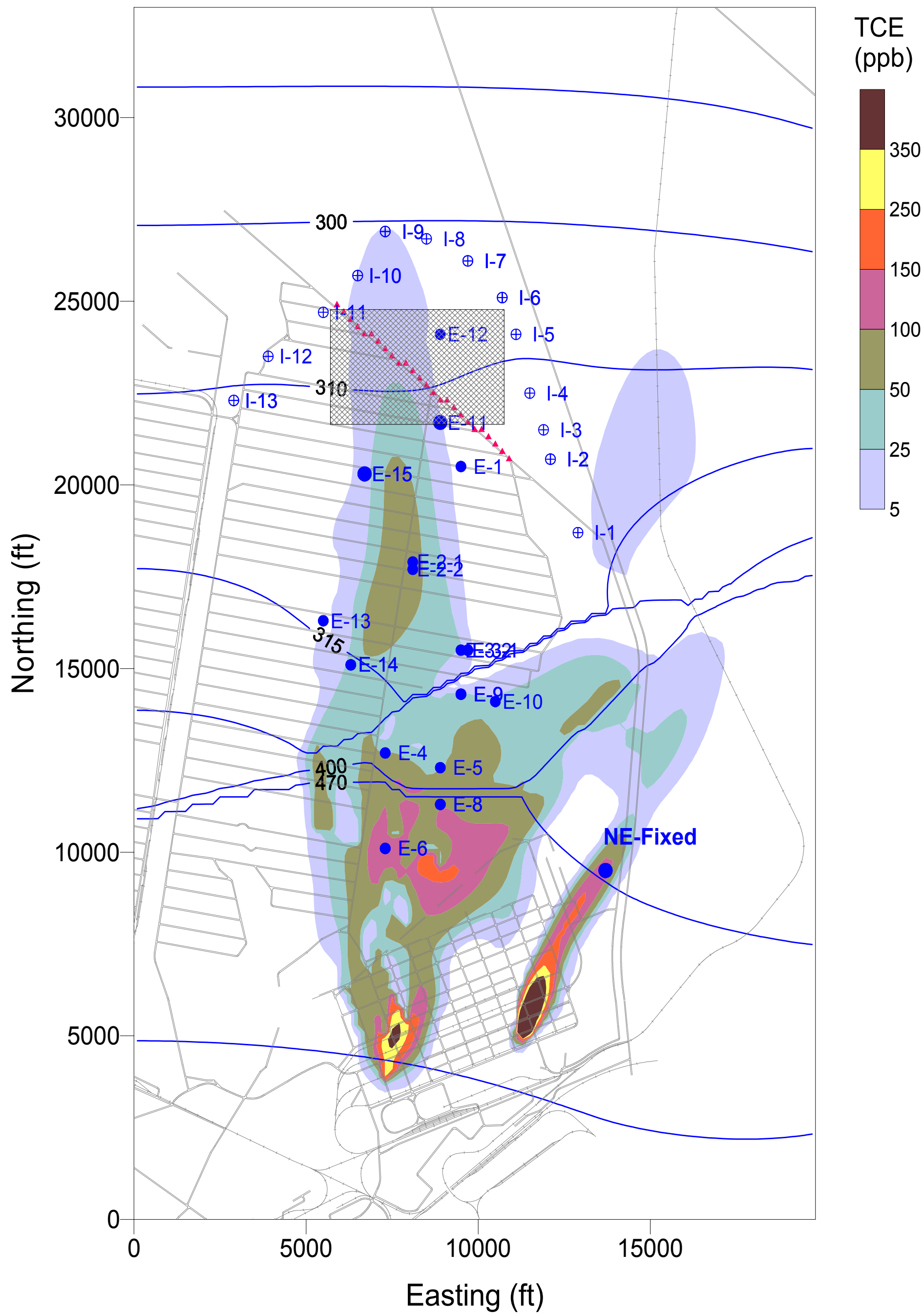


Figure 2.2. Locations of the "point of exposure" constraints for the main plume (POE-MP), shown as red triangles, where the TCE concentration must be at 5 ppb or lower by the end of year 3 and thereafter. The rectangle with cross-patterned lines indicates the 'moving well' region within which the optimal locations for potential new pumping/injection wells are sought. Also shown are the pumping/injection wells for the current pump-and-treat system and the calculated TCE plume in model layer 1 at the beginning of the optimization analysis.

Interestingly, Run 2 yielded a feasible solution that indicated that all existing pumping wells with the exception of E-11 and E-15 could be turned off since they apparently exerted only a small effect on meeting the POE-MP constraints. Because each pumping well, regardless of its actual pumping rate, would cost approximately $465,000 in net present value to operate for the total project duration of 21 years, it makes sense to turn off as many existing pumping wells as possible, provided that it would not lead to the installation of more new wells than otherwise necessary. The existing injection wells were also found to be insensitive to meeting the POE-MP constraints. Thus, very little could be gained by including them as decision variables in the optimization analysis. On the other hand, since it does not require any additional costs to operate any existing injection well, it is useful to keep existing injection wells for discharging extra water. This can be accomplished through the 'balance constraint' option in the MGO code by specifying a certain portion of pumped water that should be discharged to any particular injection well.

Based on the results and experiences obtained from the first two runs, Run 3 was set up to include four new pumping wells along with two existing wells (E-11 and E-15). Because a new injection well requires smaller capital costs to construct and no O&M costs to operate, Run 3 attempted to minimize the total costs by substituting each of the four new pumping well with a new injection well. The candidate locations for the new injection wells were defined in the same region as for the new pumping wells. Run 3 yielded a feasible steady-state solution that includes no new pumping wells, four new injection wells, and existing wells E-11 and E-15. In addition, an existing injection well 'I-4' is required to discharge extra pumped water including that from the fixed well for the NE Plume.

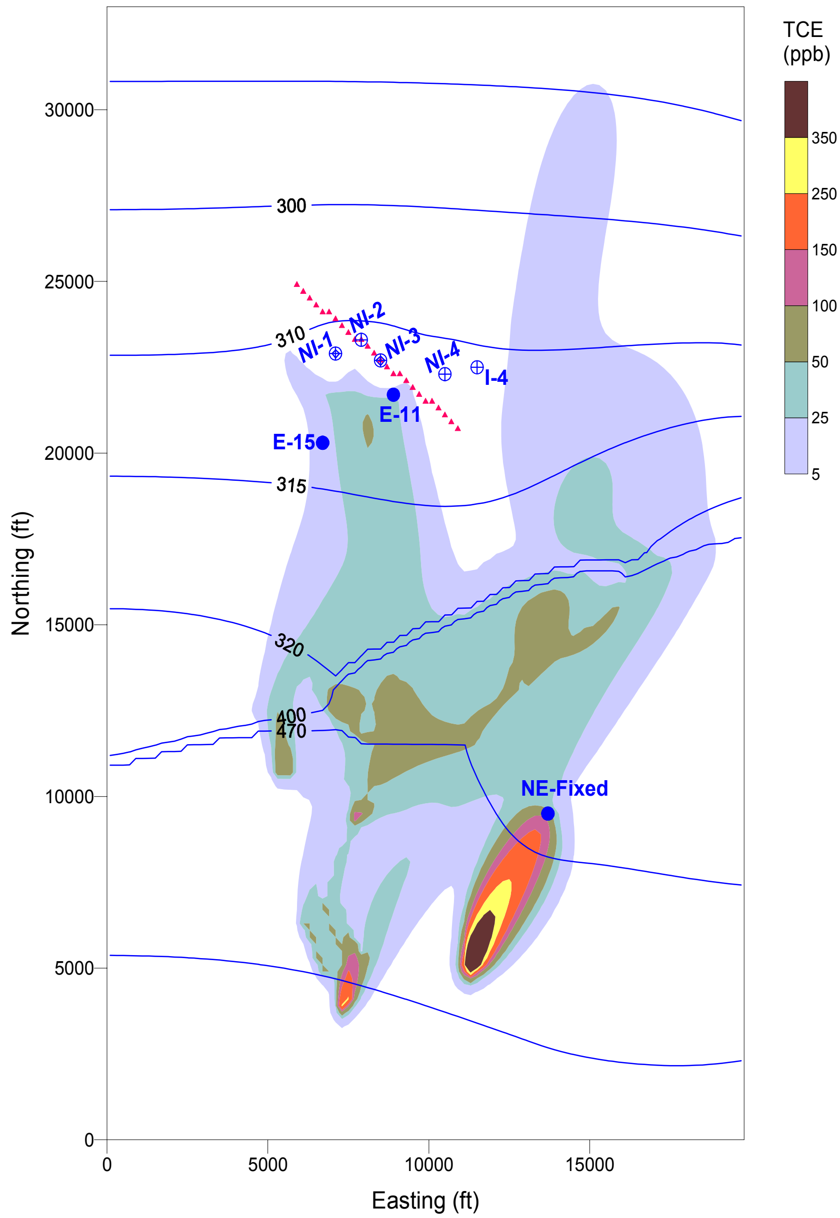
In all the runs up to this point, only steady-state solutions were sought. In other words, the well locations and flow rates were assumed to be constant throughout the entire projection duration. After the well locations were determined, a final run was carried out to develop an optimal dynamic strategy for Formulation 1. In this final run, the locations of all pumping/injection wells were fixed. The flow rate for each management period at an injection/pumping well was treated as a decision variable. The final solution is presented and discussed in the next section.

2.4 OPTIMAL SOLUTION

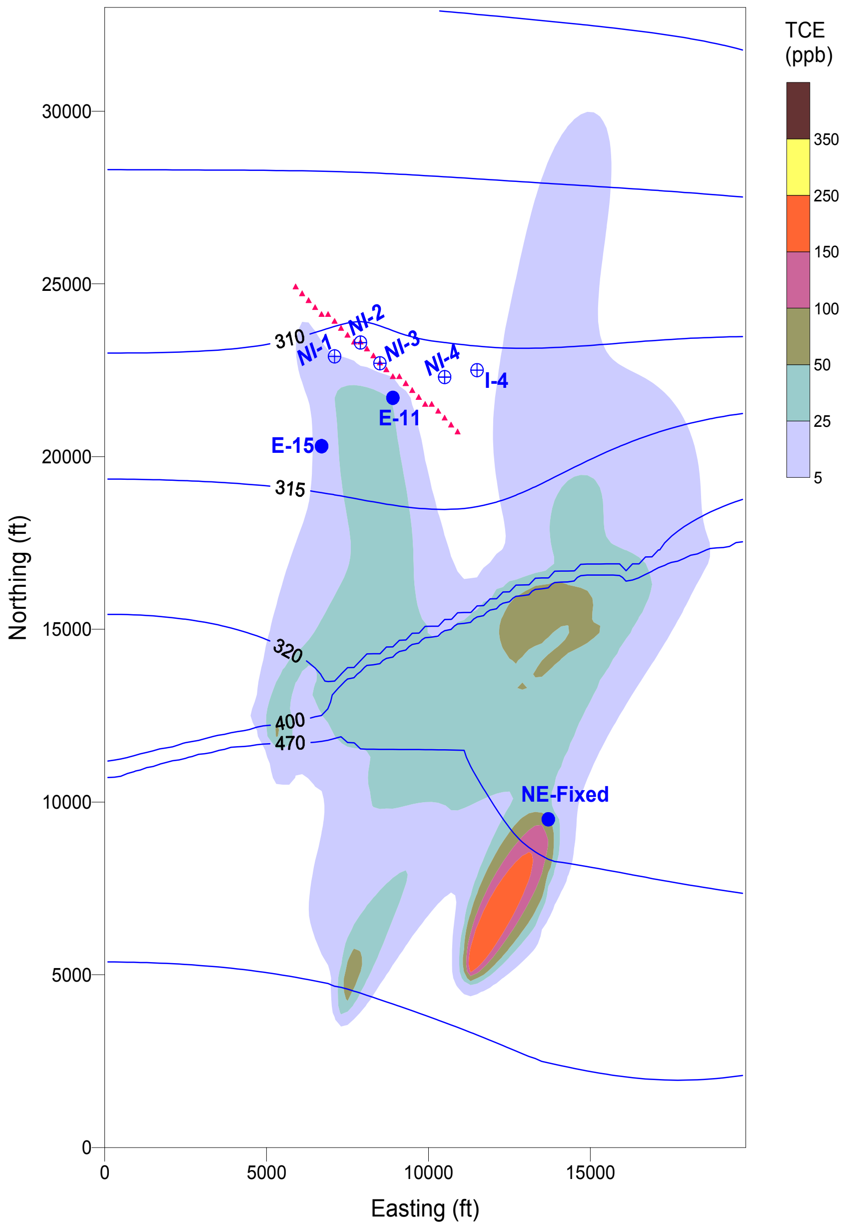
The optimal solution obtained for Formulation 1 is illustrated in Figures 2.3(a) through 2.3(c). It is noteworthy that no new pumping well is required and all existing wells are turned off except for pumping wells E-11 and E-15 and injection well I-4. One new injection (NI-1) is placed on the upgradient side of the POE-MP compliance boundary while another new injection well (NI-4) is located on the downgradient side, Two more new injection wells (NI-2 and NI-3) are located along the POE-MP compliance boundary. One new injection well (NI-2) is located in model layer 2, while the other three are all located in model layer 1. The pumped water from existing wells E-11 and E-15, in addition to that from the fixed well for the NE Plume, is discharged into the four new injection wells (NI-1 through NI-4).

The pumping and injection rates for the optimal dynamic strategy are listed in Table 2.1, and well locations are included in the input file for the MODFLOW Well Package submitted with this report. All prescribed constraints are satisfied, including the maximum TCE concentration of 5 ppb by the end of year 3 and thereafter at all POE-MP locations in all four model layers. Note that the full capacity for several new injection wells has been reached in several of the 7 management periods, which leaves very little room for dynamic adjustment of the flow rates. Most of the cost savings for the dynamic strategy comes from the existing well E-15, which can be turned off in all of the management periods except one (i.e., management 5).

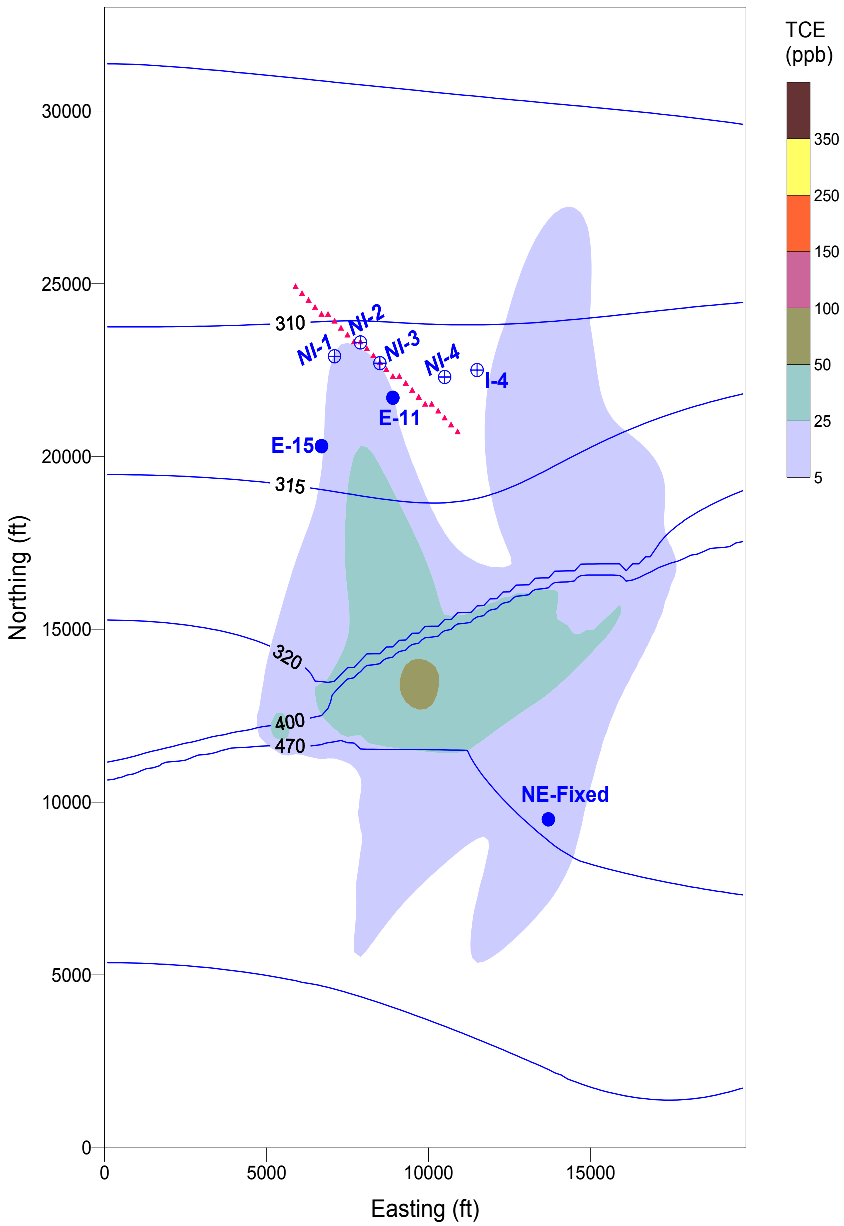
The cost objective function for the optimal strategy is $12.67 million in net present value. Of which, 56% is the fixed O&M costs which cannot be reduced as long as the pump-and-treat system is in operation. Another 32% of the total costs is related to sampling, which is dependent on the plume size. Given that containment is the primary driver for Formulation 1, it is unlikely that sampling related costs can be reduced substantially. The most significant potential for cost savings comes from shutting down most of the existing wells and replacing them with a minimum of four new injection wells. A complete cost breakdown is shown in Figure 2.4.



(a) Model layer 1



(b) Model layer 2



(c) Model layer 3

Figure 2.3. Calculated TCE plumes in (a) model layer 1, (b) model layer 2, and (c) model layer 3, at the end of the project duration (21 years). The triangles in red color indicate the POE-MP constraints where the TCE concentration must not exceed 5 ppb by the end of year 3 and thereafter. NI-1 through NI-4 are new injection wells. I-4 is an existing injection well and E-11 and E-15 are two existing pumping wells. NE-Fixed is the fixed pumping well added to address the NE plume. The total pumping from E-11, E-15 and NE-Fixed is equal to total injection at I-1 and NI-1 through NI-4 at any time.

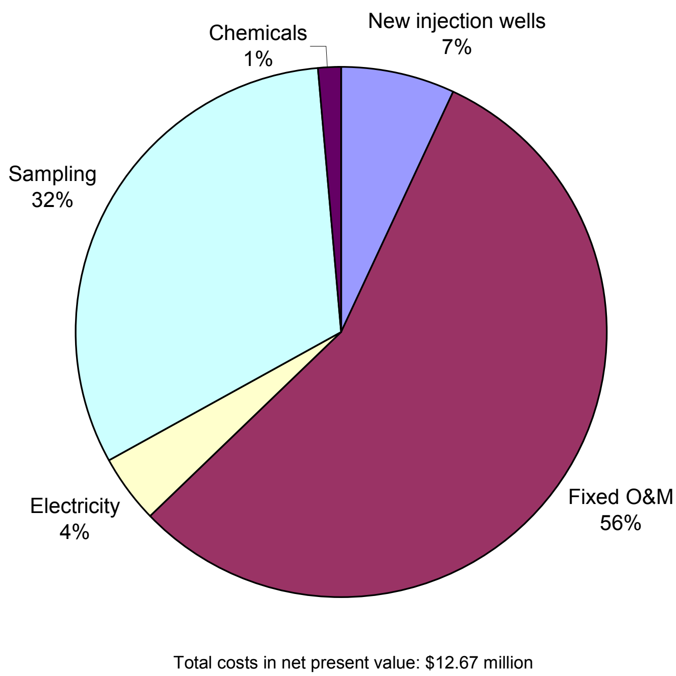


Figure 2.4. Distribution of the various cost items for the optimal solution for Formulation 1.

Table 2.1. Optimal pumping strategy for Formulation 1.

Well Name	Well Flow Rate (GPM) (- for pumping and + for injection).						
	MP 1	MP 2	MP 3	MP 4	MP 5	MP 6	MP 7
E-11	-617.5	-617.5	-617.5	-617.5	-617.5	-617.5	-617.5
E-15	0	0	0	-608.0	0	0	0
I-4	0	0	0	370.5	0	0	0
NI-1	495.1	498.8	510.6	570.0	554.2	558.1	570.0
NI-2	510.6	514.6	510.6	570.0	554.2	558.1	570.0
NI-3	526.2	514.6	510.6	570.0	554.2	558.1	570.0
NI-4	510.6	514.6	510.6	570.0	380.0	368.1	332.6
NE-Fixed	-1425.0	-1425.0	-1425.0	-1425.0	-1425.0	-1425.0	-1425.0
Net	0	0	0	0	0	0	0

* The well locations are indicated in the MODFLOW Well Package input file named ‘Formuln1.WEL’.

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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). The constraints (1) – (5) defined for Formulation 1 also apply to Formulation 2. Furthermore, there are two additional constraints that must be satisfied under Formulation 2, i.e.,

(6) The TCE concentration cannot exceed either 50% of the initial concentration or 20 ppb, whichever is larger, by the end of the first management period and thereafter, at a set of prescribed "points of compliance" on the left side of the main plume (POC-MP1) in model layers 1 and 2:

$$C^{\max} \leq \max\left(C_0/2, 20\right) \text{ at all POC-MP1 locations for } t \geq 3 \text{ years}$$

The locations of the POC-MP1 constraints are shown in Figure 3-1 as triangles in green color.

(7) The TCE concentration cannot exceed 50 ppb by the end of the first management period and thereafter, and 20 ppb by the end of the third management period and thereafter, at a set of prescribed "points of compliance" on the right side the main plume (POC-MP2) in model layers 1 and 2:

$$C^{\max} \leq 50 \text{ at all POC-MP2 locations for } 3 \leq t < 9 \text{ years}$$
$$C^{\max} \leq 20 \text{ at all POC-MP2 locations for } t \geq 9 \text{ years}$$

The locations of the POC-MP2 constraints are shown in Figure 3-1 as triangles in green color.

3.2 MODELING APPROACH

Several optimization runs were conducted for Formulation 2. The first run (Run 1) was intended to find a feasible solution that would satisfy the POC-MP1 and POC-MP2 constraints independent of other constraints. In Run 1, a total of six new pumping wells and 15 new injection wells were added near the POC-MP1 and POC-MP2 boundaries as candidate wells. The decision variables included the flow rates (*Q*) of both existing pumping/injection wells, and the newly added candidate wells. In addition, a binary 'on/off' decision variable was associated with each flow rate. Each of the *Q* decision variables was constrained between zero and their respective pumping/injection capacity. Both genetic algorithm (GA), as discussed in the previous section, and tabu search (TS), another global optimization solver available in the MGO code, were 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 with some small variations:

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)

Run 1 yielded a feasible solution that could satisfy the POC-MP1 and POC-MP2 constraints. The solution included no new pumping wells and 4 new injection wells. Because the locations of the 4 new injection wells were selected from only 15 pre-determined candidate sites, they might be suboptimal. Thus a second run (Run 2) was conducted to further optimize the locations of the 4 new injection wells.

Run 2 again used the 'moving well' option in the MGO code by allowing the 4 new injection wells to move anywhere within the candidate well region as shown in Figure 3.1 in model layers 1 and 2 until the optimal locations and associated flow rates were obtained. The results of Run 2 indicated that either 3 or 4 new injection wells would satisfy the POC-MP1 and POC-MP2 constraints. The total injection rate for the 3-well option was greater than that of the 4-well option.

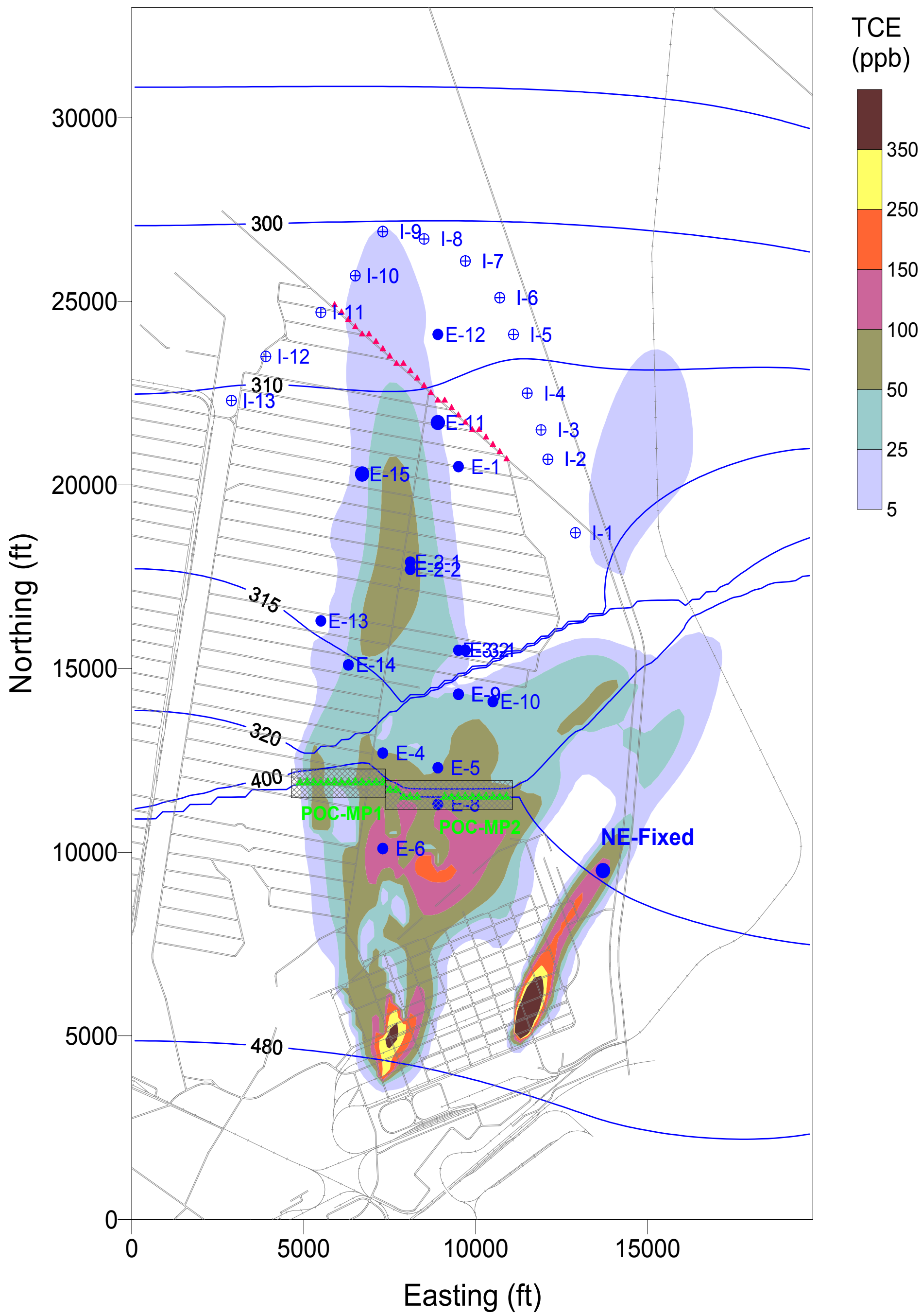


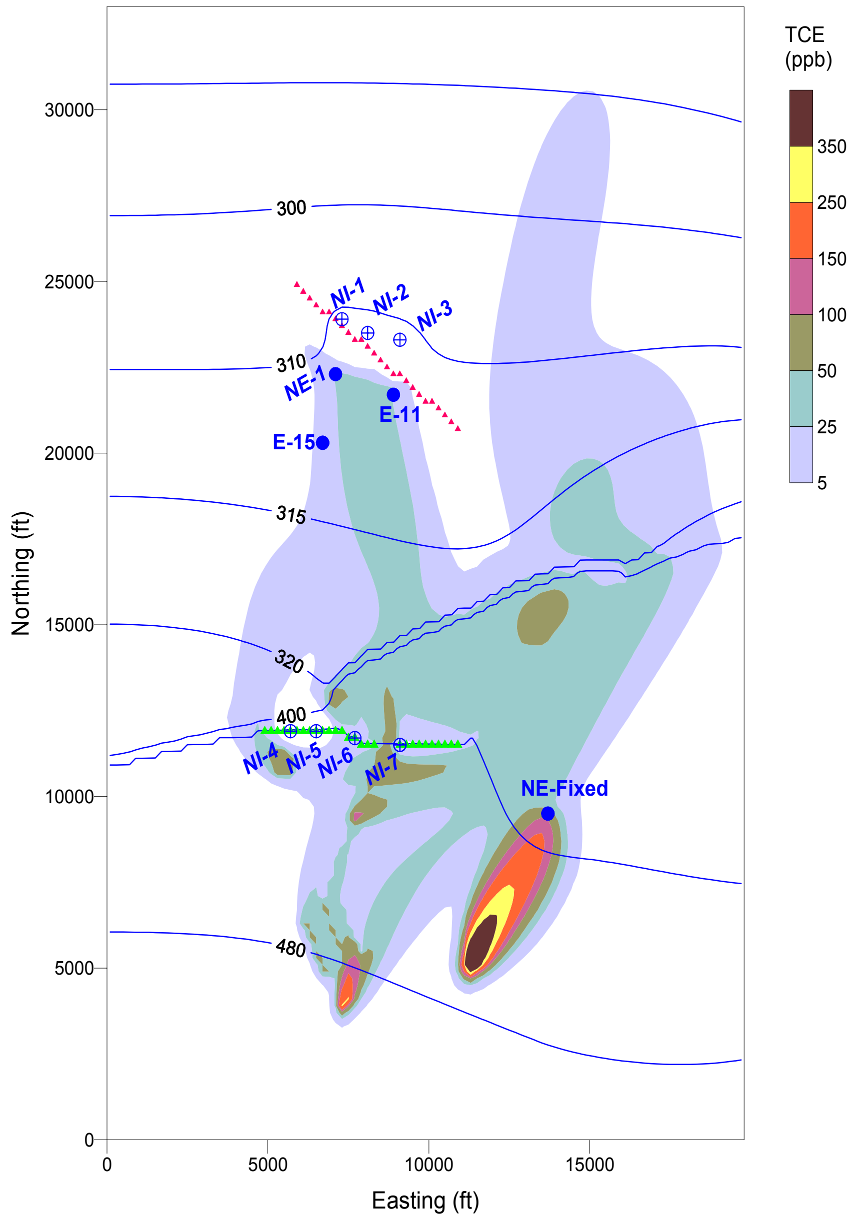
Figure 3.1. Locations of the "point of compliance" constraints for the main plume (POC-MP1 and POC-MP2) shown as green triangles. The rectangle with cross-patterned lines indicates the 'moving well' region within which the optimal locations for potential new pumping/injection wells are sought. Also shown are the pumping/injection wells for the current pump-and-treat system and the calculated TCE plume in model layer 1 at the beginning of the optimization analysis.

Based on the results and experiences obtained from the first two runs, Run 3 was carried out to develop an optimal steady-state strategy for Formulation 2 by combining the elements of Formulation 1 with the new injection wells identified to satisfy the new POC constraints. It is noteworthy that the optimal solution for Formulation 1 could not be used directly in Formulation 2 because there was not a sufficient amount of water extracted to meet the need of injection. As a result, rather than 4 new injection wells as used in Formulation 1, one new pumping well and 3 new injection wells were used in Formulation 2 to satisfy the POE constraints. The outcome of Run 3 provided the starting point for a final run to obtain an optimal dynamic strategy. In this final run, the well locations were all fixed. The flow rate for each management period at an injection/pumping well was treated as a decision variable. The final solution is presented and discussed in the next section.

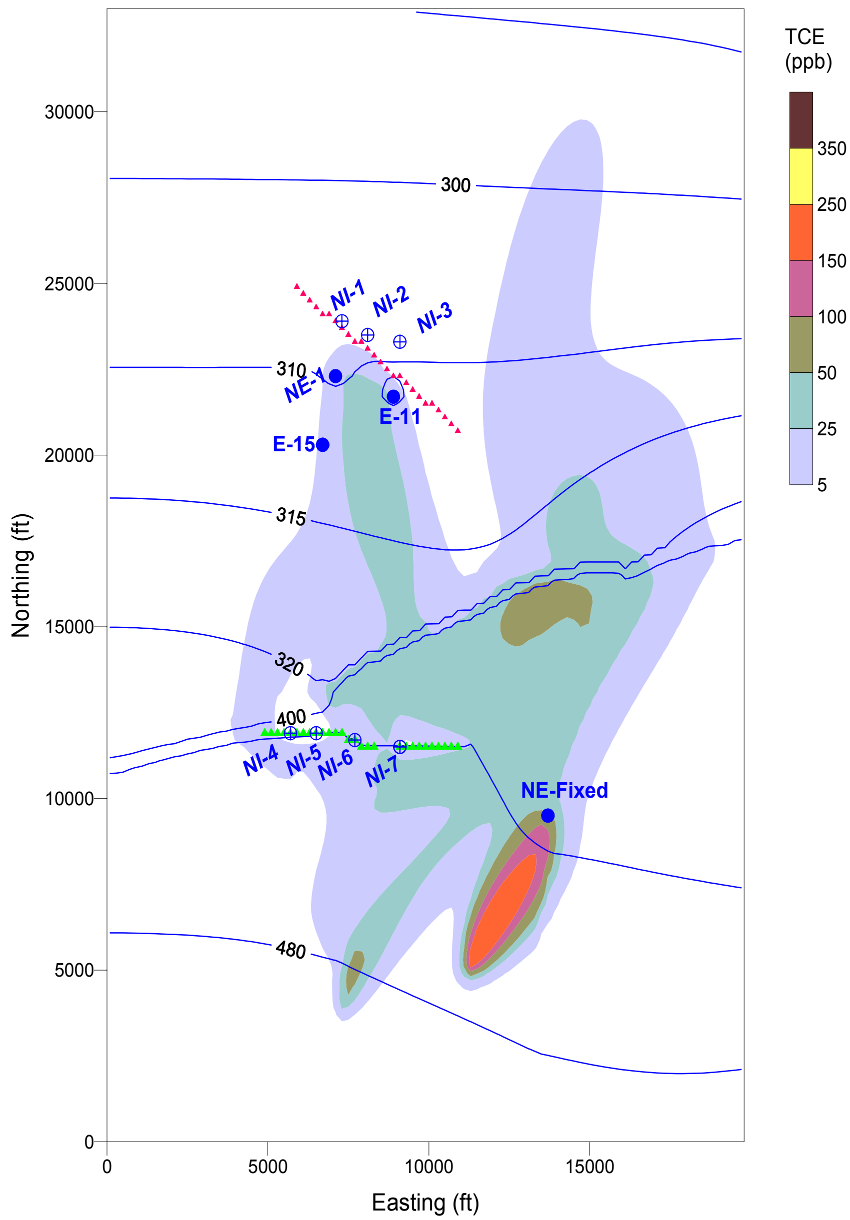
3.3 OPTIMAL SOLUTION

The optimal solution obtained for Formulation 2 is illustrated in Figures 3.2(a) – (c). It consists of one new pumping well (NE-1), 7 new injection wells (NI-1 through NI-7), and two existing pumping wells (E-11 and E-15). Three of the new injection wells are located near the POE-MP boundary, while the other four are located near the POC-MP1 and POC-MP2 boundaries. The new pumping well is screened in model layer 2. All new injection wells are screened in model layer 1 except NI-7 which is screened in both layers 1 and 2. The pumped water from the new well NE-1 and existing wells E-11 and E-15, in addition to that from the fixed well for the NE Plume, is discharged into the 7 new injection wells.

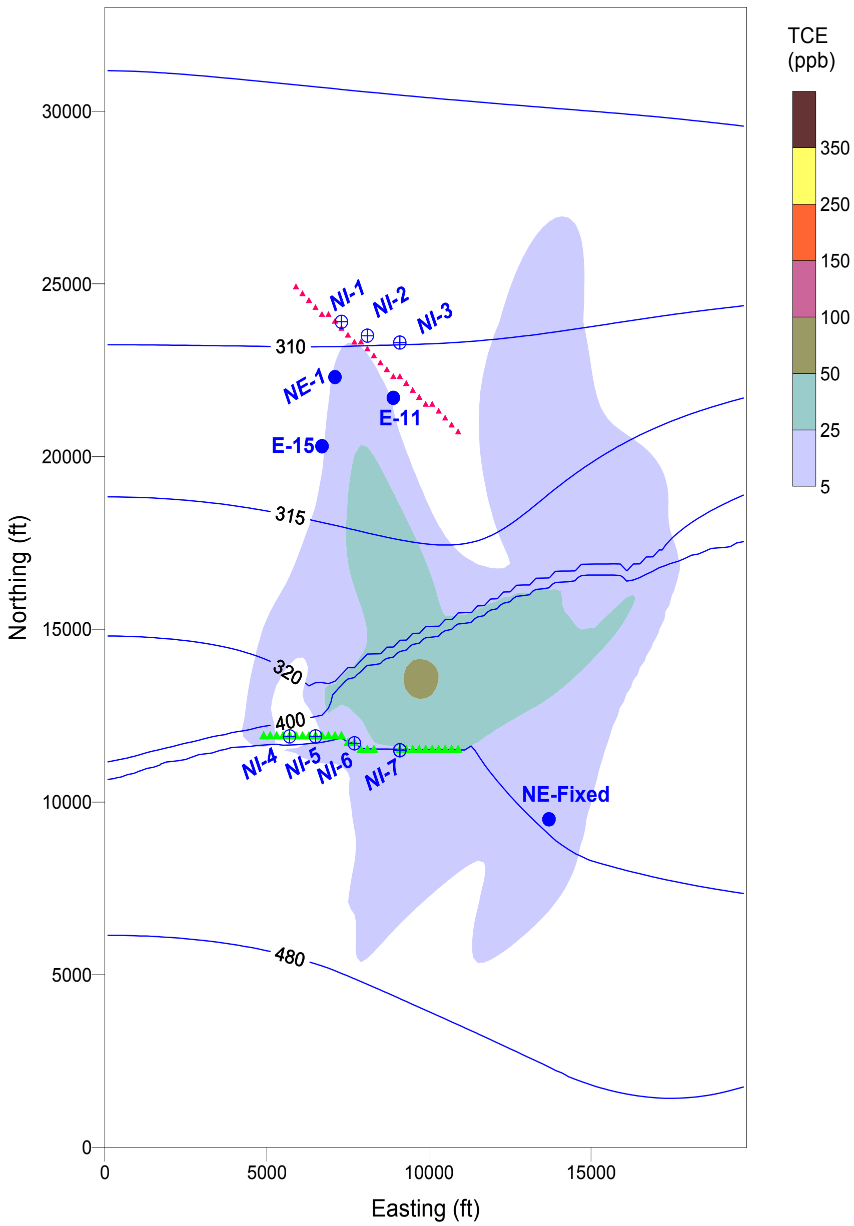
The pumping and injection rates for the optimal dynamic strategy are listed in Table 3-1, and well locations are included in the input file for the MODFLOW Well Package submitted with this report. All prescribed constraints are satisfied, including the maximum concentration limits at all POE-MP, POC-MP1, and POC-MP2 locations. The cost objective function for the optimal strategy is $14.446 million in net present value. Of which, 49% is the fixed O&M costs and another 28% is related to sampling, which is dependent on the plume size. The most significant potential for cost savings comes from shutting down most of the existing wells and replacing them with a minimum number of new pumping/injection wells. A complete cost breakdown is shown in Figure 3.3.



(a) Model layer 1



(b) Model layer 2



(c) Model layer 3

Figure 3.2. Calculated TCE plumes in (a) model layer 1, (b) model layer 2, and (c) model layer 3, at the end of the project duration (21 years). The triangles in red color indicate the POE-MP constraints and those in green indicate the POC-MP1 and POC-MP2 constraints. NI-1 through NI-7 are new injection wells. NE-1 is a new pumping well, and E-11 and E-15 are two existing pumping wells. NE-Fixed is the fixed pumping well added to address the NE plume. The total pumping from NE-1, E-11, E-15 and NE-Fixed is equal to total injection at NI-1 through NI-7 at any time.

Table 3.1. Optimal pumping strategy for Formulation 2.

Well Name	Well Flow Rate (GPM) (- for pumping and + for injection).						
	MP 1	MP 2	MP 3	MP 4	MP 5	MP 6	MP 7
E-11	-616.9	-617.5	-617.5	-617.5	-617.5	-617.5	-617.5
E-15	0.0	0.0	-217.0	-237.0	0.0	-161.0	-49.8
NE-1	-380.0	-357.0	-380.0	-380.0	-343.0	-380.0	-380.0
NI-1	390.0	120.0	400.0	570.0	400.0	570.0	440.0
NI-2	570.0	570.0	530.0	570.0	550.0	570.0	570.0
NI-3	350.0	570.0	570.0	570.0	570.0	570.0	550.0
NI-4	500.0	520.0	520.0	540.0	540.0	505.0	504.0
NI-5	250.0	250.0	250.0	120.0	130.0	227.0	227.0
NI-6	100.0	140.0	140.0	60.0	20.0	20.0	22.0
NI-7	261.9	229.5	229.5	229.5	175.5	121.5	159.3
NE-Fixed	-1425.0	-1425.0	-1425.0	-1425.0	-1425.0	-1425.0	-1425.0
Net	0.0	0.0	0.0	0.0	0.0	0.0	0.0

* The well locations are indicated in the MODFLOW Well Package input file named 'Formuln2.WEL'.

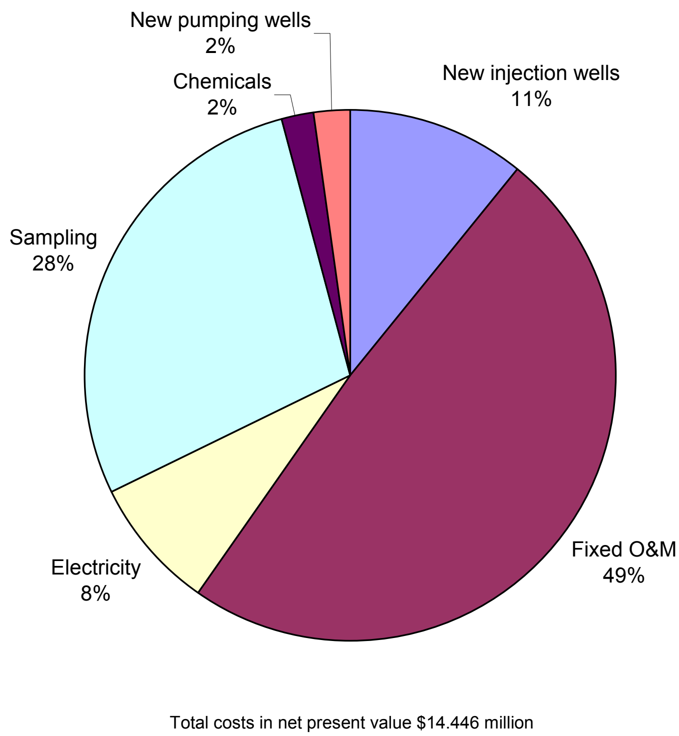


Figure 3.3. Distribution of the various cost items for the optimal solution for Formulation 2.

4

Optimal Solution: Formulation 3

4.1 OBJECTIVE FUNCTION AND CONSTRAINTS

The objective function for Formulation 3 is identical to that for Formulation 1 as expressed in equation (2.1). The constraints (1) – (7) defined for Formulation 2 also apply to Formulation 3. Furthermore, there are three additional constraints that must be satisfied under Formulation 3, i.e.,

(8) The number of new extraction wells (*NW*) cannot exceed 4 over the entire project duration (excluding the fixed well specified for the NE Plume), i.e.,

$$NW \leq 4$$

(9) The number of new injection wells (*NI*) cannot exceed 4 over the entire project duration, i.e.,

$$NI \leq 4$$

(10) TCE concentrations cannot exceed 50 ppb at all cleanup locations, i.e.,

$$C^{\max} \leq 50 \text{ ppb}$$

The locations of the cleanup constraints are shown in Figure 4.1 as all model nodes within the rectangular box. The star and cross symbols indicate contaminant sources and other "buffer" cells, where the cleanup constraint was not applied.

4.2 MODELING APPROACH

Because more than 4 injection wells have already been used to satisfy the POE and POC constraints and because several extraction wells would be required to satisfy the cleanup constraints defined over the entire main plume, it was clear prior to actual optimization analysis that Formulation 3 was unlikely to have a feasible solution. Thus the major effort associated with this formulation was to confirm that Formulation 3 would be infeasible. To that end, the first run (Run 1) was set up that included, as decision variables, all existing pumping wells, and 4 new injection and 4 pumping wells, respectively. To reduce the solution search space, the existing injection wells were treated as 'balance constraints' by allocating a certain percentage of pumped water that should be discharged into each injection well. As pointed out previously, existing injection wells did not have a significant effect on meeting any of the constraints, and thus little could be gained by including them as decision variables.

The genetic algorithm (GA) solver as implemented in the MGO code was used to solve Formulation 3. The GA method employs a penalty method which adds, for a minimization problem, a certain amount of penalty to the objective function whenever a constraint is violated. The amount of penalty added is proportional to the amount of violation. This way the selection process favors those interim solutions that have fewer and smaller violations.

Run 1 yielded no feasible solution that could satisfy all the constraints defined for Formulation 3. Thus, in an optional follow-up work, we explored two alternative formulations (Formulations 3-1 and 3-2). First, what is the smallest number of new wells that would be required to achieve a feasible solution? Second, what is the least-cost solution if the numbers of new injection and pumping wells are both allowed to exceed 4? To solve the first alternative formulation, we added additional new wells, with both flow rates and well locations as decision variables, until a feasible solution was obtained. As many existing wells as possible were used in the solution, even if new wells could be installed to satisfy the same constraints less costly. To solve the second alternative formulation, as many new wells as necessary were added to minimize the cost objective function. Only steady-state pumping/injection strategies for the alternative formulations were developed.

The results for the two alternative formulations are presented and discussed in the next section.

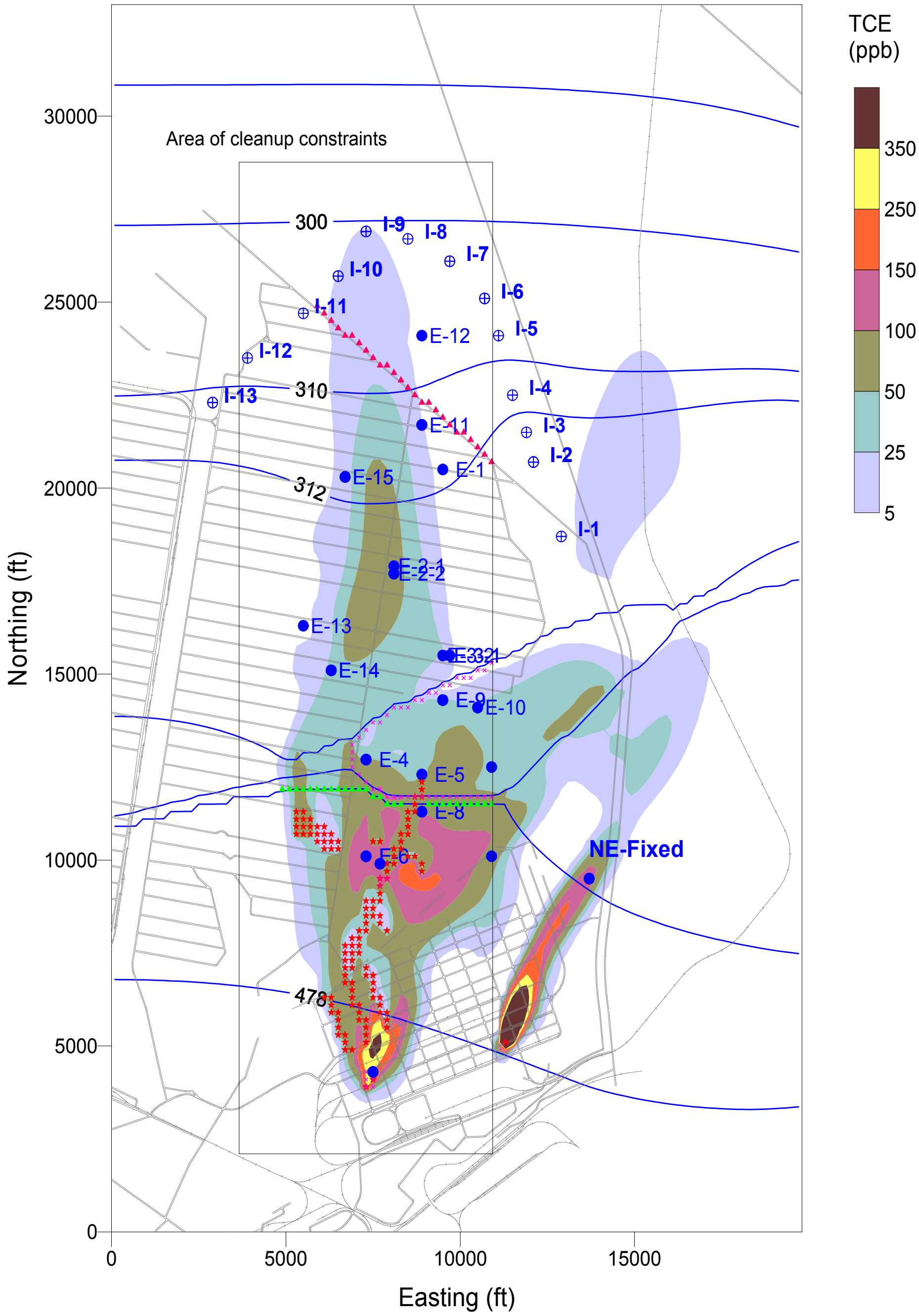


Figure 4.1. Locations of the "cleanup" constraints for the main plume shown as the area within the rectangular box. The star and cross symbols indicate the contaminant sources and other "buffer" cells, where the cleanup constraint was not applied. Also shown are the POE and POC constraints, along with the pumping/injection wells for the current pump-and-treat system and the calculated TCE plume in model layer 1 at the beginning of the optimization analysis.

4.3 SOLUTIONS FOR ALTERNATIVE FORMULATIONS

The optimal solution obtained for the first alternative formulation (Formulation 3-1) is illustrated in Figures 4.2. It consists of 4 new pumping wells, 6 new injection wells, and 6 existing pumping wells. Three of the new injection wells are located near the POE-MP boundary, while the other three are located near the POC-MP1 and POC-MP2 boundaries. The new pumping well 'NE-1' is screened in both model layers 1 and 2, while the other three are all screened in model layer 1 only. Three new injection wells are screened in model layer 1 only: NI-1, NI-3, and NI-4. The new injection well 'NI-2' is screened in layer 1, while NI-5 and NI-6 are screened in both model layers 1 and 2. Most of the pumped water from the new and existing wells, including that from the fixed well for the NE Plume, is discharged into the 6 new injection wells. The remainder is distributed among the existing injection wells. The exact locations and flow rates of all pumping and injection wells are contained in the input file for the MODFLOW Well Package. The total costs for the Formulation 3-1 are $19.26 million in net present value. A complete breakdown of the costs is shown in Figure 4.3.

The optimal solution obtained for the second alternative formulation (Formulation 3-2) is illustrated in Figures 4.4. It consists of 5 new pumping well, 7 new injection wells, and 3 existing pumping wells. The well layout for this alternative is similar to that of the first alternative. The main difference is the installation of the new pumping well 'NE-5', which, along with a new injection well, makes it possible to shut down 3 existing wells. The exact locations and flow rates of all pumping and injection wells are listed in Appendix A. The total costs for Formulation 3-2 are $18.62 million in net present value. A complete breakdown of the costs is shown in Figure 4.5.

An important assumption in the development of the above solutions is that existing wells could be slightly modified to extract water from the layers above the current screen levels. For example, E-11 is currently screened in model layer 2, but in the optimal solution, it is assumed to extract water from layer 1. This assumption is reasonable since a minimal amount of effort and expense would be involved in pumping from a shallower screen interval. This would not be the case to extract water from a greater depth than the current screen level.

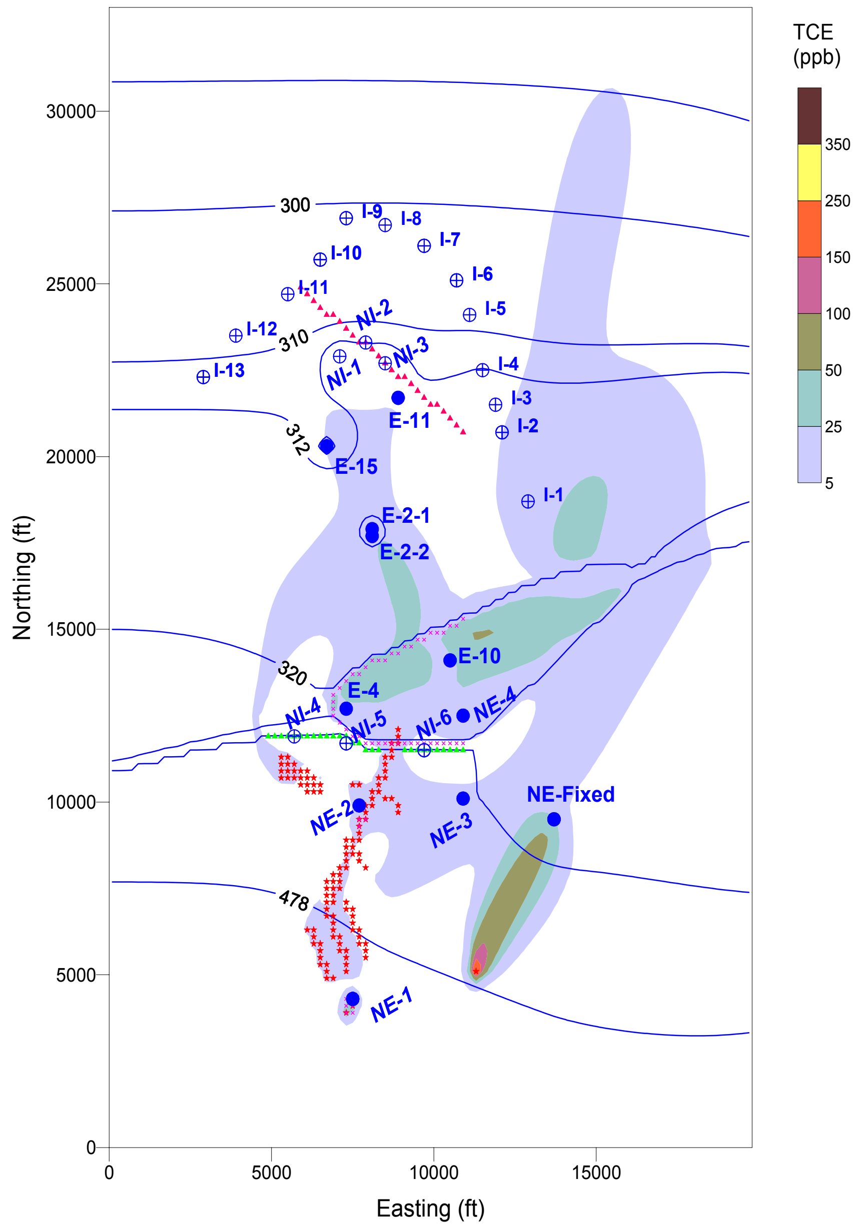


Figure 4.2. Calculated TCE plume and well layout for Formulation 3-1 in model layer 1 at the end of the project duration of 21 years. NI-1 through NI-6 are new injection wells. NE-1 through NE-4 are new pumping wells. Wells labeled with prefixes E and I are existing pumping and injection wells, respectively.

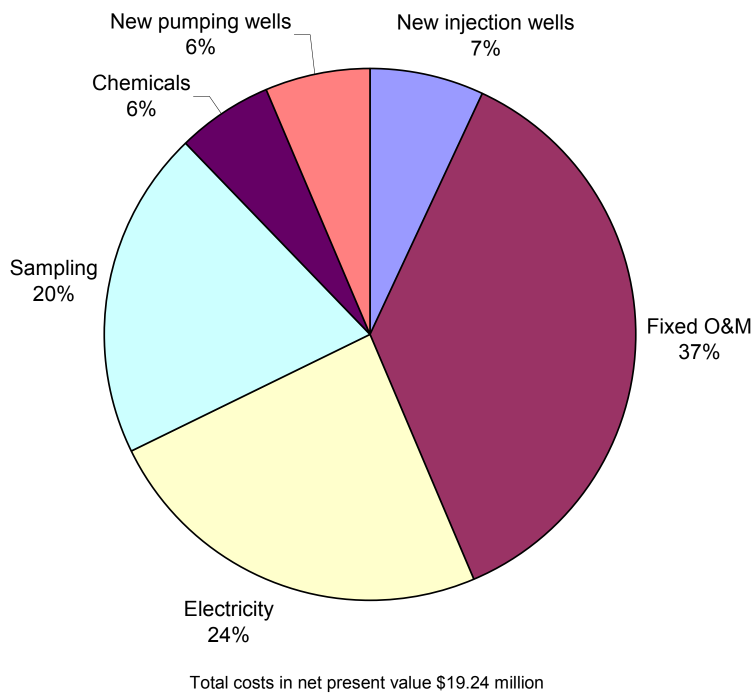


Figure 4.3. Distribution of the various cost items for the optimal solution for Formulation 3-1.

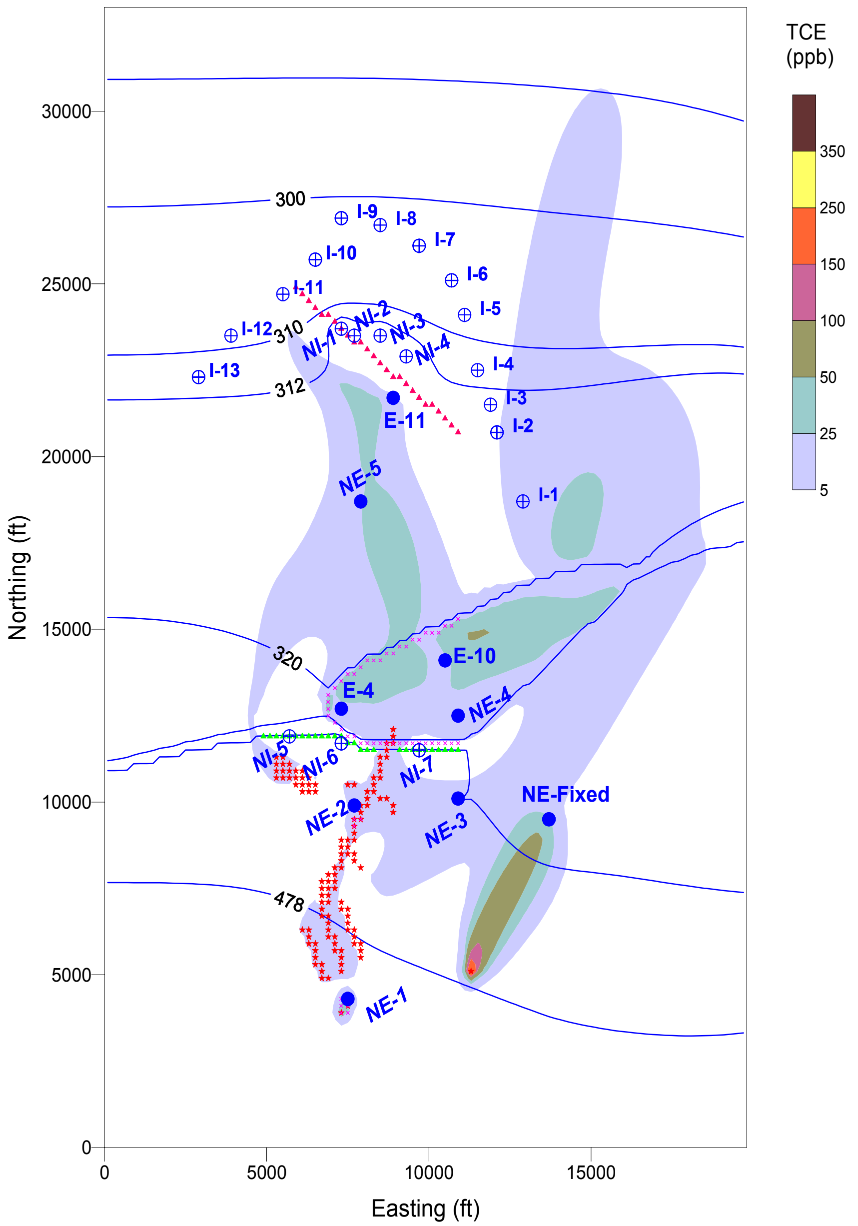


Figure 4.4. Calculated TCE plume and well layout for Formulation 3-2 in model layer 1 at the end of the project duration of 21 years. NI-1 through NI-6 are new injection wells. NE-1 through NE-4 are new pumping wells. Wells labeled with prefixes E and I are existing pumping and injection wells, respectively.

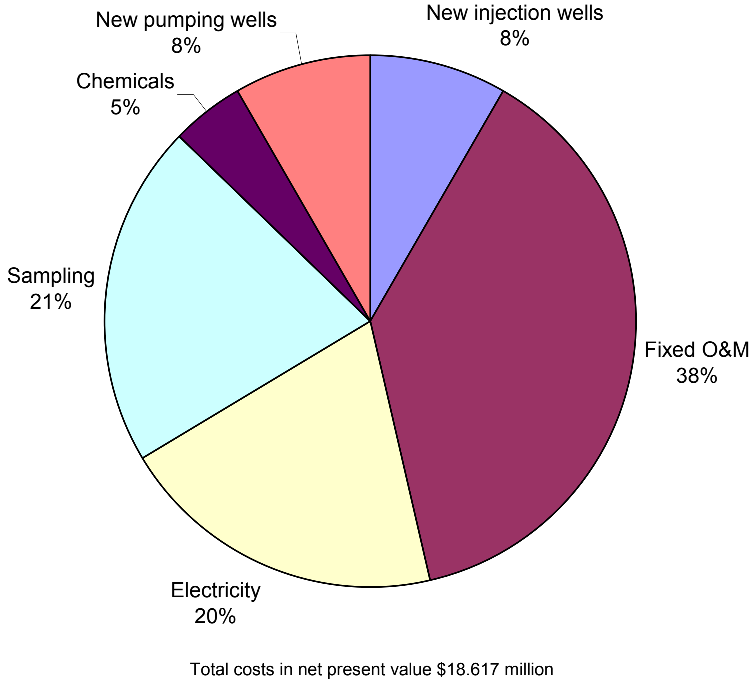


Figure 4.5. Distribution of the various cost items for the optimal solution for Formulation 3-2.

5

Summary and Discussions

5.1 SUMMARY OF STRATEGIES

Table 5.1 summarizes the optimal solutions developed for the Tooele site. Feasible solutions were obtained for Formulations 1 and 2 with a cost objective function value of $12.67 million and $14.45 million, respectively. No feasible solution was identified for Formulation 3 that would satisfy the cleanup constraints using only 4 new injection and 4 pumping wells. Optimal solutions for two alternatives to Formulation 3 are presented in Table 5.2. The solution to Formulation 3-1 indicates that the cleanup can be achieved using 4 new pumping and 6 new injection wells. The solution to Formulation 3-2 indicates that the cleanup can be achieved using a minimum cost of $18.62 million.

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

Formulation	**1**	**2**	**3**
Feasible Solution?	Y	Y	N
Objective Function Value	$12.671 M	$14.446 M	
Number of New Extraction Wells Installed	0	1	
Number of New Injection Wells Installed	4	7	
Number of Existing Pumping Wells Used	2	2	

Figure 5.2. Optimal solutions for alternatives to Formulation 3.

Alternatives for Formulation 3	**3-1**	**3-2**
Constraint Relaxation	Number of new injection wells is allowed to exceed **4**	Numbers of both new injection and extraction wells are allowed to exceed **4**
Objective Function Value	$19.234 M	$18.617 M
Number of New Extraction Wells Installed	4	5
Number of New Injection Wells Installed	6	7
Number of Existing Pumping Wells Used	6	3

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 as discussed in the previous sections, 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.

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 6000-8000 flow and transport simulations were run for each formulation by the optimization code. Each flow and transport simulation run took an average of about 3-4 minutes on PCs equipped with a Pentium III 1-Ghz CPU and 512 MB RAM or more.

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.

6

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