Environmental Security Technology Certification Program

Final Technical Report, Volume II

For

Application of Flow and Transport Optimization Codes to Groundwater Pump and Treat Systems

September, 2003

Prepared by:

Barbara Minsker, PhD, Minsker Consulting
Yan Zhang, GeoTrans, Inc.
Robert Greenwald, GeoTrans, Inc.
Richard Peralta, PhD, Utah State University
Chunmiao Zheng, PhD, University of Alabama
Karla Harre, Naval Facilities Engineering Service Center
Dave Becker, Army Corps of Engineers HTRW-CX
Laura Yeh, Naval Facilities Engineering Service Center
Kathy Yager, Environmental Protection Agency

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Appendix D: Formulation Document and Final Reports, Umatilla

Formulation Document

Transport Optimization Umatilla Army Depot
Draft Mathematical Formulations
3/21/01

Three different transport optimization formulations, consisting of an objective function to be minimized and a set of constraints to be satisfied, are described below. These formulations are based on data from the system operated from 1997 to the present, and from input provided by the installation and the Army Corp of Engineers Seattle District (collectively referred to herein as "the Installation").

Each formulation consists of a function to minimize subject to constraints. The Installation has expressed interest in achieving cleanup for both RDX and TNT. The current model indicates that a feasible solution exists for cleaning up both RDX and TNT within 20 years. The Installation has also expressed interest in determining the benefit of increasing the capacity of the treatment plant above the current capacity of 1300 gpm. Those two formulations address these interests of the Installation. For comparison purpose, a simpler objective function, minimizing mass remaining, is also constructed. The formulations are provided in detail in the following pages and can be summarized as follows:

Formulation 1: serves as baseline. The objective function is to minimize the cost subject to that 1) the current capacity of the treatment plant is held constant, 2) the cleanup is determined by both RDX and TNT within 20 years.

Formulation 2: same as Formulation 1 but allows the capacity of the treatment plant to increase to a maximum of 1950 gpm.

Formulation 3: same as Formulation 1 but the objective function is to minimize the total mass remaining (RDX plus TNT) in layer 1 within 20 years.

Formulation #1 (Baseline)

Formulation 1 -- Important Notes:

1) All cost coefficients are in thousands of dollars.

2) A site close-out cost associated with monitoring that will continue for 5 years after cleanup is assumed to be "in common" for all potential solutions, and therefore is not explicitly included in the formulations (although a slight difference in these close-out costs would result due to discounting, according to when cleanup occurs, that is not considered significant).

3) The system currently operates at a rate of 1300 gpm but is only expected to operate at that rate approximately 90% of the time (i.e., 10% down-time for GAC changeout, etc.). Therefore, modeling a steady rate should account for only 90% of the actual operating rate when system is "on". Limits on simulated flow rates are adjusted accordingly in the formulations.

4) Extraction well 2 (EW-2, easting = 2274143.6, northing = 789103.62), which currently is not in service, is located approximately 100ft northwest of extraction well 4 (EW-4).

5) The Installation provided operating costs for wells with maximum extraction rates of 400 gpm and 1000 gpm, approximately $4,000 and $19,000 respectively. Two linear relationships have been developed based on these operating costs, one to estimate costs for operating wells with extraction rates between 0 gpm and 400 gpm and the other for operating wells with extraction rates between 400 gpm and 1000 gpm. While these relationships suggest the use of variable-rate pumps, they are not intended to do so. Rather, they suggest that if optimization recommends pumping a well at a rate between 0 gpm and 400 gpm or between 400 gpm and 1000 gpm, that the Installation would install an appropriately sized fixed-rate pump with operating costs scale accordingly.

6) For this optimization study, the MODFLOW WEL package is used to simulate infiltration recharge basins instead of RCH package. There is no limit to recharge basin size. Because one recharge basin can contain more than one model cell, an additional column (after layer, row, column, and rate) is needed in the WEL package for a recharge basin cell to indicate the recharge basin number. There are 3 recharge basins in the current system, thus any new recharge basin has to start at number 4 and in ascending order thereafter, e.g., 4, 5, 6, ….

7) Site modifications must be made at the beginning of the first time step of a management period. Thus, if a new extraction well is to be installed in the first management period, it must extract water from the inception of the simulation. If a pumping rate is adjusted for the second management period, this new flow rate must be effective for every time step in that management period.

8) All measurements or observations of modeled rates (i.e., pumping and recharge) for

evaluating the objective function or the constraints must be made at the beginning of the time step of a modeling year, and observations are taken from the end of the previous time step. For example, the mass removed from the system in a year is used to calculate the variable costs of changing GAC units for that year. To calculate this cost for the first year of a management period, multiply the new flow rate (which will remain constant throughout that management period) and the concentration at the end of the last time step of the previous management period. Likewise, to obtain the mass for the second year of that management period multiply the same flow rate by the concentration at the end of the last time step of the previous year.

9)
- The formulations are presented in units most familiar to the reader, which are concentration in micrograms per liter (ug/l), flow rates in gallons per minute (gpm), and mass in kilograms.
- The model used for the optimization simulations will specify concentration in ug/l, site dimensions in feet, flow rates in cubic feet per day (ft^3/year), time in years, and mass per time in ug/l×ft^3/year.
- The objective function requires mass in kilograms (kg) for calculating the cost of changing GAC units.
- The implementation of the formulation will require unit conversions from the model units.

$$\frac{\text{ft}^3}{\text{year}} \Rightarrow \text{gpm} \qquad \text{USE} \qquad \frac{7.481\,\text{gal}}{1\ \text{ft}^3}\times\frac{1\,\text{year}}{525600\,\text{min}} = 1.4238\times 10^{-5}\ \frac{\text{gal}\cdot\text{year}}{\text{ft}^3\cdot\text{min}}$$

$$\frac{\text{ìg}}{\text{L}}\times\text{ft}^3 \Rightarrow \text{kg} \qquad \text{USE} \qquad \frac{3.785\,\text{L}}{\text{gal}}\times\frac{7.481\,\text{gal}}{1\,\text{ft}^3}\times\frac{1\,\text{kg}}{10^9\ \text{ìg}} = 2.832\times 10^{-8}\ \frac{\text{L}\cdot\text{kg}}{\text{ft}^3\cdot\text{ìg}}$$

$$\frac{\text{ìg}}{\text{L}}\times\frac{\text{ft}^3}{\text{year}} \Rightarrow \frac{\text{kg}}{\text{year}} \qquad \text{USE} \qquad \frac{3.785\,\text{L}}{\text{gal}}\times\frac{7.481\,\text{gal}}{1\ \text{ft}^3}\times\frac{1\,\text{kg}}{10^9\ \text{ìg}} = 2.832\times 10^{-8}\ \frac{\text{L}\cdot\text{kg}}{\text{ft}^3\cdot\text{ìg}}$$

$$\frac{\text{ìg}}{\text{L}}\times\frac{\text{gal}}{\text{min}} \Rightarrow \frac{\text{kg}}{\text{year}} \qquad \text{USE} \qquad \frac{1\,\text{kg}}{10^9\ \text{ìg}}\times\frac{1440\ \text{min}}{1\,\text{d}}\times\frac{365\,\text{d}}{1\,\text{year}}\times\frac{3.785\ \text{L}}{1\ \text{gal}} = 1.989\times 10^{-3}\ \frac{\text{kg}\cdot\text{L}\cdot\text{min}}{\text{year}\cdot\text{ìg}\cdot\text{gal}}$$

Formulation 1 -- Definitions

year – the modeling year defined by

$$year = \text{Roundup}(elapsed\ modeling\ years)$$

- January 1, 2003 corresponds to zero elapsed modeling years.
- 2003 corresponds to *year* =1.
- The end of June 2004 corresponds to about 1.5 elapsed modeling years and *year* =2.
- Roundup() is a function to convert a real number into an integer by rounding up (i.e., 1.0 → 1 but 1.1 → 2).

ny – the modeling year in which cleanup is achieved. That is the modeling year when

$$\left\|C_{RDX}\right\|_{\infty} \leq 2.1\,m\text{g/L} \qquad \text{and} \qquad \left\|C_{TNT}\right\|_{\infty} \leq 2.8\,m\text{g/L}$$

$\left\|C_{RDX}\right\|_{\infty}$ is the infinity-norm, which returns the maximum value of two-dimensional array C_{RDX}, which is the two-dimensional concentration array in layer 1 for RDX.

- For example, if during the 17th year of the simulation "cleanup" is achieved, then costs are incurred for 17 full years.

d – represents the conversion of capital and annual costs incurred to present value (i.e., discounted) with the following discount function:

$$PV = \frac{cost}{(1+rate)^{year-1}}$$

- PV is the present value of a *cost* incurred in *year* with a discount rate of *rate.*
- No discounting is done for all costs for *year*=1(i.e., 2003).
- All costs in subsequent years are discounted at the ends of those years.
- Example 1: Assuming a discount rate of 5% and a $1000 cost incurred at any time during 2003 (*year*=1) the present value of the cost is $1000.
- Example 2: Assuming a discount rate of 5% and a $1000 cost incurred in 2004 (*year*=2), the present value of that cost is $1000/1.05=$952.38.

management period – 5-year periods during which the site cannot be modified. Modifications may only be made during the initial time step of each management period. Therefore, modifications can first be made in January 2003 (beginning of *year*=1) and then again in January 2008 (beginning of *year*=6), 2013 (beginning of *year*=11), 2018 (beginning of *year*=16).

Formulation 1-- Objective Function

This function minimizes total cost up to and including *ny* (i.e., the year of cleanup). This function must be evaluated at the end of every year, rather than after every management period, to properly account for discounting of annual costs and to ensure that costs are not incurred for the time between *ny* and the end of that management period.

MINIMIZE (CCW + CCB + CCG + FCL + FCE +VCE+VCG + VCS)

CCW: Capital costs of new wells

$$CCW = (25 \times IEW2)^d + \sum_{i=1}^{ny} (75 \times NW_i)^d$$

ny is the modeling year when cleanup occurs.
NW_i is the total number of new extraction wells (except EW-2) installed in year *i*. New wells may only be installed in years corresponding to the beginning of a 5-yr management period. Capital costs are not incurred for operating a well that previously has been in service (i.e., already installed).
IEW2 is a flag indicator; 1 when EW-2 is first put into service, 0 otherwise.
$75K is cost of installing a new well.
$25K is the cost of putting existing well EW-2 into service.
d indicates application of the discount function to yield Net Present Value (NPV).

CCB: Capital costs of new recharge basins

$$CCB = \sum_{i=1}^{ny} (25 \times NB_i)^d$$

ny is the modeling year when cleanup occurs.
NB_i is the total number of new recharge basins installed in year *i*. New recharge basins may only be installed in years corresponding to the beginning of a management period, and must have infiltration evenly distributed throughout the basin.
$25K is the cost of installing a new recharge basin independent of its location.
d indicates application of the discount function to yield Net Present Value (NPV).

CCG: Capital cost of new GAC unit. This term is nonzero only for Formulation 2 as the treatment capacity of the plant is constrained to its current value for Formulations 1 and 3. Installation of a GAC unit is permanent once it occurs and the treatment capacity of the plant permanently reflects the addition of that unit. Up to two GAC units may be added during the 20-year modeling period.

$$CCG = \sum_{i=1}^{ny} (150 \times NG_i)^d$$

where

$$NG_i = 0 \quad \text{for} \quad (Q^* / \alpha) \le Q_1$$
$$NG_i = 1 \quad \text{for} \quad Q_1 < (Q^* / \alpha) \le Q_2$$
$$NG_i = 2 \quad \text{for} \quad Q_2 < (Q^* / \alpha) \le Q_3$$

ny is the modeling year when cleanup occurs.
$150K is the cost of converting a current GAC changeout unit into an adsorption unit.
NG_i is total number of new GAC units installed in year *i*. New GAC units may only be installed in years corresponding to the beginning of a management period.
d indicates application of the discount function to yield Net Present Value (NPV).
Q^* is the total pumping rate in the model.
α is a coefficient accounting for 10% system downtime (90% uptime), α=0.90.
Q_1 is the initial pumping rate of the system, (1300 gpm).
Q_2 is 1625 gpm, which is the initial flow rate plus the flow capacity of one additional GAC unit.
Q_3 is 1950 gpm, which is the initial flow rate plus the flow capacity of two additional GAC units.

FCL: Fixed cost of labor

$$\text{FCL}=\sum_{i=1}^{ny}(237)^d$$

ny is the modeling year when cleanup occurs.
$237K is the fixed annual O&M labor cost.
d indicates application of the discount function to yield Net Present Value (NPV).

FCE: Fixed costs of electricity (lighting, heating, etc.)

$$\text{FCE}=\sum_{i=1}^{ny}(3.6)^d$$

ny is the modeling year when cleanup occurs.
$3.6K is the fixed annual electrical cost.
d indicates application of the discount function to yield Net Present Value (NPV).

VCE: Variable electrical costs of operating wells

$$\text{VCE}=\sum_{i=1}^{ny}\sum_{j=1}^{nwel}\left(CW_{ij}\times IW_{ij}\right)^d$$

where

(gpm)

$$CW_{ij} = 0.01(Q_{ij}) \quad \text{for} \quad 0\,\text{gpm} < Q_{ij} \le 400\,\text{gpm}$$
$$CW_{ij} = 0.025(Q_{ij}) - 6 \quad \text{for} \quad 400\,\text{gpm} < Q_{ij} \le 1000\,\text{gpm}$$

(ft^3/year)

$$CW_{ij} = 1.423 \times 10^{-7}(Q_{ij}) \quad \text{for} \quad 0\ \text{ft}^3\text{/year} < Q_{ij} \le 2.811 \times 10^{7}\ \text{ft}^3\text{/year}$$
$$CW_{ij} = 3.556 \times 10^{-6}(Q_{ij}) - 6 \quad \text{for} \quad 2.811 \times 10^{7}\ \text{ft}^3\text{/year} < Q_{ij} \le 7.027 \times 10^{7}\ \text{ft}^3\text{/year}$$

ny is the modeling year when cleanup occurs.
nwel is the total number of extraction wells.
CW_{ij} is the electrical cost for well *j* in year *i*. Costs differ for wells depending on the extraction rates of well *j* in year *i*, Q_{ij}, which remain constant over a 5-yr management period.
IW_{ij} is a flag indicator; 1 if the well *j* is on in year *i*, 0 otherwise.
d indicates application of the discount function to yield Net Present Value (NPV).

VCG: Variable costs of changing GAC units

$$\text{VCG} = \sum_{i=1}^{ny} \left[g(\bar{c}_i) \times m_i \right]^d$$

where

ny is the modeling year when cleanup occurs.
d indicates application of the discount function to yield Net Present Value (NPV).
$g(\bar{c}_i)$ is the cost of mass removed (thousands of dollars per kilogram) as a function of average influent concentration (ppb) into the treatment plant.

$$g(\bar{c}_i) = \frac{-0.5(\bar{c}_i) + 225}{1000}$$

$\bar{c}_i$ is the average influent concentration (RDX plus TNT) into the treatment plant from all of the extraction wells, measured in ppb.

$$\bar{c}_i = \frac{\sum_{j=1}^{nwel} Q_j \bar{c}_{ij}}{\sum_{j=1}^{nwel} Q_j}$$

Q_j is the pumping rate of extraction well *j*.
m_i is the mass of contaminant removed (kg) during year *i*.

$$m_i = \sum_{j=1}^{nwel} Q_j \bar{c}_{ij} \times b$$

b is the conversion from $\text{ug/L}\times\text{ft}^3/\text{year}$ to kg/year $\left(\text{i.e., } 2.832 \times 10^{-8} \frac{\text{L} \cdot \text{kg}}{\text{ft}^3 \cdot mg}\right)$

VCS: Variable cost of sampling

$$\text{VCS}=\sum_{i=1}^{ny} \left[150\times (A_i / IA)\right]^d$$

ny is the modeling year when cleanup occurs.
IA is the initial plume area as measured in January 2003.
$150K is the sampling cost (as of January 2001) and considers both labor and analysis.
d indicates application of the discount function to yield Net Present Value (NPV).
A_i is the plume area during year i. The plume area is only measured at the beginning of a management period; therefore, A_i can only change during years corresponding to the beginning of a management period. A_i is measured as the summed area of all model grid cells in layer 1 that are not "clean" for either constituent at the beginning of the management period, where "clean" is less than or equal to 2.1 µg/l for RDX and 2.8 µg/l for TNT.

$$A_i = \sum_{j=1}^{m} \sum_{k=1}^{n} \left[\Delta x_j \Delta y_k \times IC_{jk}\right]$$

m is the number of grid cells in the x direction
n is the number of grid cells in the y direction
Δx_j is length of the jth grid space in the x direction.
Δy_k is the length of the kth grid space in the y direction.
IC_{jk} is a flag

$$\begin{aligned} &If\ ((C_{RDX}^{jk} > 2.1\,\text{ug/L})\ \text{ OR }\ (C_{TNT}^{jk} > 2.8\,\text{ug/L})\ ) \\ &\qquad \text{then } IC_{jk} = 1, \\ &\qquad \text{else } IC_{jk} = 0 \end{aligned}$$

C_{RDX}^{jk} is the concentration of RDX in the grid cell with indices j and k.
C_{TNT}^{jk} is the concentration of TNT in the grid cell with indices j and k.

Formulation 1 – Constraints

1) The modeling period consists of four 5-year management periods (20 years total) beginning January 2003 (*year*=1).

2) Modifications to the system may only occur at the beginning of each management period (i.e., the beginning of modeling years 1, 6, 11, and 16).

3) Cleanup must be achieved within modeling period (by the end of year 20).

$$ny \leq 20$$

4) The total modeled pumping rate, when adjusted for the average amount of uptime, cannot exceed 1300 gpm, the current maximum treatment capacity of the plant. This constraint prohibits installation of additional of GAC units (term CCG of the objective function).

$$Q^* / \alpha \leq 1300 \text{ gpm}$$

α: a coefficient that accounts for the amount of average amount of uptime, α=0.90
Q^*: the modeled flow rate.

When Evaluated: The beginning of each 5-year management period

5) The extraction system must account for limits imposed by the hydrogeology of the site. Extraction wells in Zone 1 may pump at a maximum rate of 400 gpm. Extraction wells in Zone 2 may pump at a maximum rate of 1000gpm. See Figure 1 for definitions of Zones 1 and 2.

$$\begin{array}{ll} \text{If} & \text{Zone}(i,j) = 1, \\ & \text{then} \quad Q^* / \alpha \leq 400 \text{ gpm} \\ & \text{else} \quad Q^* / \alpha \leq 1000 \text{ gpm} \end{array}$$

Zone(i,j): A function of the grid space indices i and j that returns 1 if (i,j) corresponds to Zone 1 and returns 2 if (i,j) corresponds to Zone 2
Q^*: the modeled extraction rate from a well located at grid location (i,j)

When Evaluated: The beginning of each 5-year management period

6) RDX and TNT concentration levels must not exceed their respective cleanup levels in

locations beyond an area based on the zone in the model Richard Smith made “inactive” for transport (i.e. plume cannot spread above cleanup levels to any cell adjacent to that inactive area, illustrated on Figure 2).

At any time, *t*, and for all grid indices *i* and *j* in layer 1,

$$\begin{aligned}&\text{If BRDX}(i,j) = 0\\&\quad \text{then } C_{RDX}^{ij} \leq 2.1\ \mu g/L\\&\text{and}\\&\text{If BTNT}(i,j) = 0\\&\quad \text{then } C_{TNT}^{ij} \leq 2.8\ \mu g/L\end{aligned}$$

BRDX(*i*,*j*): a function of model grid indices *i* and *j* that returns 1 if (*i*,*j*) corresponds to a location within the buffer zone for RDX and 0 if (*i*,*j*) corresponds to a location outside of the buffer zone for RDX

BTNT(*i*,*j*): a function of model grid indices *i* and *j* that returns 1 if (*i*,*j*) corresponds to a location within the buffer zone for TNT and 0 if (*i*,*j*) corresponds to a location outside of the buffer zone for TNT

C_{RDX}^{ij} : the concentration of RDX at grid location (*i*,*j*)
C_{TNT}^{ij} : the concentration of TNT at grid location (*i*,*j*)

When Evaluated: The end of each 5-year management period.

7) ABS(Total simulated pumping - total simulated recharge through recharge basins) ≤ 1 gpm

When Evaluated: The beginning of each 5-year management period

Formulation #2

Formulation 2 – Important Notes

Same as Formulation 1

Formulation 2 – Definitions

Same as Formulation 1

Formulation 2 -- Objective Function

Same as Formulation 1

Formulation 2 -- Constraints

Same as Formulation 1, except modify constraint 4) as follows:

4) The total modeled pumping rate, when adjusted for the average amount of uptime, cannot exceed 1950 gpm, the current maximum treatment capacity of the plant. This constraint allows the installation of up to two additional GAC units each with a capacity of 325 gpm.

$$Q^{*} / \alpha \leq 1950 \text{ gpm}$$

α: a coefficient that accounts for the amount of average amount of uptime, α=0.90
Q^{*}: the modeled flow rate.

When Evaluated: At the beginning of each 5-year management period

Formulation #3

Formulation 3 – Important Notes

Same as Formulation 1.

Formulation 3 – Definitions

Same as Formulation 1 (note discount rate is not required since cost is not directly calculated).

Formulation 3 -- Objective Function

This function minimizes total mass remaining in layer 1 within 20 years. This function must be evaluated at the end of every year, rather than after every management period.

MINIMIZE ($\mathbf{M_{RDX} + M_{TNT}}$)

$\mathbf{M_{RDX}}$: Total mass remaining of RDX in layer 1.

$$\mathrm{M_{RDX}} = \sum_{i=1}^{m} \sum_{j=1}^{n} V_{ij} \times C_{ij} \times f_{RDX} \times \boldsymbol{b}$$

m is the number of grid cells in the x direction.
n is the number of grid cells in the y direction.
C_{ij} is the concentration, measured in ug/L.
V_{ij} is the volume, measured in ft^3.

$$V_{ij} = \Delta x_i \times \Delta y_j \times (Head_{ij} - BotElev_{ij})$$

Dx_i is length of the ith grid space in the x direction.
Dy_j is the length of the jth grid space in the y direction.
$Head_{ij}$ is the water level in layer 1, measured in ft.
$BotElev_{ij}$ is the bottom elevation of layer 1, measured in ft.
f_{RDX} is a dimensionless factor considering porosity and sorbed contaminant mass.

$$f_{RDX} = (\boldsymbol{q} + \boldsymbol{r}_d \times K_d)$$

$\boldsymbol{q}$ is porosity.
$\boldsymbol{r}_d$ is bulk density (kg/ft^3).
K_d is distribution coefficient of RDX (ft^3/kg).
$\boldsymbol{b}$ is the unit conversion from ug/L×ft^3 to kg $\left(\text{i.e., } 2.832 \times 10^{-8} \dfrac{\text{L} \cdot \text{kg}}{\text{ft}^3 \cdot m\text{g}} \right)$

$\mathbf{M_{TNT}}$: Total mass remaining of TNT in layer 1.

$$\mathrm{M_{TNT}} = \sum_{i=1}^{m} \sum_{j=1}^{n} V_{ij} \times C_{ij} \times f_{TNT} \times \boldsymbol{b}$$

m is the number of grid cells in the x direction.
n is the number of grid cells in the y direction.
C_{ij} is the concentration, measured in ug/L.

V_{ij} is the volume, measured in ft^3.

$$V_{ij} = \Delta x_i \times \Delta y_j \times (Head_{ij} - BotElev_{ij})$$

Dx_i is length of the *i*th grid space in the *x* direction.
Dy_j is the length of the *j*th grid space in the *y* direction.
$Head_{ij}$ is the water level in layer 1, measured in ft.
$BotElev_{ij}$ is the bottom elevation of layer 1, measured in ft.
f_{TNT} is a dimensionless factor considering porosity and sorbed contaminant mass.

$$f_{TNT} = (q + r_d \times K_d)$$

q is porosity.
r_d is bulk density (kg/ft^3).
K_d is distribution coefficient of TNT (ft^3/kg).
b is the unit conversion from ug/L×ft^3 to kg $\left(\text{i.e., } 2.832 \times 10^{-8} \frac{\text{L} \cdot \text{kg}}{\text{ft}^3 \cdot m\text{g}}\right)$

Formulation 3 -- Constraints

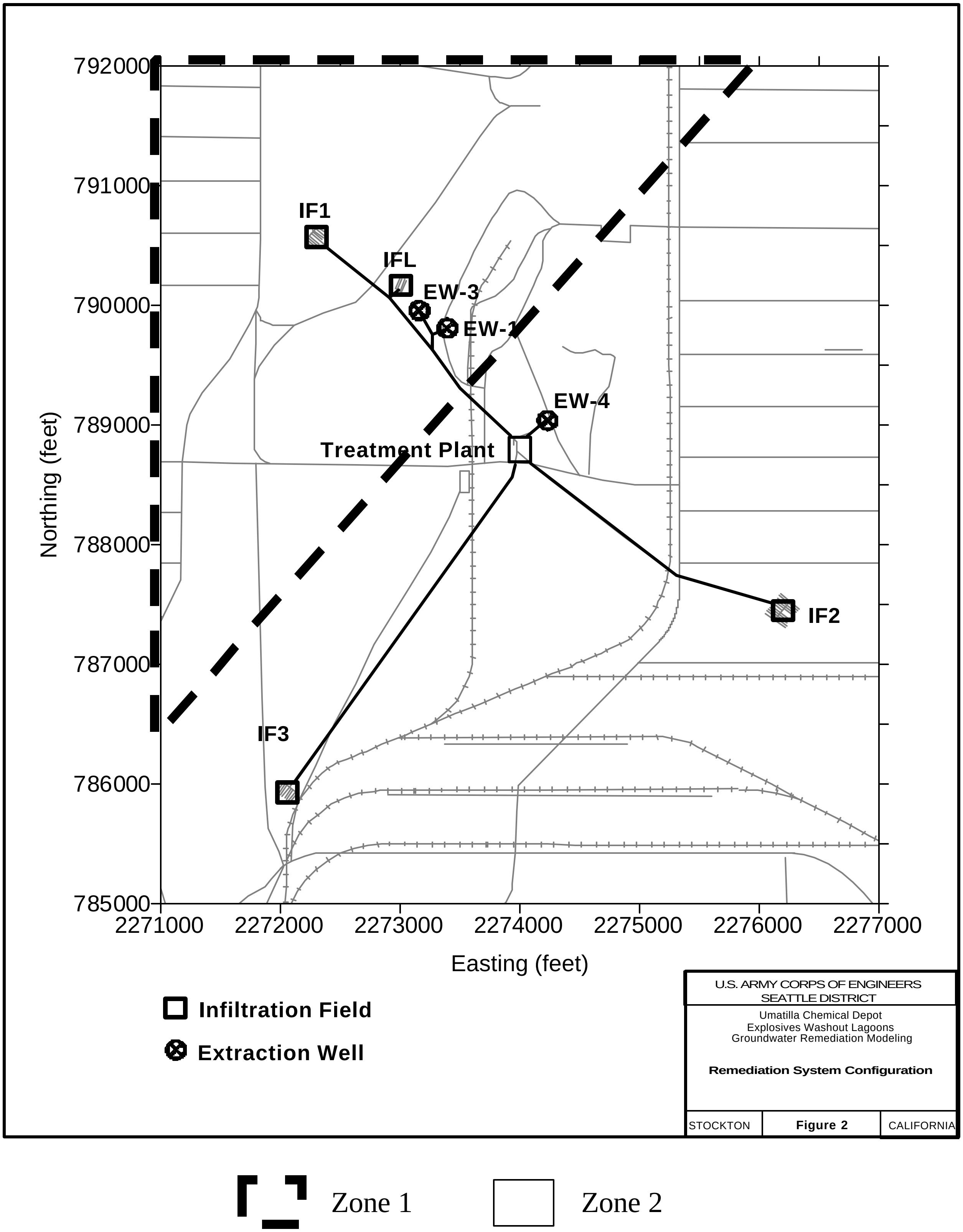
Same as Formulation 1, plus the following constraints:

8) Maximum number of new wells ever installed ≤ 4

   When Evaluated: The beginning of each 5-year management period

9) Maximum number of new recharge basins ≤ 3

   When Evaluated: The beginning of each 5-year management period


792000
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2273000
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2277000
Easting (feet)
IF1
IFL
EW-3
EW-1
EW-4
Treatment Plant
IF2
IF3
Infiltration Field
Extraction Well
U.S. ARMY CORPS OF ENGINEERS
SEATTLE DISTRICT
Umatilla Chemical Depot
Explosives Washout Lagoons
Groundwater Remediation Modeling
Remediation System Configuration
STOCKTON
Figure 2
CALIFORNIA
Zone 1
Zone 2

Figure 1

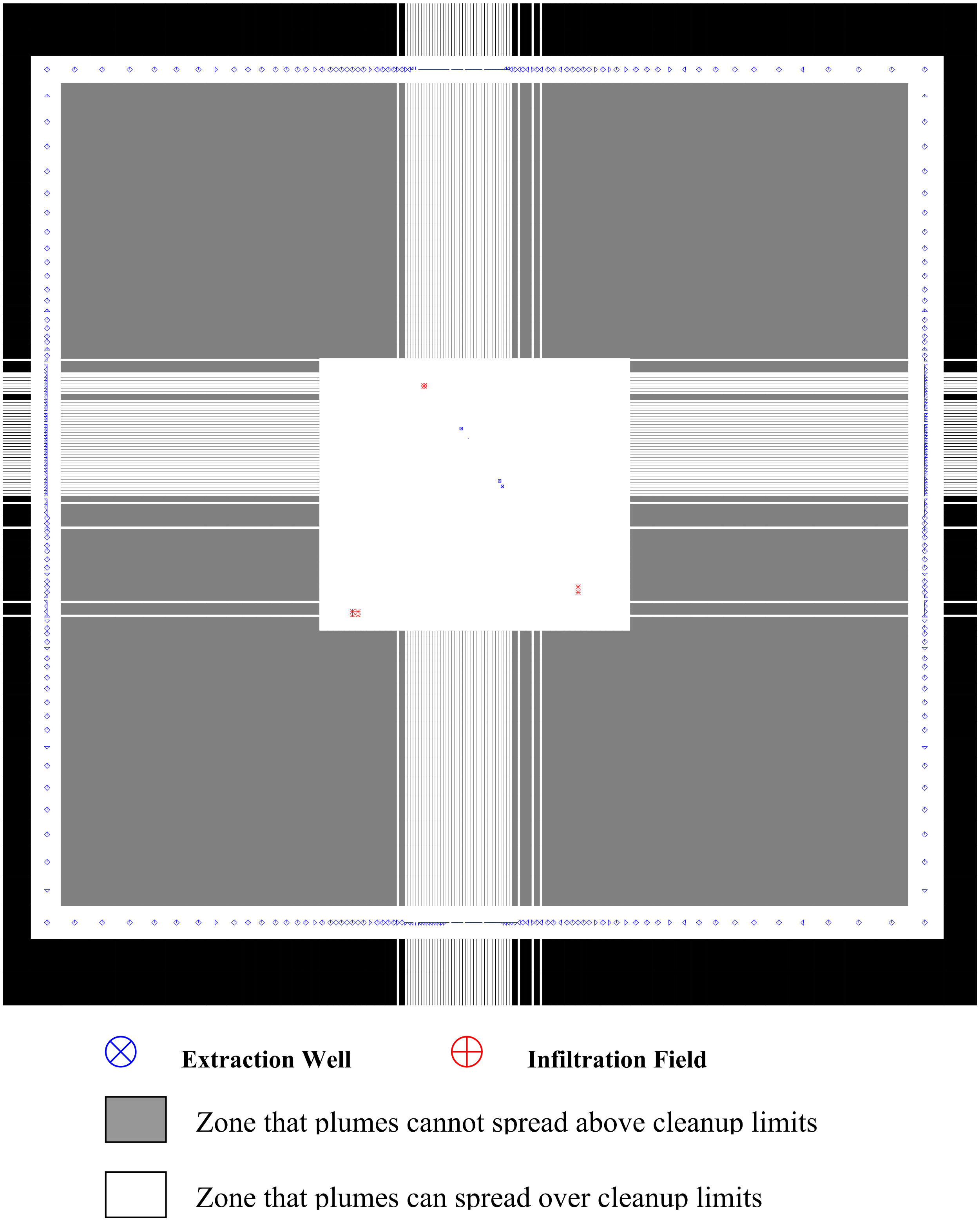
Extraction Well
Infiltration Field
Zone that plumes cannot spread above cleanup limits
Zone that plumes can spread over cleanup limits

Figure 2

GeoTrans Report on Umatilla

OPTIMIZATION RESULTS: GEOTRANS

ESTCP TRANSPORT OPTIMIZATION PROJECT
SITE #1: UMATILLA ARMY DEPOT

Prepared By:

Yan Zhang and Rob Greenwald
GeoTrans, Inc.
2 Paragon Way
Freehold, New Jersey 07728

NOTICE

This work was performed for the U.S. Environmental Protection Agency (U.S. EPA) under Dynamac Contract No. 68-C-99-256, Task # WA-1-ST-1. The technical work was performed by GeoTrans under Subcontract No. AD01-106M.

PREFACE

The goal of the ESTCP Transport Optimization project ("the project") is to evaluate the effectiveness and cost/benefit of transport optimization software for pump and treat system optimization. When coupled with a site-specific solute transport model, transport optimization software implements complex mathematical algorithms to determine optimal site-specific well locations and pumping rates. This demonstration project is intended to address the following scientific questions:

1) Do the results obtained from these optimization software packages (e.g. recommended optimal pump and treat scenarios) differ substantially from the optimal solutions determined by traditional "trial-and-error" optimization methods?

2) Do the results obtained from these optimization software packages warrant the additional effort and costs when compared to traditional "trial-and-error" optimization methods?

The project involves the determination of optimal extraction and pumping well scenarios at three Department of Defense (DoD) pump and treat systems. The installations are encouraged (but not required) to implement optimization suggestions resulting from the demonstration.

For each of the three sites, three site-specific optimization problems ("formulations") will be defined. Each of three modeling groups will independently attempt to determine the optimal solution for each of the optimization formulations. Two of the modeling groups will use their own independently developed transport optimization software, and the other group (GeoTrans) will use a traditional "trial-and-error" optimization method. Thus, the optimization recommendations from two separate transport optimization software programs will be compared to each other and to the recommendations from an experimental control.

This report presents the "trial-and-error" results determined by GeoTrans for Site #1, which is the Umatilla Army Depot in Hermiston, Oregon. The three formulations for this site are described in detail in a separate document.

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1.0 OPTIMIZATION TECHNIQUE

GeoTrans applied "trial-and-error" optimization for each of the three formulations. The simulation period consisted of four 5-year management periods (20 years total), beginning January 2003. Each trial-and-error simulation involved modifying pumping wells (locations and rates) and recharge of treated water (represented as injection well locations and rates) in the MODFLOW/MT3D well package. Pumping and recharge could be modified at the beginning of each of the 5-year management periods within a specific simulation.

The general optimization approach utilized by GeoTrans is described below.

Step 1: Program FORTRAN Postprocessor

For each simulation, it was necessary to evaluate the objective function value, to determine if that simulation produced an improved solution relative to previous simulations. For each simulation it was also necessary to determine if all constraints were satisfied. For "trial-and-error" optimization, it was essential that the evaluation of objective function and constraints be done efficiently. Therefore, GeoTrans coded a FORTRAN program to read specific components of model input and output, and then print out the objective function value (broken into individual components) and all constraints that were violated. GeoTrans provided this FORTRAN code to the other modeling groups, to allow those groups to check their solutions (i.e., to make sure they had not made any errors in programming associated with their methods that would invalidate their results).

Step 2: Develop "Animation" approach for RDX and TNT

The purpose of the animations was to clearly illustrate the plume movement over time, for both RDX and TNT, based on simulation results. The animations for each constituent were developed by creating a concentration contour map for model layer 1 at the end of each year in the simulation, using SURFER, and then compiling those into a Microsoft PowerPoint file to allow the plume movement over time to be displayed as an "animation". This was only done for model layer 1 because the components of the optimization formulations only apply to model layer 1 at this site.

Step 3: Modify Pumping/Recharge, Run FORTRAN Code, and Create/Evaluate Animation

This is the classic "trial-and-error" method. After the simulation, the FORTRAN code allowed immediate determination regarding the objective function value, and whether or not the run was feasible (i.e., all constraints satisfied). Based on evaluation of the animations for RDX and TNT, modified pumping/recharge strategies were selected for one or more subsequent simulations, to better address areas of relatively high concentrations and/or areas where cleanup was not progressing fast enough.

2.0 OPTIMIZATION RESULTS

2.1 Current System

2.1.1 Layout of Wells and Recharge Basins for Current System

Pre-remediation concentration distributions for RDX and TNT are illustrated on Figure 2-1. The remedial design configuration for the current system is also shown in Figure 2-1. The current pump-and-treat system has 4 extraction wells installed (EW-1, EW-2, EW-3, and EW-4) and 3 recharge basins (IF1, IF2, and IF3). Wells EW-1, EW-3 and EW-4 have pumps and piping, and are being used to extract groundwater. Well EW-2 is located approximately 100 feet northwest of EW-4 and does not have a pump or any associated piping. Groundwater remediation at the site began with official plant startup on 15 January 1997. The system has operated since that time with the exception of an extended period of shutdown for treatment system adjustment during the first quarter of operation, intermittent power outages, and periodic granular active carbon (GAC) replacement events.

Contaminants (RDX and TNT) are removed in th treatment plant by GAC, and treated water is discharged to the infiltration basins. The current GAC capacity is 1300gpm. The representative extraction rates and recharge rates for the current system, as specified in the model provided by the installation, are listed below (these rates in the model account for 10% system downtime, such that actual rates when pumping are approximately 10% higher).

Well	Recharge Basin	Rate (gpm)
EW-1		128.23
EW-2		0
EW-3		105.05
EW-4		887.24
	IF1	232.80
	IF2	405.27
	IF3	482.40

2.1.2 Cleanup Time and Mass Removal for Current System

Based on the modeling results for the current system, RDX cleanup (2.1 ug/l) in the alluvial aquifer is predicted to take 8 years, and TNT cleanup (2.8 ug/l) in the alluvial aquifer is predicted to take 17 years. These times are based on simulations that begin in January, 2003, which is specified as the initial time for the transport optimization simulations.

Formulation 3 is based on minimizing the combined mass of RDX and TNT remaining in model layer 1 after 20 years, starting in January 2003. Based on the modeling results for the current system, the remaining mass of RDX and TNT in layer 1, after 20 years, is as follows:

	Time = 20 yrs
RDX Mass (kg)	0.204
TNT Mass (kg)	1.561
Total Mass (kg)	1.765

A plot of mass versus time, for the current system, is included as Figure 2-2.

2.1.3 Costs for Current System

For formulations 1 and 2, a cost function to be minimized was developed (in conjunction with the installation) that combines the "Up-Front Costs" with the "Total of Annual Costs" over the time it takes to reach cleanup for both RDX and TNT, assuming a discount rate of 5%. The components of cost are:

MINIMIZE (CCW + CCB + CCG + FCL + FCE + VCE + VCG + VCS)

where

CCW: Capital costs of new wells
CCB: Capital costs of new recharge basins
CCG: Capital cost of new GAC unit (formulation 2 only)
FCL: Fixed cost of labor
FCE: Fixed costs of electricity (lighting, heating, etc.)
VCE: Variable electrical costs of operating wells
VCG: Variable costs of changing GAC units
VCS: Variable cost of sampling

The specifics of the cost function are provided in the detailed problem formulation (separate document). All costs are in thousands of dollars.

Based on the modeling results, the value of the cost function for the current system (over the 17 years until both RDX and TNT are cleaned up) is 3836.285 (i.e., $3.836 million).

2.2 Formulation 1: Minimize Cost to Cleanup, Current Plant Capacity

2.2.1 Objective Function and Constraints

The objective function is to minimize the cost function over the time until cleanup levels are achieved for both RDX and TNT (see Section 2.1.3), subject to the following constraints:

- The modeling period consists of four 5-year management periods (20 years total) beginning January 2003;

- Modifications to the system may only occur at the beginning of each management period;
- Cleanup, for both RDX and TNT, must be achieved within modeling period (by the end of year 20);
- The total modeled pumping rate, when adjusted for the average amount of uptime, cannot exceed 1300gpm, the current maximum treatment capacity of the plant;
- The extraction system must account for limits imposed by the hydrogeology of the site (limit of 400 gpm or 1000 gpm, depending on location, adjusted for system downtime);
- RDX and TNT concentration levels must not exceed their respective cleanup levels in locations beyond a specified area;
- The total pumping rate and total recharge rate have to be balanced.

The specifics of the cost function are provided in the detailed problem formulation (separate document).

2.2.2 Optimal Solution

A total of 39 simulations were performed by GeoTrans for Formulation 1. The best solution was found in simulation 28, and has the following details:

	Current System	Optimal Solution
RDX Cleanup	8 yrs	6 yrs
TNT Cleanup	17 yrs	6 yrs
Objective Function (Total)	$3,836,285	$2,230,905
Objective Function (Components)		
CCW: Capital costs of new wells	$0	$133,764
CCB: Capital costs of new recharge basins	$0	$19,588
CCG: Capital cost of new GAC unit	$0	$0
FCL: Fixed cost of labor	$2,805,552	$1,263,086
FCE: Fixed costs of electricity	$42,616	$19,186
VCE: Variable electrical costs of operating wells	$251,405	$91,952
VCG: Variable costs of changing GAC units	$16,338	$14,301
VCS: Variable cost of sampling	$720,374	$689,028

Two new wells and one recharge basin are included in the optimal solution. Extraction rates and recharge rates are listed below:

Well or Recharge Basin	New or Existing	Current System (gpm)	Optimal Solution Period 1 (gpm)	Optimal Solution Period 2 (gpm)
EW-1	Existing	128.23	280	350
EW-2	Existing	0	0	0
EW-3	Existing	105.05	0	360
EW-4	Existing	887.24	660	0
NW-1	New		0	100
NW-2	New		230	360
Total Extraction		**1120.52**	**1170**	**1170**
IF1	Existing	232.80	282.33	585
IF2	Existing	405.27	405.27	0
IF3	Existing	482.40	482.40	0
RCH4	New		0	585
Total Injection		**1120.47**	**1170**	**1170**

Locations of wells and recharge basins are presented in Figure 2-3. A chart illustrating objective function value versus simulation number is provided in Figure 2-4. Note that the optimal solution (simulation 28) is only about 10 percent better than the solution found in simulations 2, 3, and 4. A chart illustrating mass remaining after each year is provided in Figure 2-5.

2.2.3 General Approach to Determining the Optimal Solution

It was evident from the cost function that total cost could be reduced substantially by shortening the cleanup horizon (which is also a component of the objective function that can be easily attacked via trial-and-error). The current system had a cleanup time of 8 years for RDX and 17 years for TNT. Therefore, the focus by GeoTrans was to reduce the total cleanup time. The general approach to finding the optimal solution via trial-and-error can be summarized as follows:

Simulations 1-4

Since RDX was largely cleaned up after Period 1, pumping was accelerated within the TNT plume starting in Period 2. By the end of 4 simulations, total cleanup time was reduced to 7 years (6 years for RDX, 7 years for TNT).

Simulations 5-7

The goal of these simulations was to accelerate RDX cleanup to 5 years or less, by adding new recharge basins. TNT cleanup was not a focus of these runs. By the end of simulation 7, RDX cleanup within 5 years was achieved.

Simulations 8-17

Combine the RDX strategy from simulations 5-7 with the TNT strategy from simulations 1-4. By simulation 17, solutions were achieved with RDX cleanup of 5 years and TNT cleanup of 8 years.

Simulations 18-19

Increase pumping within TNT plume in Period 1, with corresponding reduction in pumping beyond TNT plume. By the end of simulation 19, cleanup time was again reduced to 7 years (6 years for RDX, 7 years for TNT).

Simulations 20-22

Add new well locations at various locations within the TNT plume, in attempt to reduce TNT cleanup to 6 years or less. By the end of simulation 22, cleanup time was still 7 years (6 years for RDX, 7 years for TNT).

Simulations 23-28 (***Optimal Solution, Simulation 28***)

In addition to new wells in TNT plume, shift additional pumping from RDX plume (EW-4) to within TNT plume, in attempt to reduce TNT cleanup to 6 years or less. By the end of simulation 28, cleanup time was reduced to 6 years (6 years for RDX, 6 years for TNT). This was the best solution found by GeoTrans. No attempt was made to optimize the individual components of the objective function, because GeoTrans felt that the most significant management variable was cleanup time and variations in other components of the cost function would be minor.

Simulations 29-39

Attempt to find reduced cleanup time by adding recharge basins in center of TNT plume (dilution) and extraction wells at edge of TNT plume. However, this tended to cause unintended spreading of the TNT and/or RDX plume, and no improved solutions were found.

2.3 Formulation 2: Minimize Cost to Cleanup, Increased Plant Capacity Allowed

2.3.1 Objective Function and Constraints

The objective function is to minimize the cost function over the time until cleanup levels are achieved for both RDX and TNT (see Section 2.1.3), subject to the same constraints as Formulation 1, except that treatment plant capacity could be increased in steps of 325 gpm, from the current capacity of 1300 gpm to a maximum capacity of 1950 gpm.

2.3.2 Optimal Solution

A total of 25 simulations were performed by GeoTrans for Formulation 2. The best solution was found in simulation 25, and has the following details:

	Current System	Optimal Solution
RDX Cleanup	8 yrs	4 yrs
TNT Cleanup	17 yrs	4 yrs
Objective Function (Total)	$3,836,285	$2,015,909
Objective Function (Components) CCW: Capital costs of new wells CCB: Capital costs of new recharge basins CCG: Capital cost of new GAC unit FCL: Fixed cost of labor FCE: Fixed costs of electricity VCE: Variable electrical costs of operating wells VCG: Variable costs of changing GAC units VCS: Variable cost of sampling	 $0 $0 $0 $2,805,552 $42,616 $251,405 $16,338 $720,374	 $150,000 $0 $300,000 $882,410 $13,404 $98,329 $13,279 $558,487

Two new wells are included in the optimal solution (no new recharge basins are included). Extraction rates and recharge rates are listed below:

Well or Recharge Basin	New or Existing	Current System (gpm)	Optimal Solution (gpm)
EW-1	Existing	128.23	305
EW-2	Existing	0	0
EW-3	Existing	105.05	360
EW-4	Existing	887.24	774.565
NW-1	New		190.435
NW-2	New		125
Total Extraction		**1120.52**	**1755**
IF1	Existing	232.80	715
IF2	Existing	405.27	520
IF3	Existing	482.40	520
Total Injection		**1120.47**	**1755**

Locations of wells and recharge basins are presented in Figure 2-6. A chart illustrating objective function value versus simulation number is provided in Figure 2-7. Note that the optimal solution (simulation 25) is only about 10 percent better than the solution found in simulation 3. A chart illustrating mass remaining after each year is provided in Figure 2-8.

2.3.3 General Approach to Determining the Optimal Solution

The general approach was to increase pumping according to the increased capacity allowed, in an attempt to lower cleanup time to either 5 or 4 years (since 6 years had been achieved with Formulation 1).

Simulations 1-2

Increase pumping of three existing wells to their full individual capacities (each run had different distribution of recharge). Achieved cleanup time of 7 years (5 years for RDX and 7 years for TNT).

Simulation 3

Additionally add a new well in TNT plume, to reach full capacity of new plant. Achieved cleanup time of 5 years (5 years for RDX and 5 years for TNT).

Simulation 4

Same as Simulation 3, but attempt to speed TNT cleanup with new recharge basin at southern edge of TNT plume. Achieved cleanup time of 6 years (6 years for RDX and 5 years for TNT).

Simulations 5-6

Attempt to get cleanup in 5 years with only one new GAC unit (i.e., capacity only increased to 1625 gpm rather than 1950 gpm). Achieved cleanup time of 6 years (6 years for RDX and 6 years for TNT).

Simulations 7-23

Starting from Simulation 2, try various combinations of pumping/recharge, including addition of a second new well in TNT plume, in attempt to reduce cleanup time to 4 years. Achieved cleanup time of 5 years (4 years for RDX and 5 years for TNT).

Simulation 24

Add a new recharge basin closer to TNT plume to try to reduce TNT cleanup to 4 years. Achieved cleanup time of 5 years (5 years for RDX and 5 years for TNT).

Simulation 25 (***Optimal Solution, Simulation 25***)

Noticed that Simulation 20 was 1 gpm below capacity. Added the 1 gpm to NW-1 inside the TNT plume. Achieved cleanup time of 4 years (4 years for RDX and 4 years for TNT). Decided going after cleanup time of 3 years was not worth the effort (could not be accomplished). No attempt was made to optimize the individual components of the objective function, because GeoTrans felt that the most significant management variable was cleanup time and variations in other components of the cost function would be minor.

2.4 Formulation 3: Minimize Combined Mass of RDX and TNT Remaining After 20 Years

2.4.1 Objective Function and Constraints

The objective function is to minimize the total mass remaining (RDX plus TNT) in layer 1 at the end of 20 years. The constraints are the same as Formulation 1, except the maximum number of new wells cannot exceed 4, and the maximum number of new recharge basins cannot exceed 3.

2.4.2 Optimal Solution

A total of 24 simulations were performed by GeoTrans for Formulation 3. The best solution was found in simulation 9, and has the following details:

	Current System	Optimal Solution
Total Mass Remaining After 20 Years	RDX: 0.204 kg TNT: 1.561 kg Total: 1.765 kg	RDX: 0.231 kg TNT: 0.145 kg Total: 0.376 kg
RDX Cleanup	8 yrs	7 yrs
TNT Cleanup	17 yrs	7 yrs

Two new wells are included in the optimal solution (no new recharge basins are included). Extraction rates and recharge rates are listed below:

Well or Recharge Basin	New or Existing	Current System (gpm)	Optimal Solution Period 1 (gpm)	Optimal Solution Period 2 (gpm)	Optimal Solution Period 3 (gpm)	Optimal Solution Period 4 (gpm)
EW-1	Existing	128.23	110	0	0	0
EW-2	Existing	0	0	0	0	0
EW-3	Existing	105.05	0	210	210	210
EW-4	Existing	887.24	600	600	600	600
NW-1	New		360	0	0	0
NW-2	New		100	360	360	360
Total Extraction		**1120.52**	**1170**	**1170**	**1170**	**1170**
IF1	Existing	232.80	282.33	282.33	282.33	282.33
IF2	Existing	405.27	405.27	405.27	405.27	405.27
IF3	Existing	482.40	482.40	482.40	482.40	482.40
Total Injection		**1120.47**	**1170**	**1170**	**1170**	**1170**

Locations of wells and recharge basins are presented in Figure 2-9. A chart illustrating objective function value versus simulation number is provided in Figure 2-10. A chart illustrating mass remaining after each year is provided in Figure 2-11.

On Figure 2-10, two different "optimal solutions" are actually indicated. Simulation 23 actually has a slightly better objective function value than Simulation 9 (0.332 kg versus 0.376 kg), but was considered sub-optimal by GeoTrans because it required 4 new wells (as opposed to two), and two of the locations are in the bottom right corner of the modeled area and do not make sense with respect to future implementation..

2.4.3 General Approach to Determining the Optimal Solution

Simulation 1

Start with the optimal solution for Formulation 1 in stress period 1, keep same pumping for the entire 20 year simulation. That achieves total mass remaining of 0.645 kg.

Simulations 2-5

Try different combinations of pumping to lower mass remaining. Achieved total mass remaining of 0.465 kg.

Simulations 6-7

Add several new recharge basins at edge of RDX plume, makes objective function worse.

Simulation 8

Similar to Simulations 2-5, but add 2 extraction wells within RDX plume. Achieved total mass remaining of 0.466 kg.

Simulation 9 (***Optimal Solution, Simulation 9***)

Similar to Simulation 4, but slightly different combination of pumping rates. Achieved total mass remaining of 0.376 kg.

Simulations 10-16

Attempt various combinations of new wells and/or recharge basins, and varying combinations of rates. No improvement achieved.

Simulations 17-24

Add 2 new wells in lower right corner of active area where mass is determined. It was noted that some mass was accumulating there in the model, apparently moving up from layers 2 and 3. All of these solutions represented mathematical improvements (0.332 kg to 0.371 kg), but GeoTrans considers these sub-optimal because they include two extra wells, and do not make sense with respect to potential implementation.

3.0 COMPUTATIONAL PERFORMANCE

Preliminary Items

Development of the three formulations, and development of the FORTRAN postprocessing code, were considered separate tasks from the actual solution of the problems, and are not described herein (since each of the other optimization groups started after the formulations and FORTRAN postprocessor were provided to them). However, those costs should be accounted for when evaluating the cost of the overall optimization process.

Solution of the Three Formulations

GeoTrans worked within a pre-specified budget of approximately $32,000 for developing optimal solutions for each of the three formulations. Development of the SURFER/PowerPoint animation technique accounted for approximately $2000 of this $32,000, and the remaining $30,000 went towards solving the problems.

Each flow and transport simulation required approximately 10 minutes on a Pentium III, 500 MHZ computer. Running the FORTRAN code required less than one minute. Creating the SURFER grid files, contour maps, and subsequent animations required approximately 1 hour per simulation. The remaining time was spent reviewing the results, deciding what modifications to make to pumping/recharge, and modifying the well package for the subsequent run.

GeoTrans ultimately made 88 simulations, as follows:

formulation 1: 39 simulations
formulation 2: 25 simulations
formulation 3: 24 simulations

Based on a cost of approximately $30,000 allocated towards solving the problems, this represents a cost of approximately $340 per simulation. That represents approximately 3.5 hours for project level staff (Yan Zhang) and approximately 1 hour for senior level staff (Rob Greenwald) for each simulation, associated with setting up, running, and postprocessing the simulation, and determining what to implement for the subsequent simulation.

As noted in Section 2, solutions nearly as good as the optimal solutions were generally found within just a few simulations. For example, for Formulation 1 the optimal simulation (Simulation 28) was only about 10% better than Simulations 2-4, and for Formulation 2 the optimal simulation (Simulation 25) was only about 10% better than Simulations 3. The major difference between these early simulations, versus the optimal simulation, was achieving a cleanup time one year lower. This represents a somewhat artificial “step function” that in real world terms is probably not significant (i.e., cleanup in 5.9999 years results in costs incurred for six years in the objective function, whereas cleanup in 6.0001 years results in costs incurred for 7 years in the objective function).

GeoTrans would not have performed as many trial-and-error simulations if work was not being performed within the context of this project. GeoTrans would have also recommended revising Formulation #3 prior to performing the simulations, if not performed in the context of this project.

4.0 SITE SPECIFIC INFORMATION

The following observations pertain to aspects of this particular site and/or problem statement that GeoTrans feels may not be true of all sites where transport optimization may be attempted.

<u>One Model Layer</u>

The objective function and constraints only applied to one model layer (layer 1). This simplified the problem significantly, and made the trial-and-error process much more simple to perform. Firstly, the graphics and animation procedures employed as part of the trial-and-error approach were easier to generate and evaluate because they were limited to one model layer. Secondly, there were no multi-aquifer wells, which simplified the logistics of specifying well rates. Thirdly, the number of possible alternatives to consider was limited because all extraction and recharge was specified in only one model layer.

<u>Limited Management Periods Required For Formulations 1 and 2</u>

Although the formulation allowed up to four 5-year management period, the solutions for Formulations 1 and 2 quickly indicated cleanup within the first two management periods. This limited the potential number of trial-and-error alternatives to consider.

<u>No continuing Source in the Model</u>

The sources of contamination were assumed to no longer exist in the model. This allowed solution of problems based on achieving cleanup levels (Formulations 1 and 2). Formulations based on cleanup time may not be feasible when continuing sources above cleanup levels are assumed in the model.

<u>Formulations Fixed at the Beginning of the Simulation Period</u>

For this project, the three formulations had to be "locked in" prior to the simulation period. This is not typical for optimization projects. In most cases it would be beneficial to start with one formulation, and based on those results develop different formulations. For instance, after determining in Formulations 1 and 2 that cleanup could be obtained in less than 10 years, the objective function for Formulation 3 (minimize mass remaining after 20 years) seems inappropriate, since pumping for a 20-year time horizon seems unnecessary.

5.0 SENSITIVITY ANALYSIS (IF PERFORMED)

Sensitivity analysis, as it relates to optimization, refers to the extent to which the optimal solution changes with respect to specific changes in the optimization formulation. GeoTrans did not attempt to solve any problems other than the three that were specified. Therefore, sensitivity analysis was not performed. The “trial-and-error” methodology is poorly suited for performing that type of sensitivity analysis, because the solution method is not automated.

6.0 SUMMARY AND LESSONS LEARNED

The trial-and-error approach yielded improved solutions relative to the current system. All three optimal solutions represent reductions in cleanup time (4-7 years) relative to the simulation of the current system (17 years). However, comparison to the current system is somewhat unfair, since the current system was not designed based on any of these three formulations, nor was it based on the specific flow/transport model used for this project (i.e., the model had been updated subsequent to system installation).

More significantly, the trial-and-error approach was rigorously applied, and therefore represents a good baseline for evaluating the benefits of mathematical optimization performed by the other two modeling groups.

The trial-and-error simulations were performed at a cost of approximately $340 per simulation (associated with setting up, running, postprocessing the simulation, and determining what to implement for the subsequent simulation). The trial-and-error approach was limited to only dozens of simulations per formulation, and therefore could only explore a small portion of the potential number of pumping/recharge alternatives. This limitation of trial-and-error may have been even more severe if more than one model layer was involved in the objective function and constraints, and/or solutions to Formulations 1 and 2 were not limited to only one or two of the four potential management periods.

Solutions nearly as good as the optimal solutions were generally found within just a few simulations. For example, for Formulation 1 the optimal simulation (Simulation 28) was only about 10% better than Simulations 2-4, and for Formulation 2 the optimal simulation (Simulation 25) was only about 10% better than Simulations 3. The major difference between these early simulations, versus the optimal simulation, was achieving a cleanup time one year lower. This represents a somewhat artificial “step function” that in real world terms is probably not significant. Also, GeoTrans would not have performed as many trial-and-error simulations if work was not being performed within the context of this project (i.e., total simulations cost of $30,000 would have been lower).

GeoTrans does not believe Formulation 3 is useful to the installation. Pumping for 20 years is unlikely, based on results of the other formulations (which showed cleanup in 6 years or less). Also, most of the mass in model layer 1 is gone after 20 years in all simulations (most simulations had mass of 0.3 to 0.5 kg remaining after 20 years), and it is unclear that there is any tangible difference between any of these results from a management perspective. It would have been more useful to revise Formulation 3 to something like “minimize timeframe to reach a specified amount of remaining mass”, rather than fixing the time horizon to 20 years.

Figure 2-1 System Configuration with Pre-Pumping RDX and TNT Plumes

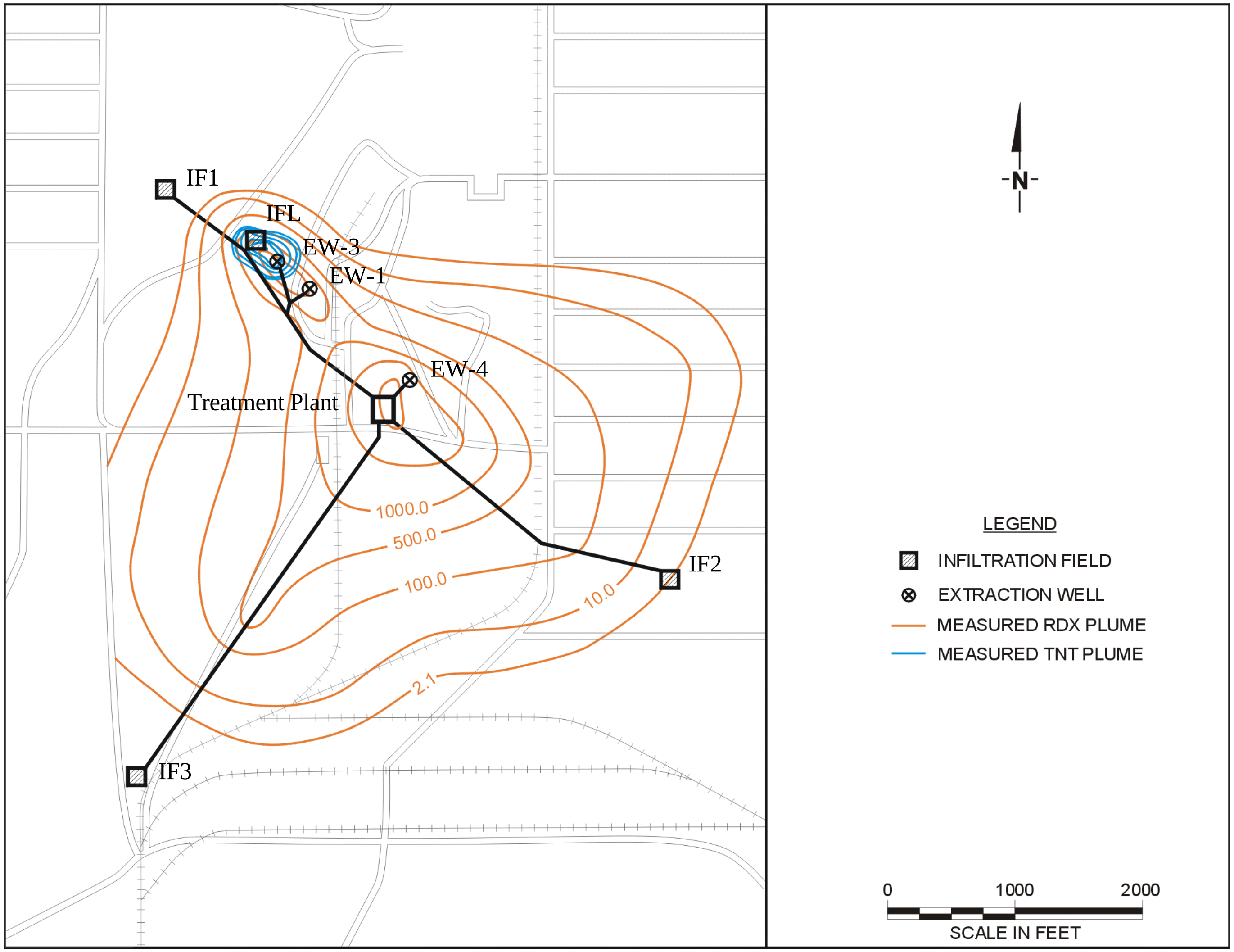


Figure 2-2 Plume Mass versus Time, Current System

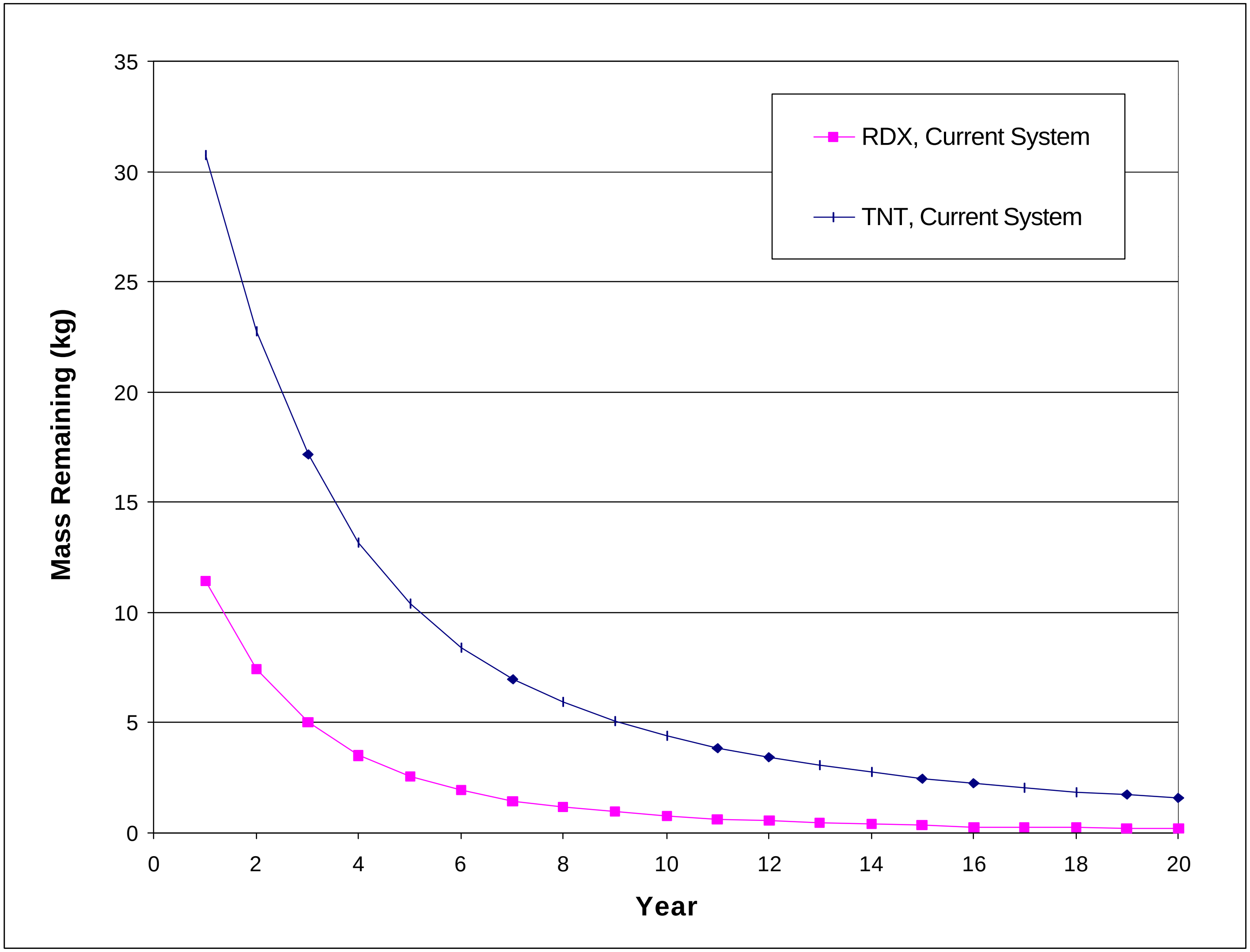


Figure 2-3   Locations of Wells and Recharge Basins, Formulation #1

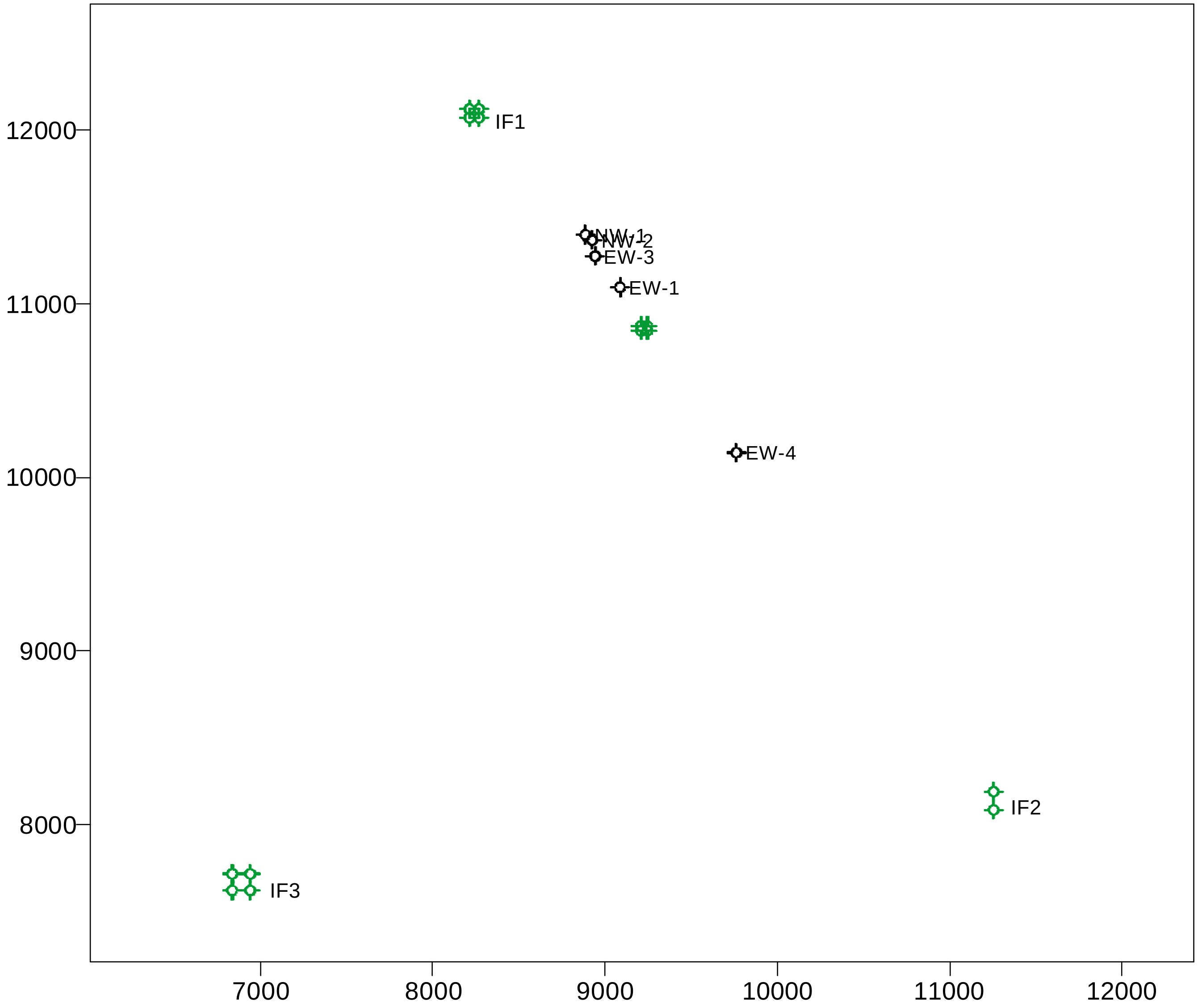


Figure 2-4   Objective Function Value, Formulation #1

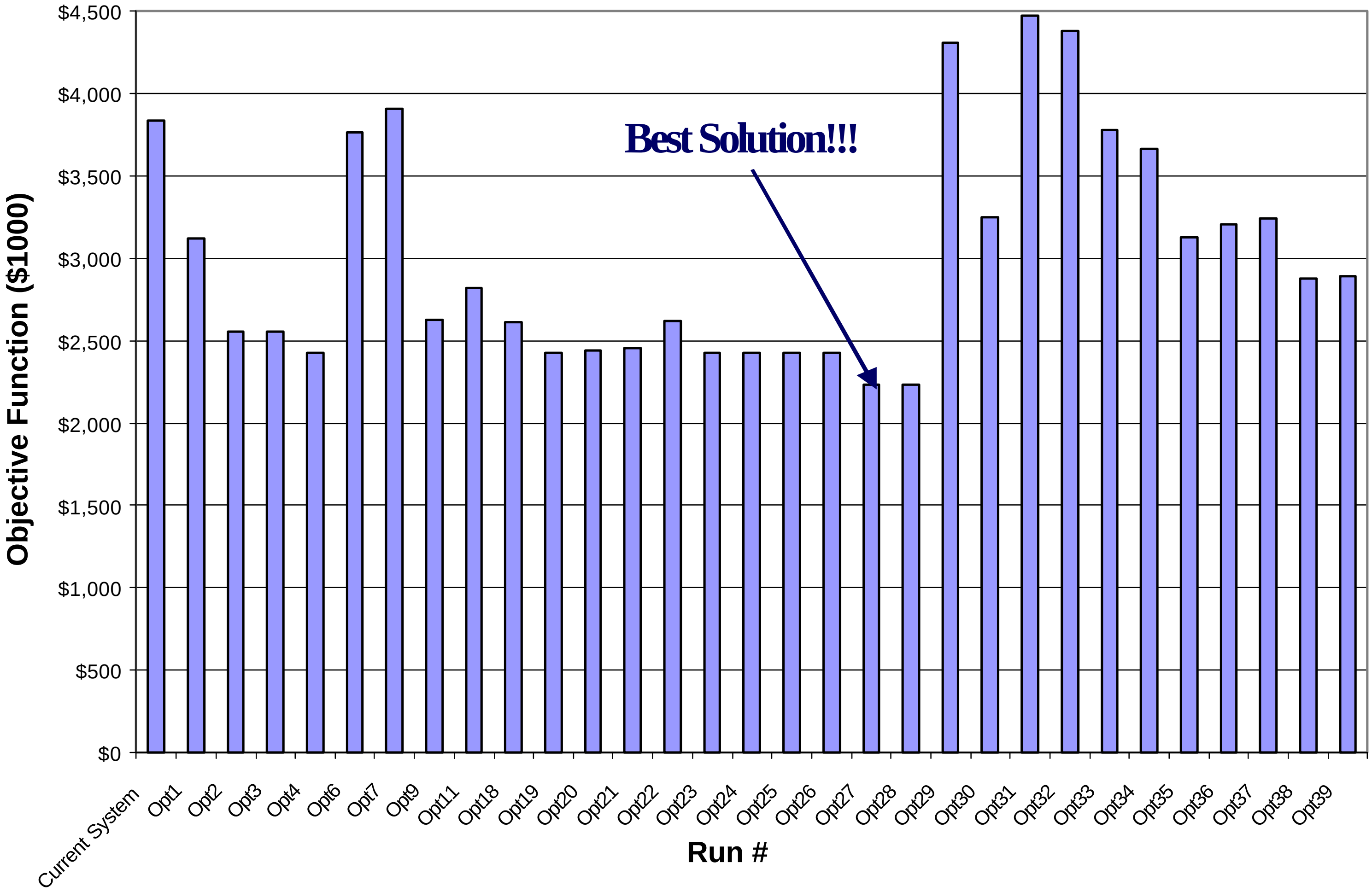


Figure 2-5 Mass Remaining in Layer 1, Current System vs. Formulation #1

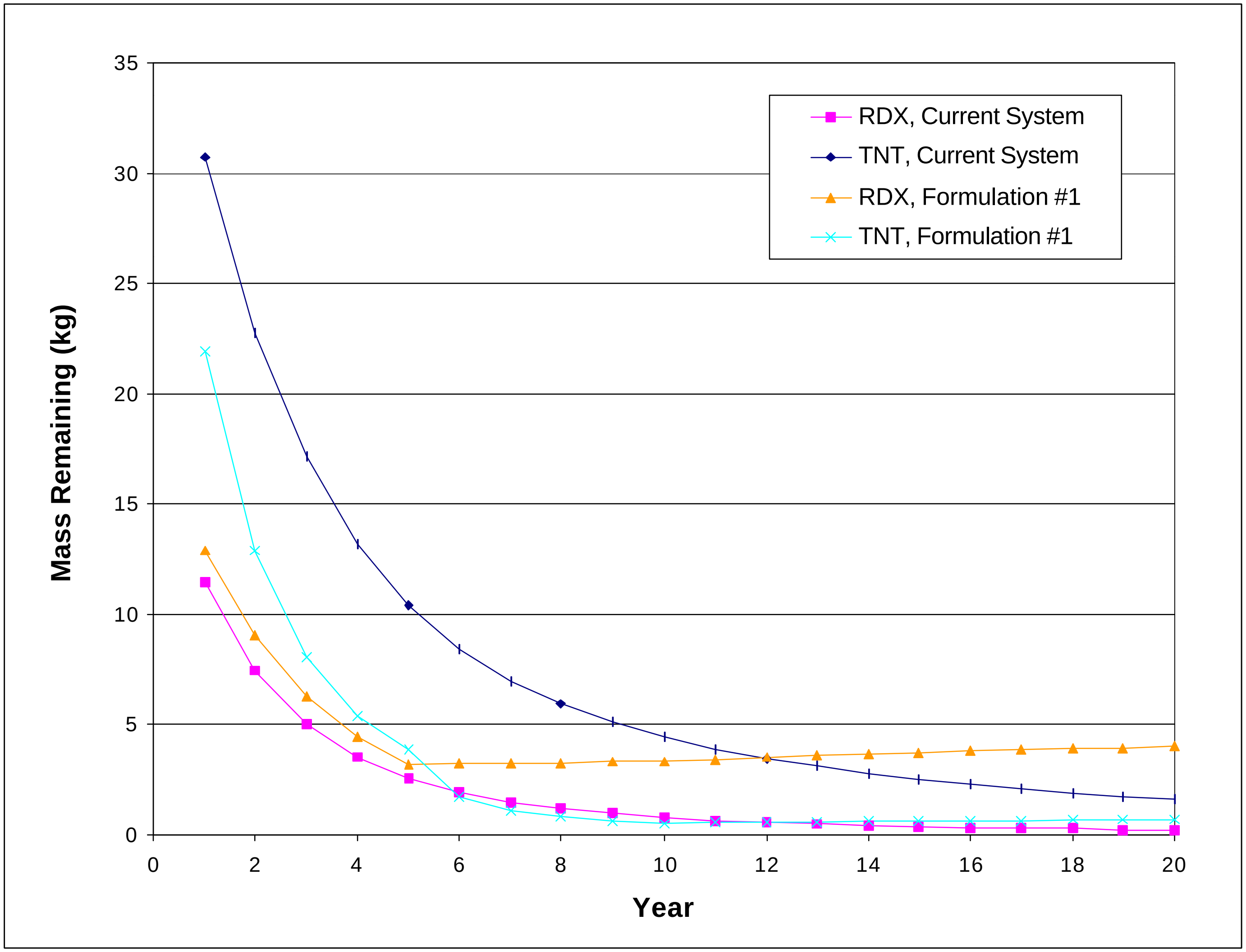


Figure 2-6   Location of Wells and Recharge Basins, Formulation #2

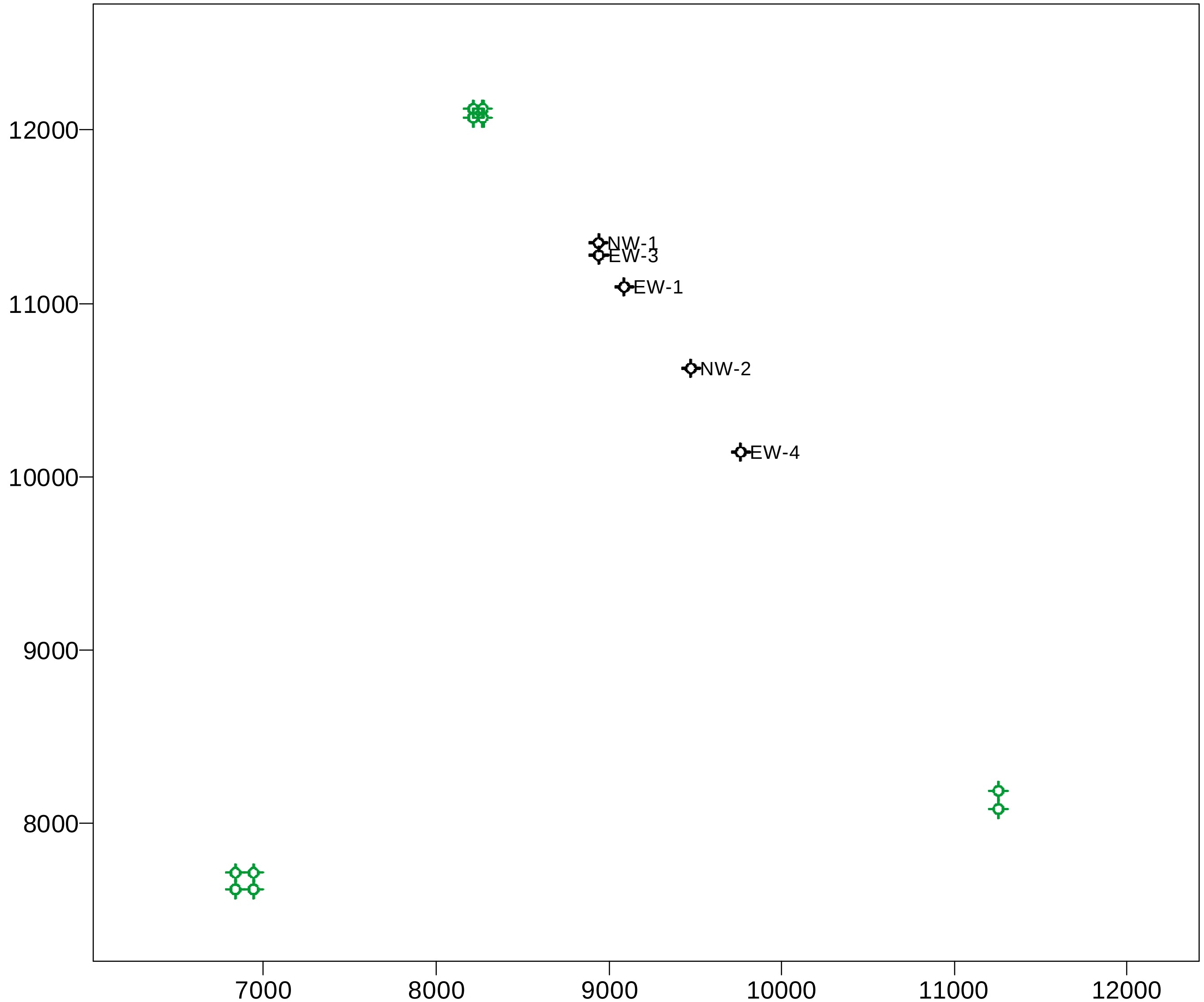


Figure 2-7 Objective Function Value, Formulation #2

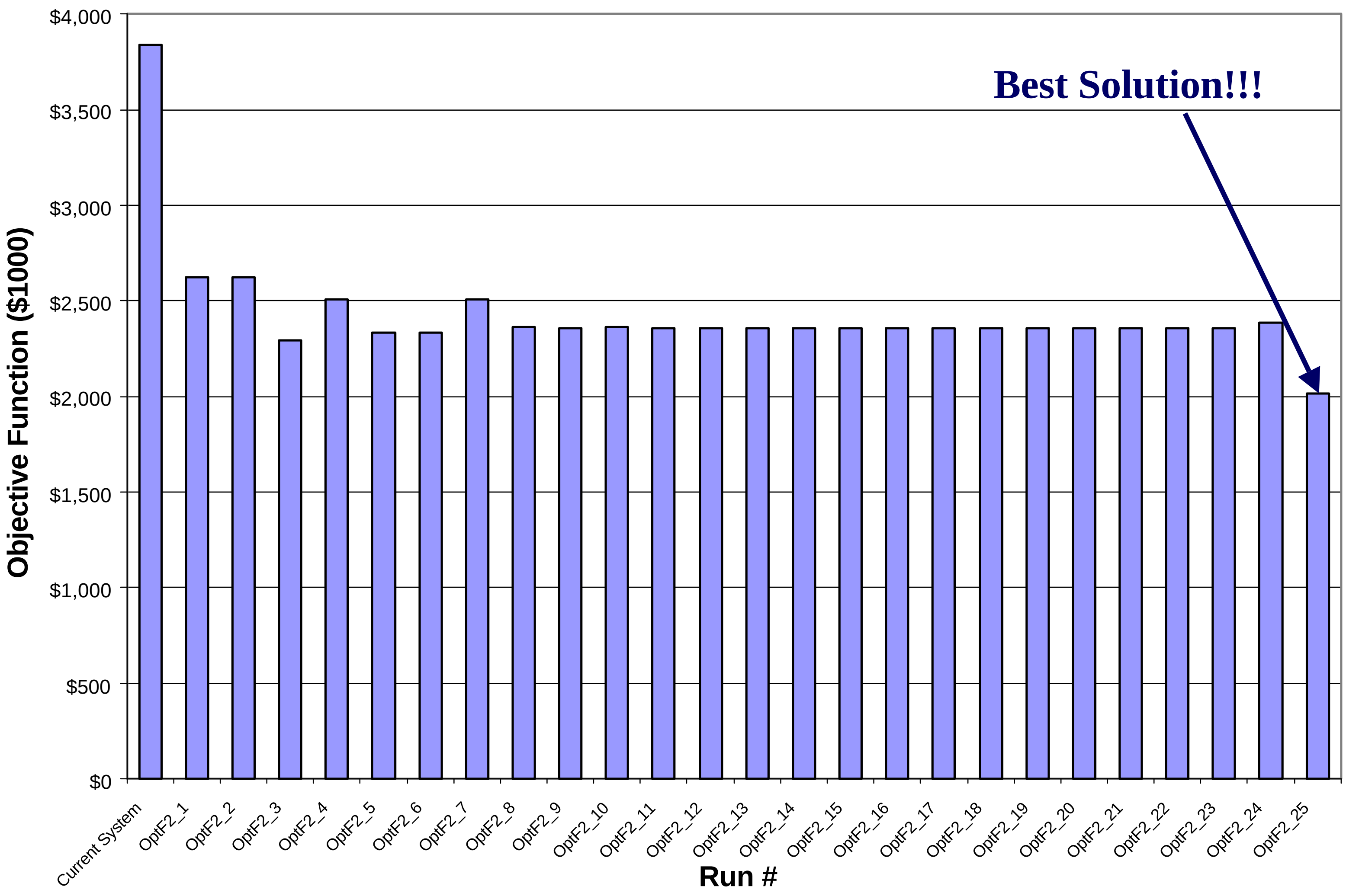


Figure 2-8 Mass Remaining in Layer 1, Current System vs. Formulation #2

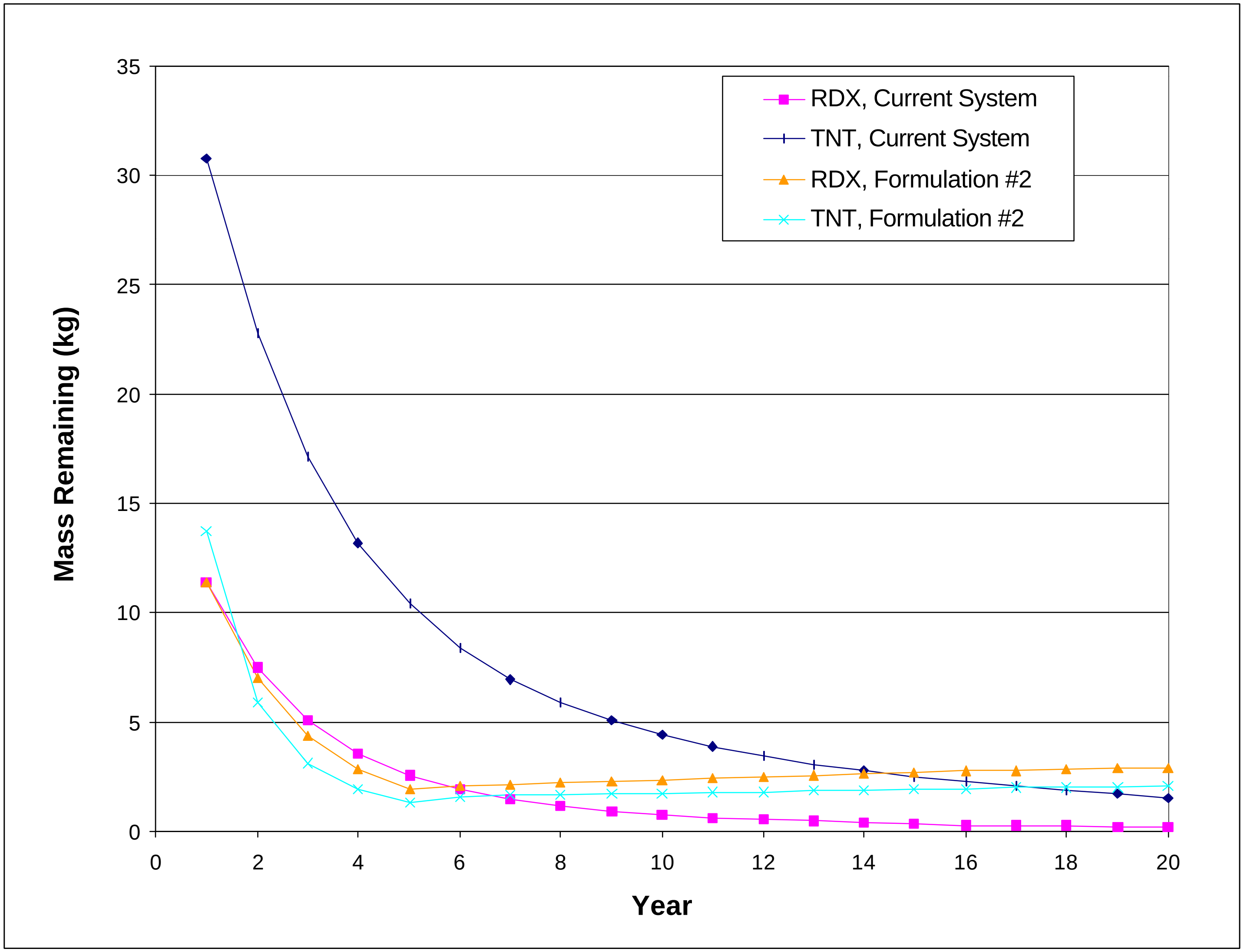


Figure 2-9 Locations of Wells and Recharge Basins, Formulation #3

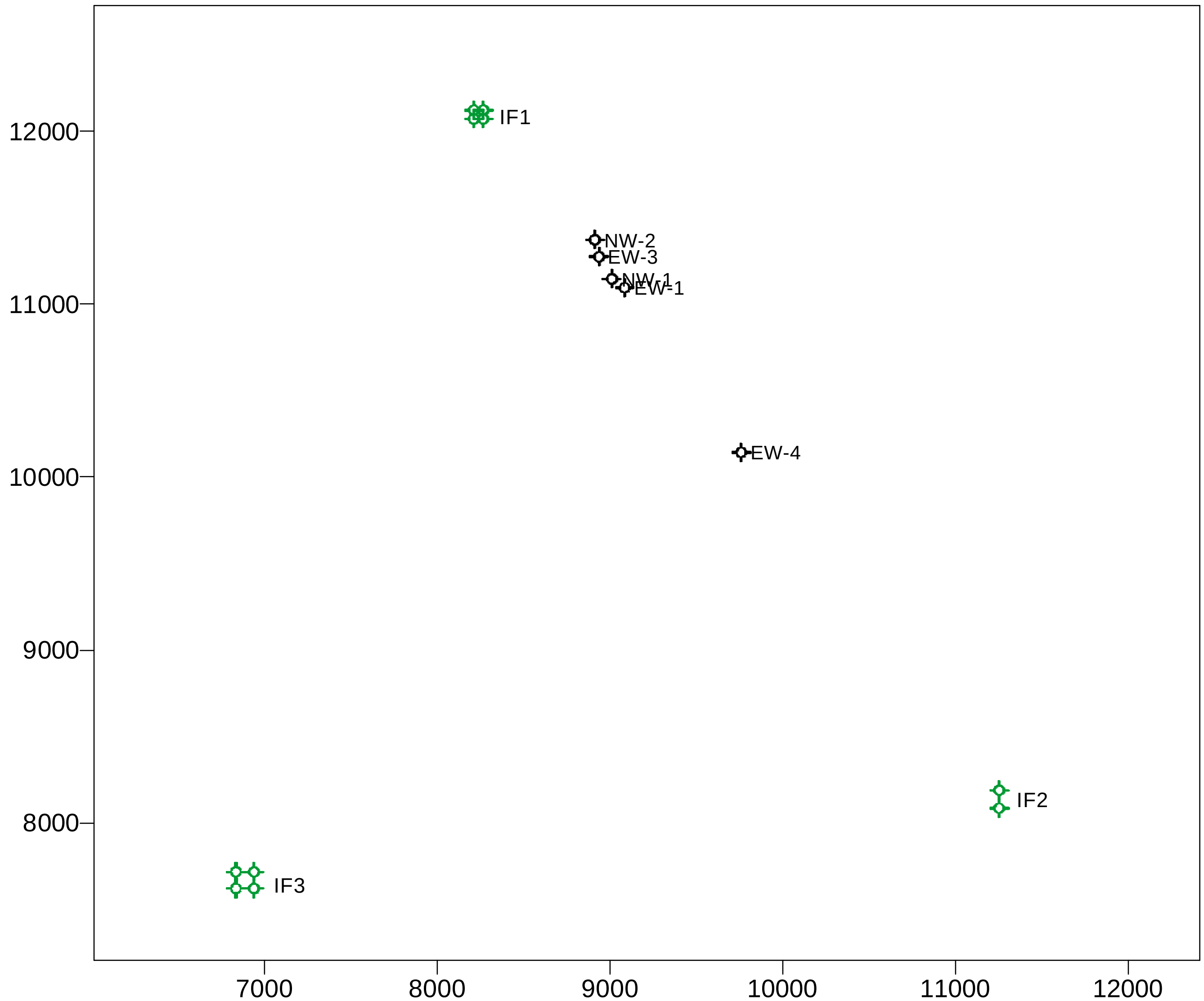


Figure 2-10   Objective Function Value, Formulation #3

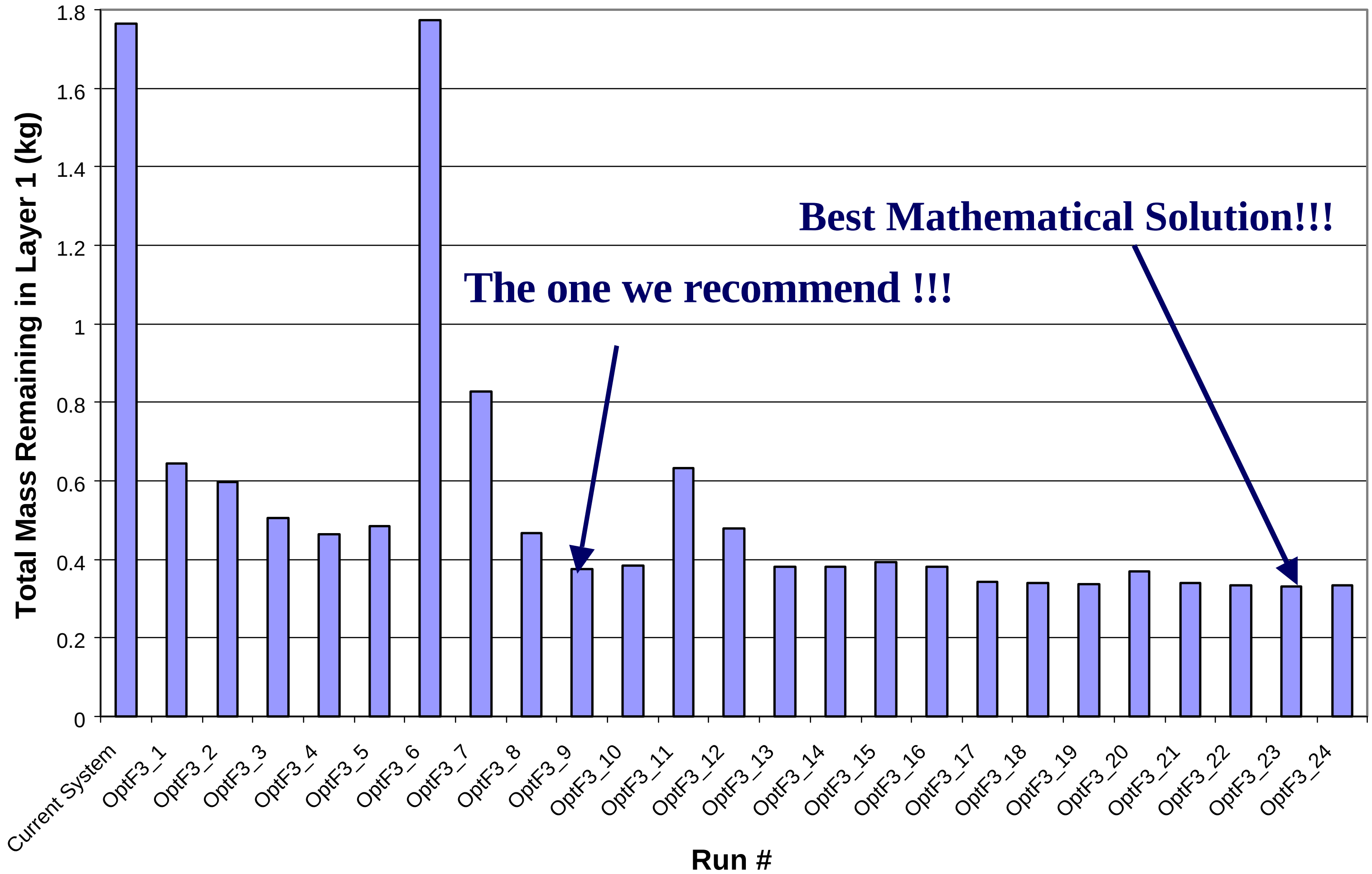
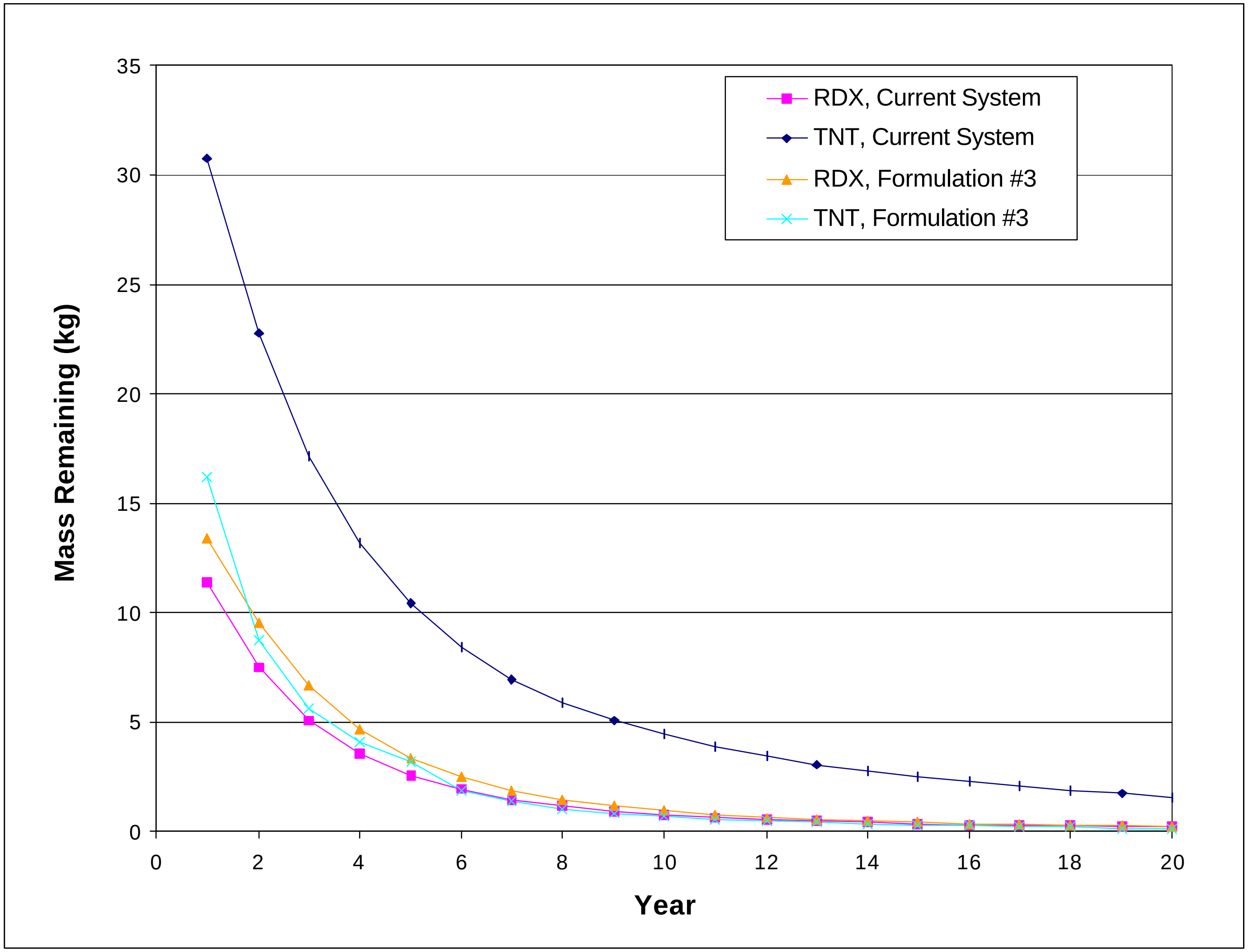


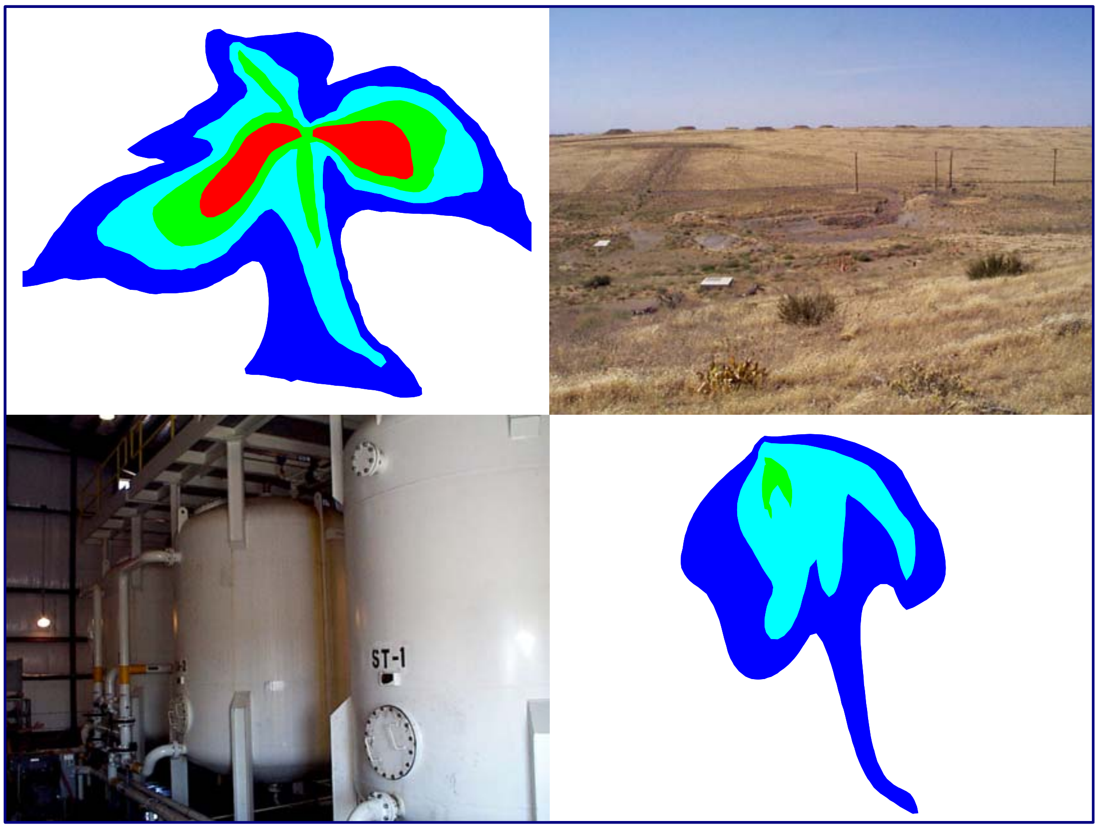
Figure 2-11 Mass Remaining in Layer 1, Current System vs. Formulation #3



UA Report on Umatilla

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

Chunmiao Zheng and Patrick Wang
The University of Alabama



The Hydrogeology Group
The University of Alabama

Technical Report
October 2001
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The University of Alabama

Prepared for
Naval Facilities Engineering Service Center
Port Hueneme, California
and
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Washington, DC

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.

1

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.

2

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.

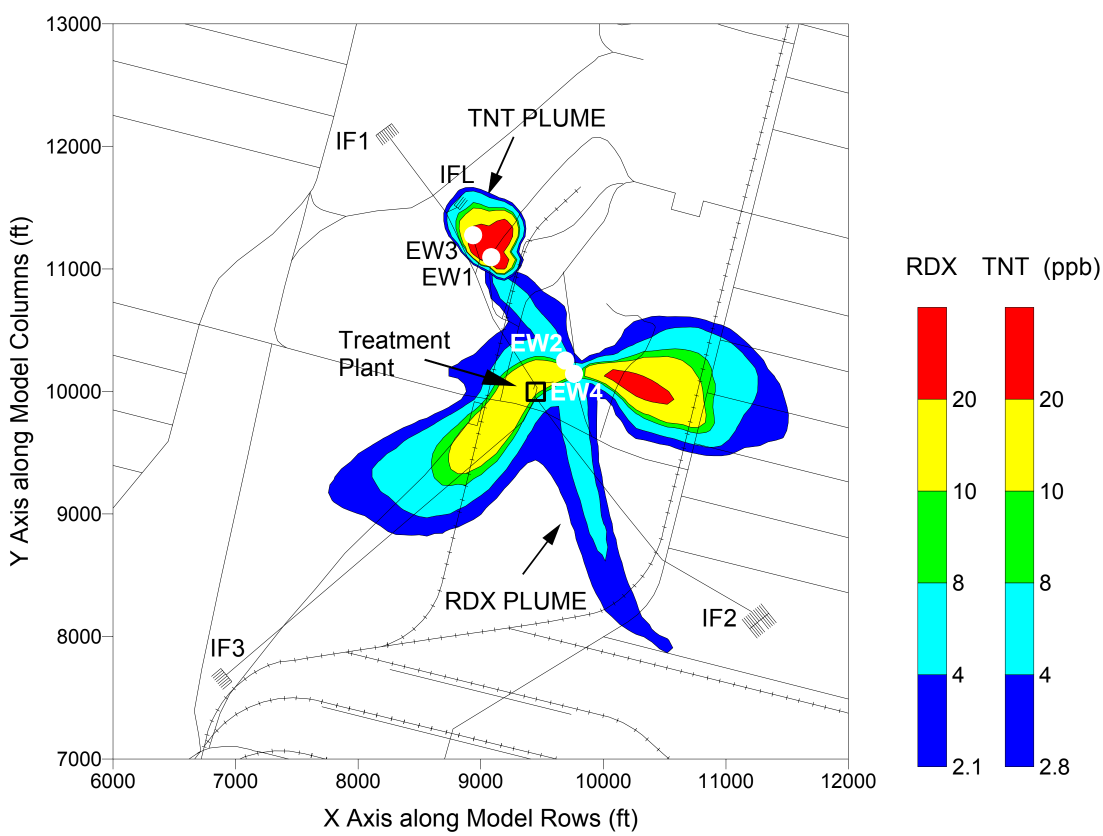


Figure 3.1. Simulated RDX and TNT plumes in the shallow aquifer at the end of year 2002 under the existing pump-and-treat system on Umatilla Army Depot, Oregon. The existing pump-and-treat system consists of three extraction wells (EW1, EW3, and EW4) and three infiltration basins (IF1, IF2, and IF3). 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:

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

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:

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

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:

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

(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:

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

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):

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

(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.

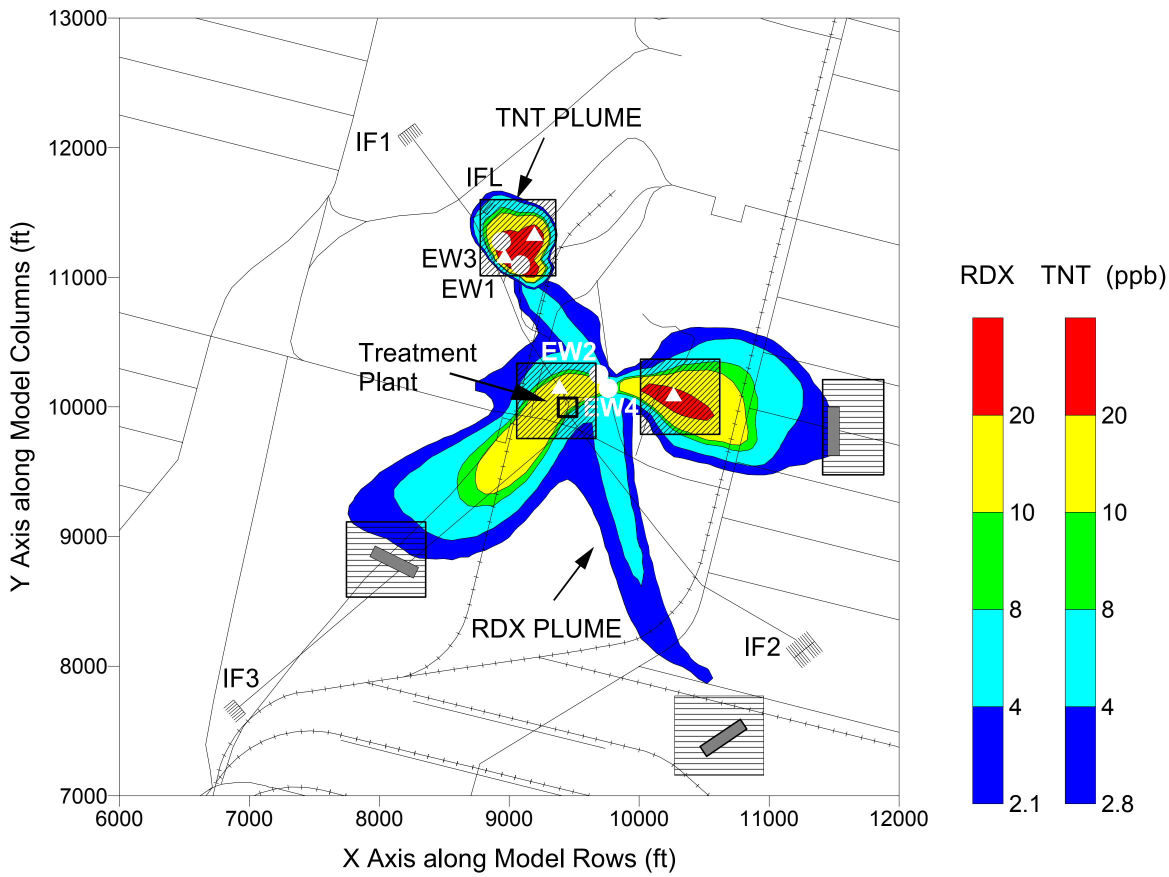


Figure 3.2. Potential new wells (shown as triangles) and new infiltration basins (shown as solid blocks) along with their respective candidate locations defined by the rectangles with line patterns.

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.

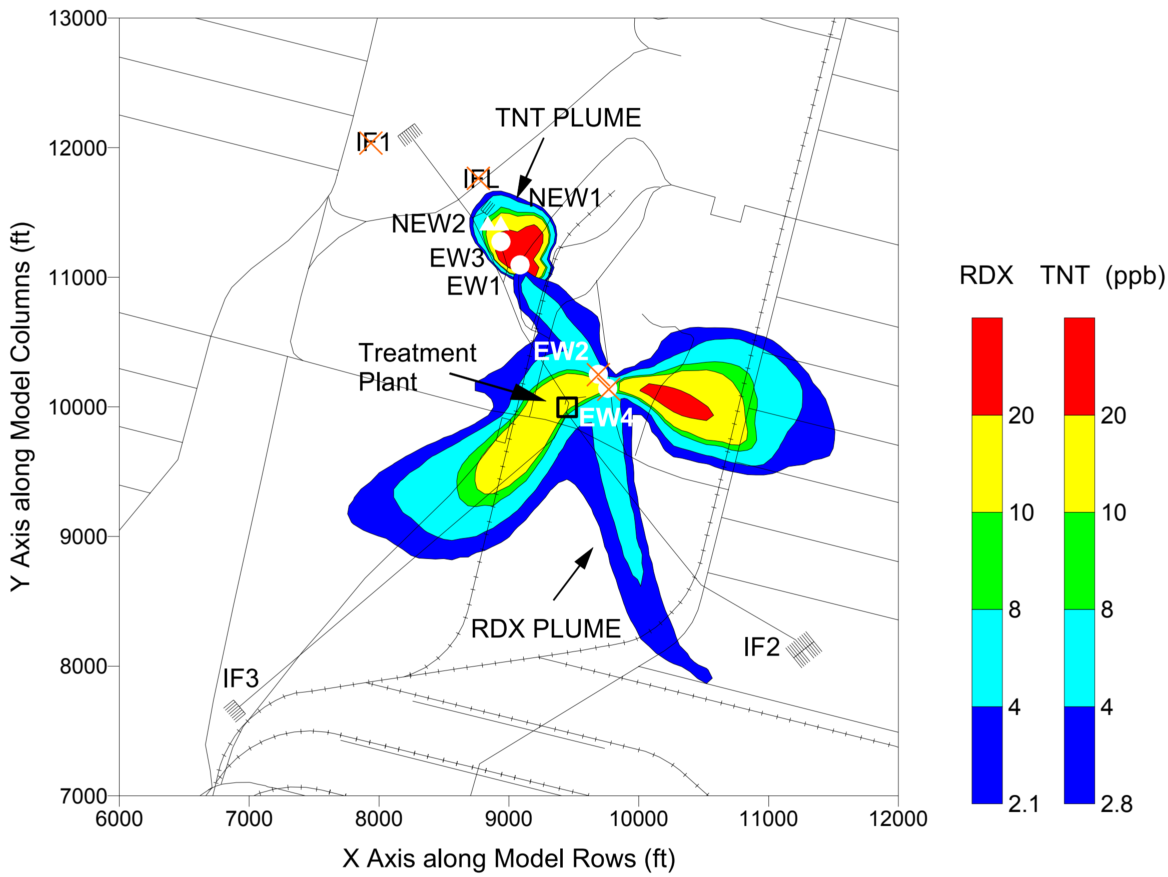


Figure 3.3. Locations of extraction wells and infiltration basins for the optimal strategy identified under Formulation 1. It consists of two existing wells (EW1 and EW3, marked as cycles) and two new wells (NEW1 and NEW2, marked as triangles), all of which are located in the TNT plume area. The existing 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.

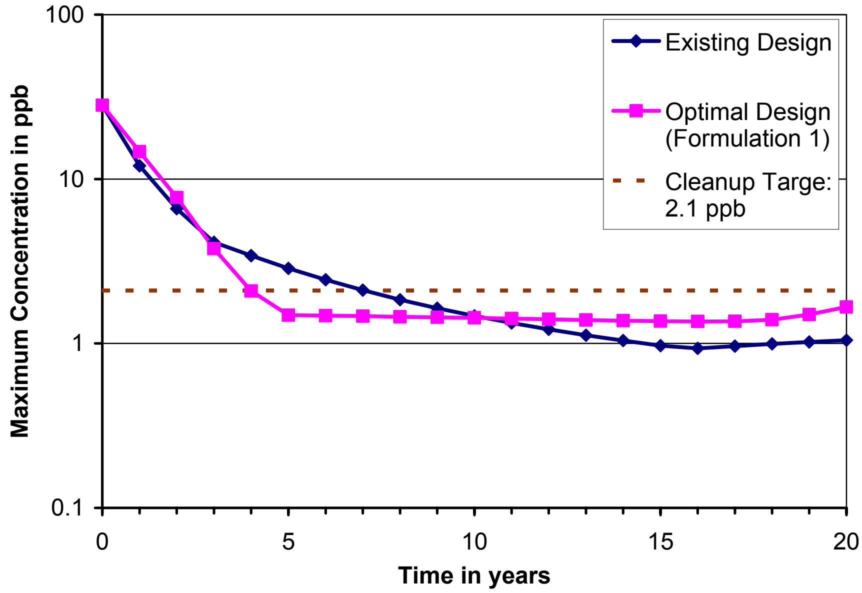
Table 3.1. Optimal pumping strategy for Formulation 1 as compared with the existing design (a negative flow rate for pumping and positive for injection).

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*

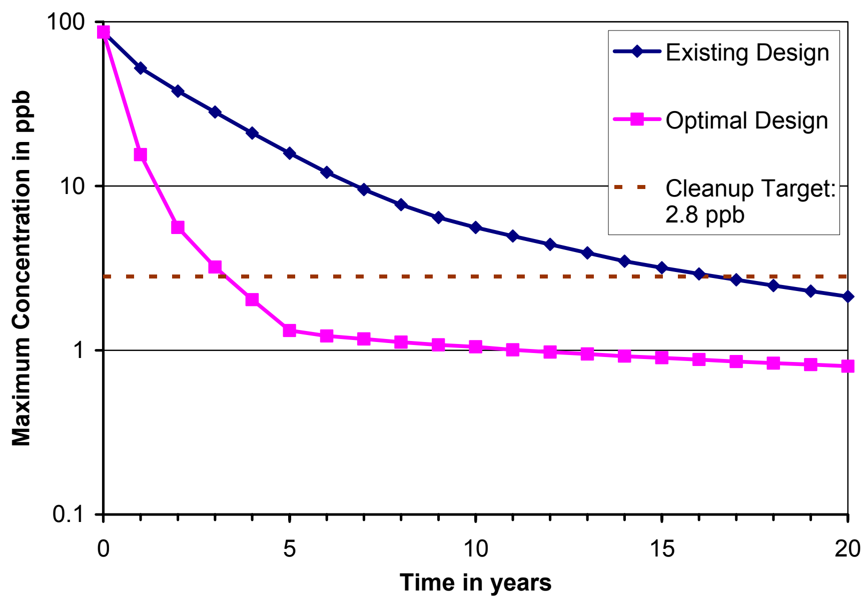
*Note: Each infiltration basin occupies more than one model cell. The exact location is indicated in the MODFLOW Well Package input file named 'Formuln1.WEL' (see Attachment A).

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:

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

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

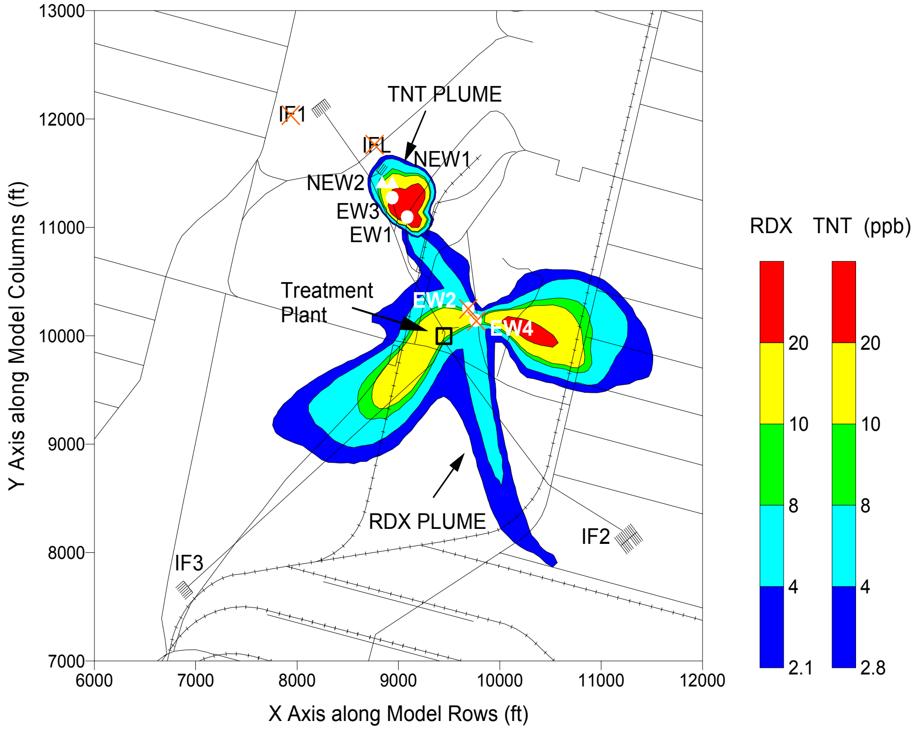
The dynamic optimal pumping strategies for the four management periods of Formulation 3 are shown in Figure 3.5(a)-(d). The optimal pumping and injection rates are listed in Table 3.3. The RDX and TNT plumes shown in each figure represent the conditions at the beginning of each management period. Moreover, 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.

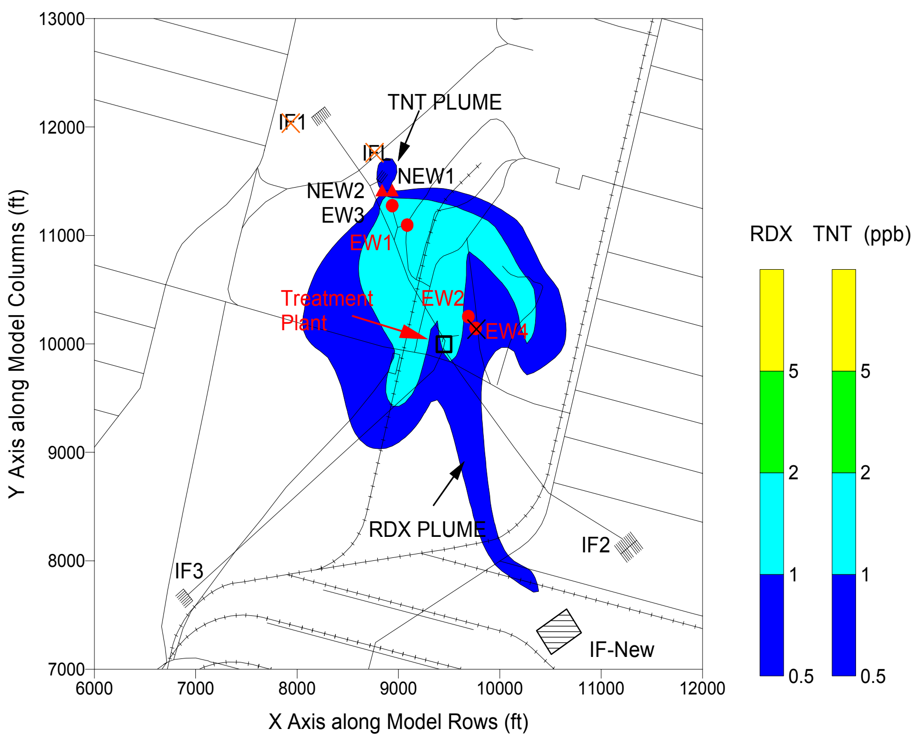
For Management Period 2 [see Figure 3.5(b)], the existing well labeled 'EW2' is utilized. This shifts more pumping back to the RDX plume as the TNT plume has been nearly all removed. Furthermore, a new infiltration basin labeled 'IF-NEW' is added to push the residual mass along a zone of low hydraulic 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%.

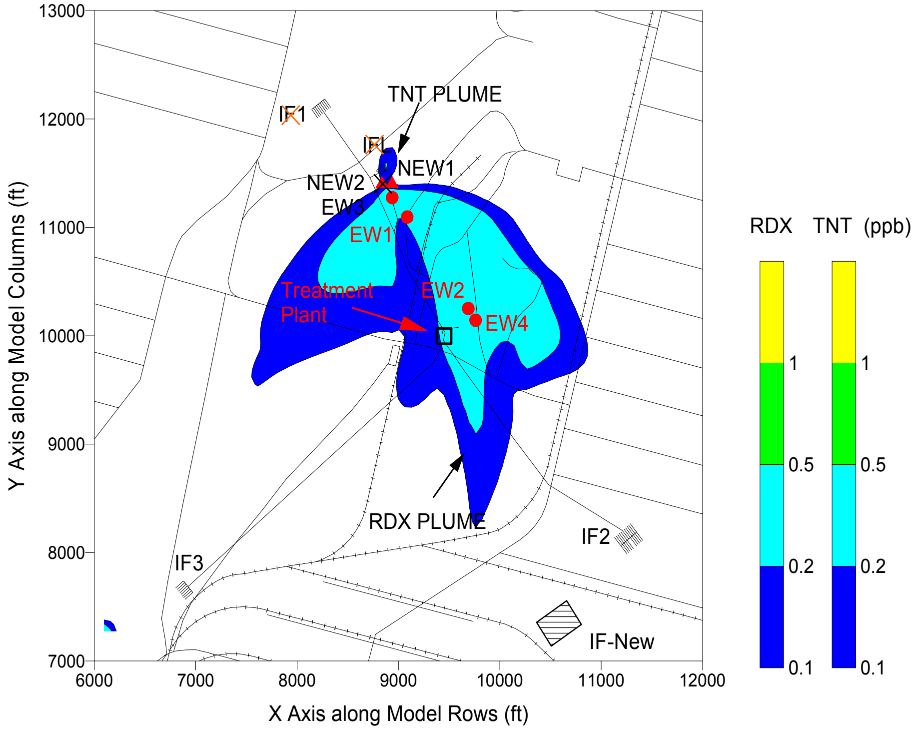


(a) Management Period 1 (Year 0-5)

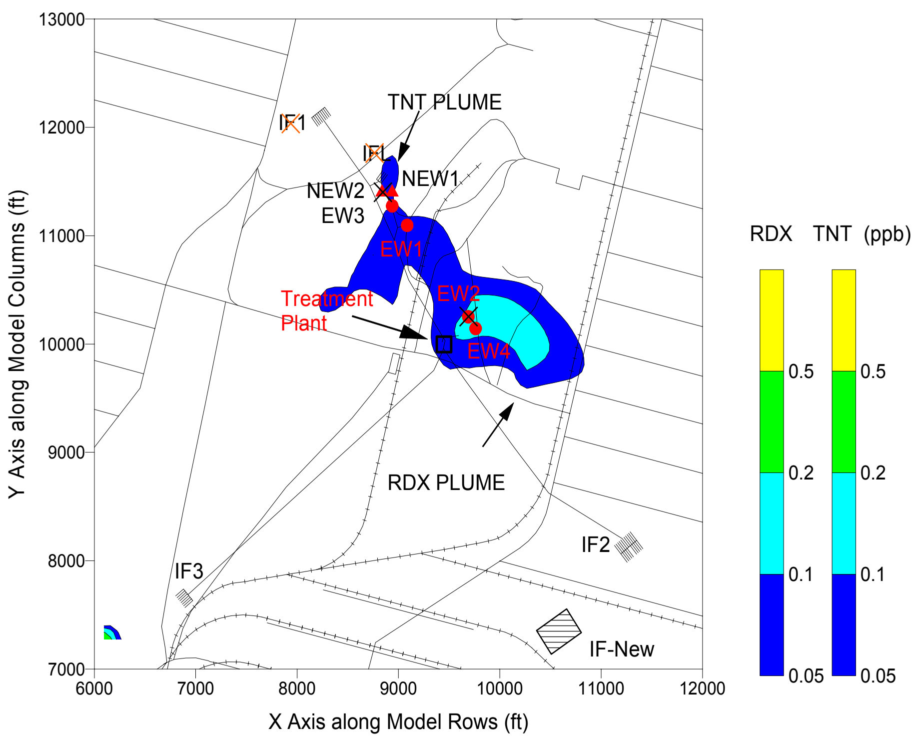


(b) Management Period 2 (Year 6-10)

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.

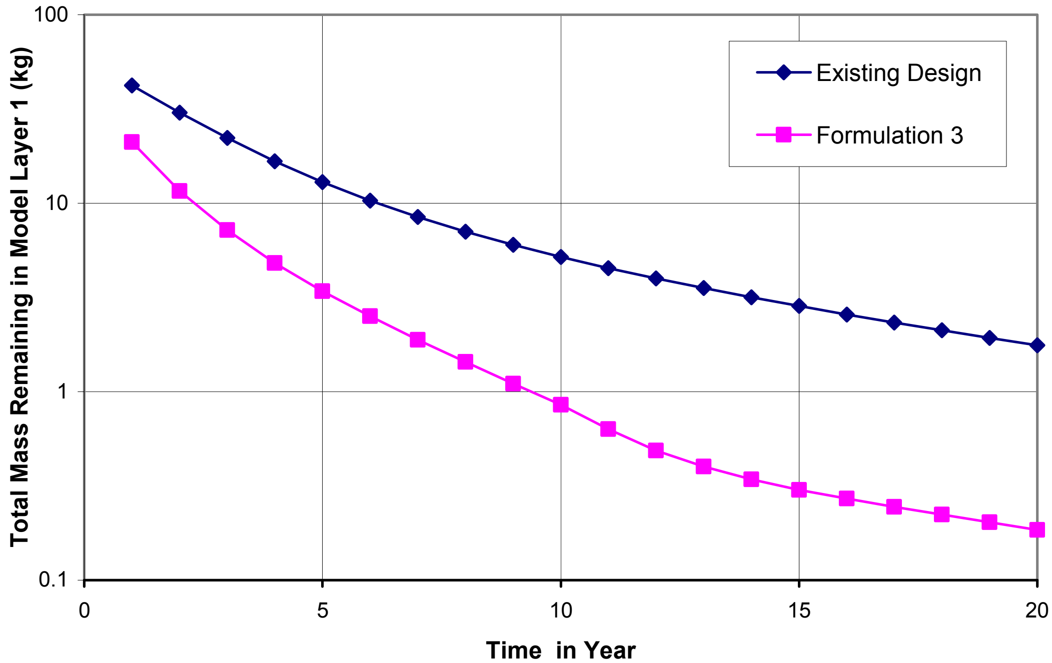


Figure 3.6. Total RDX/TNT mass remaining in the shallow aquifer under the optimal pumping strategy (Formulation 3) and under the existing design.

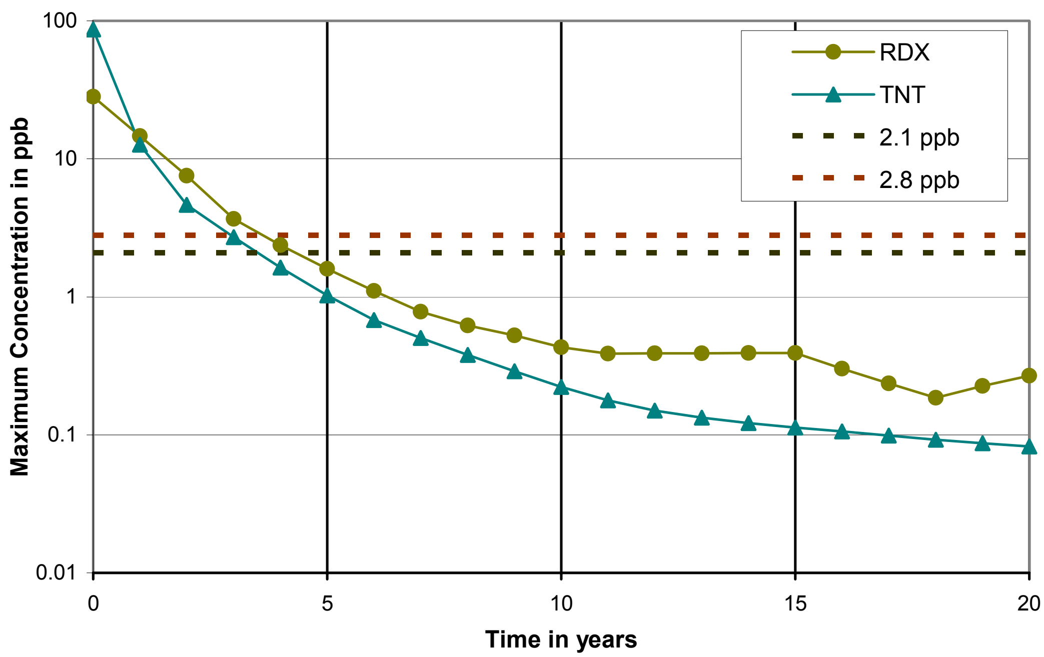
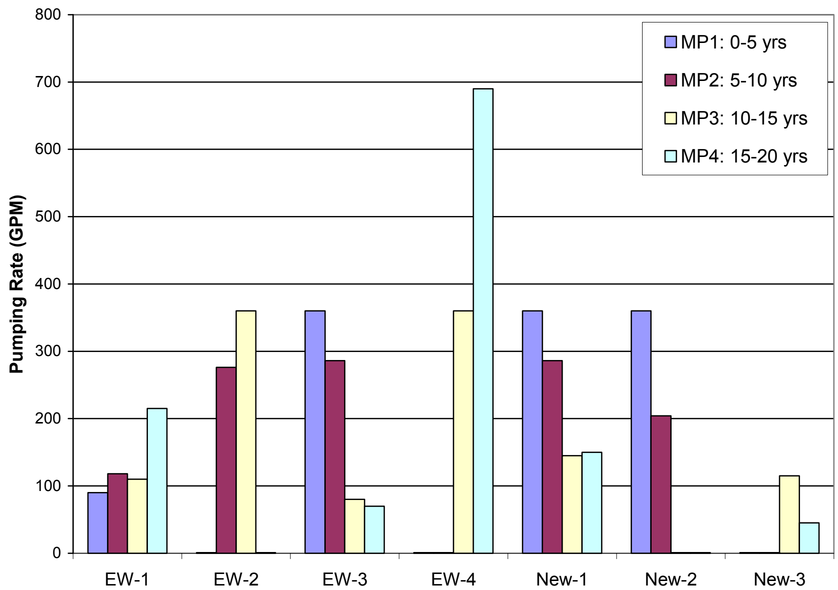
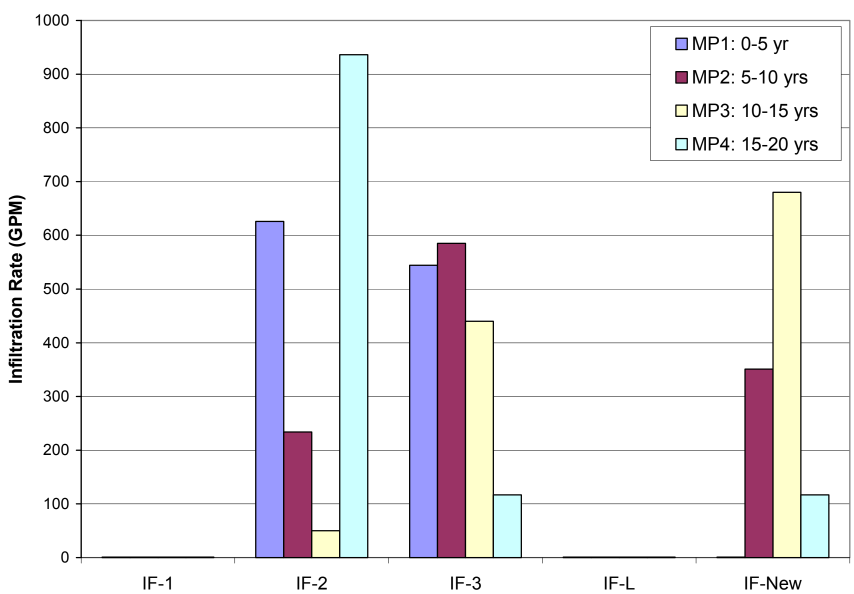


Figure 3.7. Calculated maximum concentrations under the optimal pumping strategy (Formulation 3). The cleanup targets of RDX = 2.1 ppb and TNT = 2.8 ppb are achieved in year 5 and year 3, respectively.



(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.

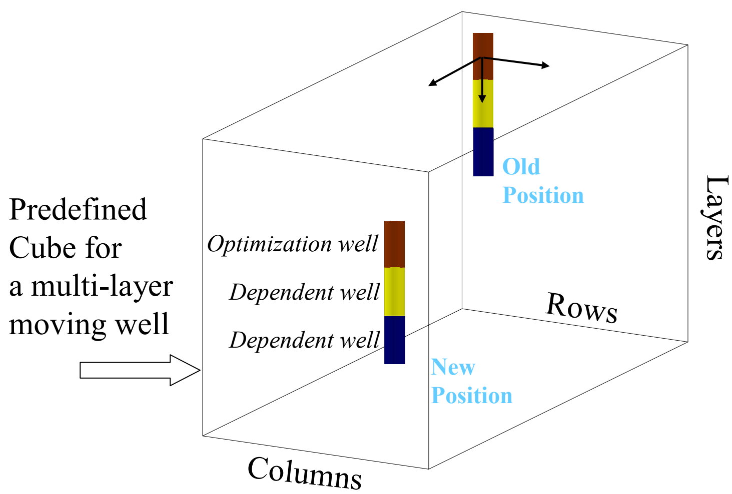


Figure 4.1. Illustration of the moving well option for defining well locations.

5

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ATTACHMENT A

MODFLOW WELL PACKAGE INPUT FILE
FOR OPTIMIZATION FORMULATION 1

```
       100
        39  /Stress Period:  1
         1         85        86         0
         1         53        59 -15422619
         1         60        65 -21605718
         1         83        84         0
         1         48        59 -25294500
         1         48        55 -19884288
         1         86        93         0
         1         86        74         0
         1         30        39         0
         1         30        40         0
         1         31        39         0
         1         31        40         0
         1        104       102  13349875     1
         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
         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         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
         0  /sp2
         0  /sp3
         0  /sp4
```

ATTACHMENT B

MODFLOW WELL PACKAGE INPUT FILE
FOR OPTIMIZATION FORMULATION 3

```
     100
      39  /Stress Period:  1                   (year 1-5)
       1        85        86         0
       1        53        59 -25294500
       1        60        65  -6323625
       1        83        84         0
       1        48        59 -25294500
       1        48        55 -25294500
       1        86        93         0
       1        86        74         0
       1        30        39         0
       1        30        40         0
       1        31        39         0
       1        31        40         0
       1       104       102  21992162      1
       1       105       102  21992162      1
       1       109        23   9555700      2
       1       109        24   9555700      2
       1       110        23   9555700      2
       1       110        24   9555700      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        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
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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

USU Report on Umatilla

FINAL

OPTIMAL PUMPING STRATEGIES
FOR
UMATILLA CHEMICAL DEPOT RDX AND TNT PLUMES

Presented to

Navy Facilities Engineering Command
NAVFACENGCOMDET-SLC

Per

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Prepared by

Systems Simulation/Optimization Laboratory
Dept. of Biological and Irrigation Engineering
Bldg EC-216
Utah State University
Logan, UT 84322-4105

31 Dec 2002

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APPENDICES

Executive Summary

We present optimal pumping strategies to address RDX and TNT plumes at Umatilla Chemical Depot (UCD). We provide strategies for four optimization problem formulations. Each strategy requires constructing 2 wells. New Well U-1 is in the same location for all strategies. The second well location can differ with formulation. The number in a strategy's name refers to the formulation it addresses. Using optimization in design is normally an iterative process involving interaction between the designer and client after preliminary optimizations are performed. This project does not permit that. To compensate, we present a second strategy for Formulation 1 (Strategy USU1B), and a Formulation 4 that include features possibly interesting to the client, yet not included explicitly within the original 3 optimization problem formulations.

For Formulation 3, Strategy USU3 minimizes the total contaminant mass remaining in aquifer layer 1 after 20 years. Within 5, 10, 15 and 20 years USU3 will remove 94.4, 98.5, and 99.4 and 99.7 percent, respectively, of the 61.5 kg existing in January 2002. After 20 years this is an improvement of 88.6 percent over the results of continuing current pumping. The 0.2 kg remaining after 20 years equals only about 7 cubic inches of solid contaminant. One is unlikely to use a Formulation 3 strategy for 20 years because contaminant removal efficiency becomes very low as concentrations diminish below Cleanup Levels (CLs).

For Formulation 1, Strategy USU1A minimizes the cost of achieving CLs for both contaminants. CLs are 2.8 ppb for TNT and 2.1 ppb for RDX. By achieving CLs within 4 years and pumping only 1154 gpm, Strategy USU1A provides a strategy costing $1,663,841. This is a 56.6 % reduction from the cost expected to result from continuing the current pumping strategy. USU1A can pump less than other strategies because its second new well would be placed where it can best affect the western lobe of the RDX plume. Within the allowed period, USU1A is also the lowest cost strategy we developed for Formulation 2.

Despite its mathematical least-cost, Strategy USU1A might not be the preferred Formulation 1 strategy. If UCD intends to continue pumping for some reason after attaining CLs, Strategy USU1B would probably be better. USU1B is designed to consider UCD preferences that are not included in the optimization problem formulation.

USU1B differs from USU1A in that it pumps 1170 gpm (costs about $400 more), and its second new well can be placed in any of hundreds of locations. The second new well location can be selected from those we tested, based on: robustness, constructability, and the management goal after CLs are achieved. A possible goal after achieving CLs is minimizing remaining contaminant mass. Robustness refers to the likelihood that the pumping strategy will achieve CLs within 4 years even if the aquifer characteristics in the field differ from those assumed in the computer model of the aquifer. We evaluated the robustness of strategies employing different second well locations, especially those near existing pipelines to simplify construction.

We propose a Formulation 4 for the likelihood that UCD might want to emphasize removing TNT mass after achieving CLs. USU4 requires constructing wells at

(row,column): (48,57) and (58,60). USU4 uses the pumping rates of USU1B during the first five years and then different pumping rates for the next 15 years. It costs the same to achieve CLs as USU1B, and is predicted to remove 2 grams more mass than USU3 after 20 years of pumping. Changing the USU1B pumping rates slightly can yield a hydraulic conductivity robustness of at least ± 15 percent.

Introduction

We present optimal pumping strategies to address the Umatilla Chemical Depot (UCD) TNT and RDX plumes as they are projected to exist in January 2002 (Figures 1 and 2). We developed these strategies using the heuristic optimization and artificial intelligence capabilities of the SOMOS simulation/optimization model (SSOL and HGS, 2001).

Simulation/optimization use should be tempered with judgment. Good judgment helps: in selecting candidate well locations; in selecting one from among many virtually identical mathematically optimal strategies; and in modifying a posed optimization problem to more satisfactorily address a real-world situation. Here we present optimal strategies developed for three single-objective optimization problem formulations posed by UCD. We tried to balance the desire for mathematical optimality with practicality.

Our developed optimal strategies are being reviewed by an external evaluator. After we submitted strategies for the first three formulations, the evaluator requested additional information. From the type of information requested, we inferred that the evaluator desired another formulation—a combination of two of the three initial formulations (objectives). Therefore we also present an optimal strategy for a fourth formulation that satisfies multiple objectives. We did this after the period of competition. The result is a pumping strategy that is probably better for UCD than any of our strategies developed for the first three formulations.

Optimization Technique

Formulations Addressed

We present optimal pumping strategies for four optimization problem formulations or scenarios. Formulations 1-3 were posed by UCD. A restriction for all formulations is that no developed pumping strategy can allow TNT or RDX to exceed cleanup levels (CLs) within a defined *exclusion* or *forbidden zone* (a region of currently uncontaminated aquifer). Cleanup levels are 2.8 ppb for TNT and 2.1 ppb for RDX.

Formulations 1 and 2 involve minimizing present value of the cost of remediating to CLs within a specified *cleanup zone* (a region that is or is becoming contaminated). Formulations 1 and 2 differ in the maximum total groundwater extraction rate that is allowed, and related costs. A Formulation 1 strategy is permitted to pump no more than 1170 gpm. A Formulation 2 strategy can pump no more than 1755 gpm, but requires expanding the existing treatment facility.

Formulation 3 involves developing a pumping strategy that minimizes the total RDX and TNT mass (adsorbed and dissolved) remaining after 20 years. A Formulation 3 strategy can extract no more than 1170 gpm and can require constructing new extraction wells and recharge basins.

We presented the results of pumping strategies for Formulations 1-3 (Tables 1-3) in our July 2001 report (SSOL, 2001). After that report, our research sponsor requested information regarding the time needed for a Formulation 3 strategy to achieve cleanup-to-CLs, and for information regarding Formulation 3 strategy costs. The sponsor seemed to desire a pumping strategy that, to the extent possible, achieves CLs economically, but would subsequently optimally decrease the contaminant mass left behind. Our Formulation 4 satisfies that need.

Formulation 4 is a combination of Formulations 1 and 3. Our Formulation 4 strategy achieves CLs within four years and continues pumping 1170 gpm to minimize the mass remaining after 20 years (Table 4). In our Formulation 4 strategy, pumping rates from the different wells can change every five years. The Formulation 4 strategy is not part of the competition that involved the other formulations.

The Optimization Procedure

Preliminaries

We developed optimal pumping strategies for Umatilla Chemical Depot (UCD) using SOMOS (SOMO3 module). The SOMO3 optimization module uses heuristic optimization and artificial intelligence capabilities. SOMO3 heuristic optimization modules include genetic algorithm (GA) and simulated annealing (SA). In one mode, it trains artificial neural networks (ANN) for state variables and uses a GA for optimization. For Umatilla optimization we employed our GA with and without the ANN.

The ANN is a *multi-layer feedforward error backpropagation neural network*. Nodes in the ANN input layer receive stimuli (pumping strategies). Each individual pumping rate is then linearly scaled into a value between –0.8 and 0.8 (reflecting the linear part of a sigmoid function). The output layer, consisting of a single node, yields a single state variable value. Between the inputs and output are weighted connections and a hidden layer of neurons. SOMO3 trains one ANN for each state variable. To learn, the ANN employs back-propagation and adaptive learning (delta-bar-delta rule). It adjusts weights to minimize the sum of squared errors (measured by the difference between the desired and actual outputs).

Generally speaking, our simulation and optimization runs are partitionable into two phases:

- Exploratory simulation and optimization. We began this phase by performing exploratory simulation runs. Then we tested and evaluated several candidate well locations using optimization.
- Optimization. We vigorously performed optimization for several sets of candidate well locations. Most runs included simulation of both RDX and TNT transport.

Since we considered Formulation 3 (minimizing mass remaining) to be the easiest problem to handle, we began by exploring candidate well locations for that formulation. We rapidly learned that cleanup can be achieved during the first five-year stress period. This simplified the optimization problem.

Figure 3 shows the optimization problem being solved when minimizing the total mass remaining after 5 years. We defined batches of candidate well locations in one or more groups and the optimization algorithm determined which well combinations yielded better results. We considered batches of candidate wells in different parts of the study area (for example: area north of the TNT hot spot; area east of the TNT hot spot, areas west of the TNT hotspot; area between existing TNT hot spot wells; and several locations in the RDX plume). The optimization algorithm determined which combinations of wells from the different batches would yield better total results.

From the preliminary optimization runs we gained understanding concerning how to minimize the mass remaining after 5 years and how to reduce RDX and TNT cleanup time (it became clear that reducing cleanup time significantly reduces cost, relevant for Formulations 1 and 2).

Preliminary GA optimization computed a pumping strategy that required constructing two extraction wells to remove about 95 percent of the initial mass within 5 years, and would reduce RDX and TNT to below their CLs within four years if we constructed two wells. We learned that reducing cleanup time required focusing candidate wells in the TNT area.

Subsequently, we worked on Formulations 1 and 3 simultaneously. Trying injection outside the RDX plume did not appreciably improve solutions. We did not consider new recharge locations within the contaminated portion of the aquifer because that would likely force contaminant mass out of the cleanup/containment zones into the exclusion (forbidden) zone or previously uncontaminated aquifer (contamination initially exists in the aquifer far beyond the MCL contour lines). Therefore, we proceeded using only extraction wells as candidates.

Formulation 3 process

After identifying candidate well locations for the first stress period for Formulation 3, we continued optimizing for the next stress periods using sequential optimization. For the later stress periods, we evaluated potential new candidate well locations within the TNT and RDX plumes. After several runs we concluded it would not be practicably cost effective to add other extraction wells (beyond the two intended for period 1)--the small increase in RDX and TNT removal would not justify the increasing cost of installing and operating additional wells. (In other words, adding another new well would not significantly reduce mass remaining).

Most mass would be removed in the first stress period. Respectively, Figures 4 and 5 show time series of mass removal (production functions) and incremental mass removal (marginal functions). Those figures show predicted results for the current strategy, and strategies USU3 and USU4.

From then on we optimized for Formulation 3 allowing installation of two new extraction wells in the first stress period. We ran sequential GA optimization runs on different computers using different candidate locations for one or both of the wells. Representative GA input parameters are listed in Table 5.

Formulations 1, 2 and 4 processes

Figure 6 shows the formal Formulation 1 cost minimization optimization problem objective function. Preliminary optimizations determined that we could achieve cleanup to CLs within 4 years using 1170 gpm and building only two wells. Initial optimization runs also indicated that no economically desirable combination of new extraction wells and recharge basins could reduce the CLs cleanup time to 3 years. Therefore, the only objective function components subject to further reductions are the last two terms shown in Figure 6 (variable costs of pumping and GAC exchange).

Variability in GAC exchange cost is much less than pumping cost variation. GAC exchange cost is proportional to contaminant mass removal. Minimizing GAC exchange cost is akin to minimizing mass removal. Because minimizing mass removal was not a goal we wanted to pursue, we chose to develop a cost minimization strategy by minimizing total pumping (while constructing only 2 wells to achieve CLs in four years). Figure 7 shows the resulting surrogate optimization problem used to address Formulation 1.

We defined batches of candidate wells in groups from which the optimization model could only use 2 wells at a time, and did GA optimization to yield the wells of strategy USU1A. Briefly applying the coupled ANN and GA reduced the pumping rates further. Representative GA and ANN input parameters are shown in Tables 5 and 6, respectively.

We also analyzed the robustness of the pumping strategies as affected by candidate well locations. USU1A resulted from GA optimization with little robustness analysis. USU1B resulted from GA optimization and well selection based on robustness.

Robustness analysis includes running simulations using, for each simulation, different values of uncertain physical parameter(s). Evaluating robustness of hydraulic conductivity includes: varying a global hydraulic conductivity multiplication factor for different simulation runs; and then determining whether all optimization problem constraints are still satisfied. In our analysis, we increased or decreased the multiplication factor in steps of 1 percent.

For several combinations of well locations a small change in multiplication factor would seriously degrade strategy results (for example, cleanup > 4 years). Other well combinations were very robust. Based on robustness and practicality, we selected 2 candidate wells for strategy USU1b. We performed several GA optimizations with those candidates to develop strategy USU1b. Table 5 shows representative Formulation 1 GA input parameters.

We used the Formulation 1 strategy as an initial guess of the optimal strategy for Formulation 2, and used additional candidate extraction well and recharge basin locations. However, we soon understood that increasing pumping and adding another GAC unit would not reduce cost. Hence, the optimal strategy for Formulation 1 will also be optimal for Formulation 2.

We formalized Formulation 4 after the initial project deadline. This formulation combines the constraints and goals of Formulations 1 and 3. To develop germane strategy USU4 we first considered strategies USU1b and USU3 and the previous robustness analysis. We adopted Strategy USU1B for the first five years and then used GA to optimize for the remaining 15 years.

Formulation results

Formulation 1 is supported by Figures 6-16 and Appendices A-D. Formulation 3 is supported by Figures 17-19 and Appendices E and F. Formulation 4 is supported by Figures 20-21 and Appendices D, G and H. Appendices A, C, E and G are MODFLOW well packages for strategies USU1A, USU1B, USU3 and USU4, respectively. Appendices B, D, F, and H are GeoTrans postprocessor outputs for those respective strategies.

Formulation 3

The Formulation 3 optimization problem is illustrated in Figure 17. We addressed the four-period problem sequentially, one five-year stress period at a time. Table 1 shows the wells that yielded the best pumping strategy from among those combinations tested during the period of competition (Strategy USU3 of Table 1; Table 3).

Figure 18 shows the head resulting from five years of pumping per USU3 strategy. The total mass remaining from USU3 after 5, 10, 15 and 20 years are 3.4206, 0.8908, 0.3879 and 0.2015 kg, respectively (Fig. 19 and Appendix F). These are improvements of 79.5, 82.8, 86.4 and 88.6 percent, respectively, over the current strategy. They can be achieved by constructing two extraction wells (wells U-1 and U-3), at cells (48,57) and (49,62). At twenty years, only 0.3 percent of the initial mass remains.

Most of the remaining 0.2 kg is RDX, which is gradually desorbing in the large area of initial contamination and especially to the west of recharge basin IF-2. The 0.2 kg is equivalent to about 7 cubic inches of solid phase contaminant. Because the concentration is very low and widely dispersed, adding more wells to very slightly decrease the mass remaining after 20 years did not seem justifiable, so we did not allow the model to do that.

As stated in our July 2001 project report, using the well locations of Formulation 1 (Strategies USU1A or USU1B) and a modified pumping strategy can also result in a very small mass remaining. We quantify this later in Formulation 4.

Least Cost Strategy USU1A

As stated above, we optimized a surrogate problem (Figure 7) to solve the posed Figure 6 problem. GA followed by brief coupled ANN-GA optimization created Strategy USU1A (Tables 1 and 2). We used the GeoTrans post-processor to compute the present value cost (Appendix B).

Figure 8 shows the time series of maximum RDX and TNT concentrations resulting from Strategy USU1A. Figures 9-11 show how the RDX plumes evolve spatially by the end of years 1-3, respectively. Figures 12-14 show TNT plume evolution. By year four, no contamination exceeds CLs.

Strategy USU1A injects at existing basins IF2 and IF3 and extracts at existing wells EW-1 and EW-3 and proposed wells U-1 and U-2, in (row,column): (48,57) and (65,60) respectively. It pumps 1154 gpm, 16 gpm less than the allowed 1170. Placing the second well (U-2) at cell (65,60) helped reduce cost because that southerly position required less pumping than other locations to capture all the western RDX lobe within four years. This is explained as follows.

The cone of depression and head contours resulting from Strategy USU1a are similar to those of Fig. 18. To satisfy the optimization problem constraints, the gradients and contaminant velocities must be sufficient to achieve cleanup within four years and plume containment. Gradients and velocities are affected by other factors, including hydraulic conductivity.

Figure 15 shows the model layer 1 hydraulic conductivity distribution. Comparing Figure 15 with the shape of the RDX plume at year 3 (Fig. 11) shows how the western plume lobe tends to move a little to the east to be able to bypass the 600 ft/day zone and move through the 3014 and 1500 ft/day zones in its northward migration. Similarly, the eastern plume lobe tries to bypass the 1500 ft/day zone and move through the 1918 and 4110 ft/day zones on its way north.

Figures 9-11 show a bulge in the RDX plume western lobe caused by the well U-2 capture zone. This indicates how the southerly location of well U-2 makes capture of the western lobe easier than a more northerly location might. We were unwilling to consider positioning this well further to the south because that would increase its distance from the TNT contamination (Fig. 1).

The location of well U-2 allows the pumping reduction that makes this strategy slightly more economical than the thousand or so other paired locations of new wells that can (teamed with existing structures) achieve cleanup within four years at rates at or near 1170 gpm. However, these 1000+ pumping strategies have objective function (OF) values within several hundred dollars of each other. OF value differences are primarily due to slight variation in pumping rates. Strategy USU1A is less than $1,000 better than other strategies that also remediate to CLs by constructing only two wells.

Alternative Near-Least-Cost Strategies USU1B

Because the OF values of the developed strategies are so similar, one should also consider other, less quantifiable, factors in recommending well locations. During the competition period, we considered: (a) reliability that the strategy will achieve cleanup even if the assumed hydraulic conductivity differs from reality; and (b) ease of connecting new wells to existing pipelines; and (c) the management goal after CLs are achieved.

Computer models are approximations of reality. The actual Umatilla hydraulic conductivity (K) field differs from the field assumed in the model. Regardless, we want the proposed strategy to achieve cleanup within four years in the field. Therefore, we evaluated how different well combinations would perform despite variation in K. This helped identify the most robust locations for new wells--locations (with appropriate pumping rates) that would still achieve cleanup in four years even if the real K were higher or lower than the assumed K.

If all other factors are equal, we prefer new well locations that are near existing pipelines to those more distant. Generally, the closer a new well is to an existing pipeline, the easier it is to connect the two. Because we do not know the flow capacity of the existing pipelines, we provide alternative new-well locations near both the major and feeder pipelines for one well.

Now we discuss how these considerations can affect positioning wells for a generic strategy termed USU1B (Tables 1 and 2). Strategy USU1B includes constructing Well U-1 at cell (48,57), to remediate TNT within four years; and constructing another well (U-2) farther south to speed RDX northward migration and to remediate it within four years.

Total USU1B pumping is 1170 gpm. If all other well and recharge basin fluxes are per strategy USU1B, well U-2 can be in virtually any cell in Figure 16 and achieve CLs within four years.

Figure 16 shows cells (wavy borders) along pipelines west of EW-1. The main pipeline runs between cell (59,57) and cell (65,60). A smaller pipeline runs between cell (65,60) and cell (58,60). A feeder pipeline runs to well EW-1.

Cells at the end of the pipeline segments contain numbers indicating the range of conductivity multipliers for which pumping at that cell will still achieve cleanup in four years. For example, pumping at our specified rate in cell (58,60) will achieve 4-year cleanup if the hydraulic conductivity in the field is between 0.84 and 1.07 times the conductivity assumed in the model. We term that range as the range of robustness for cell (58,60). The range of robustness for cells between (58,60) and (65,60) changes nonlinearly but monotonically in space.

Thus, Strategy USU1B employs 1170 gpm and has many permutations, each differing only in the location of well U-2. The pumping rates for all wells remain the same. Total pumping can be reduced somewhat (amount depends on the cell selected for well U-2), and still achieve cleanup within four years. However, reducing pumping can reduce strategy robustness, a concern if field conductivity or porosity differs from model-assumed values.

If: (a) the field conductivities are as little as 0.84 times the assumed values; or (b) pumping might continue significantly beyond four years to reduce adsorbed TNT mass; and (c) the existing feeder pipeline can convey the extra flow of well U-2; cell (58,60) would be a good choice for well U-2. Placing well U-2 at cell (58,60) provides a robustness range of 0.84-1.07, valuable if the field hydraulic conductivity is less than 90 percent of the model conductivity. Because the RDX plume lies to the south, Well U-2 would become less effective for RDX cleanup if it were placed too far north.

Once a particular cell is selected for well U-2, the pumping strategy can be optimized further, depending on the management objectives after CLs are achieved. For example, if one might want to continue pumping beyond CLs to further reduce remaining mass, one can select a U-2 location that best aids that, and then optimize pumping rates.

Formulation 2

The Formulation 2 optimization problem differs from that of Formulation 1 in that the upper limit on total groundwater extraction is 1755 gpm. For a Formulation 2 pumping strategy to be less expensive than strategy USU1A, it would have to achieve CLs within 3 years. It was not economically beneficial to increase pumping enough to achieve cleanup within three (3) years. Therefore a strategy optimal for Formulation 1 is also optimal for Formulation 2.

Formulation 4

The Formulation 4 optimization problem combines all goals and constraints of Formulations 1 and 3 (Figure 20). Its goal is to achieve CLs within four years and to minimize the mass remaining after 20 years of transient pumping. Formulation 4 applies multi-objective optimization by minimizing mass remaining after 20 years, subject to the implicit constraint that it also achieves a minimum cost. The least cost constraint is explicitly represented via cleanup-to-CLs-within-four-years constraints. We addressed this optimization problem by adopting Strategy USU1B for the first five years and then optimizing for the remaining 15 years. Contractually we felt restrained from moving the well locations determined during the period of competition.

Tables 1 and 4 summarize Strategy USU4. The mass remaining is actually slightly less (better) than that of USU3. This is possible because (58,60) was not a candidate well location for Formulation 3 optimization. The cost to CLs is about the same as all other four-year cleanup strategies. We did not estimate the cost of pumping beyond four years. The robustness range of hydraulic conductivity multiplication factors is that of USU1B, (0.84-1.07).

We found that changing the first period pumping rates increases the hydraulic conductivity robustness range to 0.85 -1.17. Figure 21 shows the resulting relationship between hydraulic conductivity multiplier and present value. The storativity/effective porosity robustness range of this modified strategy is 0.5-1.03 (we did not test multipliers lower than 0.5). Again, the mass remaining after 20 years is 0.199 kg.

Our project contract indicated there was no need to evaluate issues such as strategy robustness. We were to address the three posed optimization problem formulations and not interact with the client (UCD). Nevertheless, by evaluating robustness and developing Formulation 4 we further the project goal of demonstrating the power of optimization.

Normally, when using optimization to design a pumping strategy for a client, the developer and the client interact even after the optimization has begun (Peralta and Aly, 1994, 1995, 1996; Hegazy and Peralta, 1997; Peralta, 2001a,b). Interaction is helpful in refining a strategy because the optimization problem formulation does not always consider all factors useful for design and construction.

Saturated Thickness

The optimization formulations we were assigned did not include limits on head or saturated thickness as constraints. After presenting our optimal strategies for the three formulations in July, we reviewed the saturated thickness that would result from the optimal pumping rates. The saturated thickness resulting in cell (48,57) containing well U-1 is at the edge of what we are comfortable with. We are not used to conductivities nearly as large as those near that cell.

Strategy USU1B results in about 6 feet of saturated thickness at cell (48,57) after four years of pumping. Saturated thickness at the well casing will be less—how much less depends on the well design. If a large well diameter is used, drawdown might be only about one foot because of the huge 3000 ft/day conductivity. The transmissivity resulting from 6 feet of saturated thickness is 18,000 ft^2 /day. This is equivalent to the transmissivity of 60 ft of saturated thickness of an aquifer having a conductivity of 300 ft/day—a much more common conductivity.

The currently proposed location of well U-1 at (48,57) is a compromise position:
- It is far enough north and west to remediate all the TNT north and west of it even if field hydraulic conductivity varies somewhat.
- It is located in a slight NW-SE running depression in the aquifer bottom (Fig. 22) giving it more saturated thickness than if it were located within several cells to the west or east (Fig. 23).
- It is far enough south to have as much saturated thickness as practicable (Fig 24), while still remediating the contamination to the north. It has more saturated thickness than any more northerly cell in that vicinity.

Nevertheless, achieving more saturated thickness for well U-1 might be preferable, if there are no harmful consequences. Moving well U-1 one cell to the south or southeast might slightly improve ultimate saturated thickness while probably still achieving CLs within 4 years. Possibly one can move well U-1 two cells. Our expectation is based on early runs in which well U-1 was placed in other cells near (48,57).

Conclusions

Table 1 summarizes results from the pumping strategies developed for the several optimization problem formulations, and strategy results. Predicted results are as accurate as the simulation models they are based upon. Each of our strategies requires constructing 2 wells. Well U-1 is in the same location for all strategies. The second well location can differ with formulation.

Strategy USU3 is designed to minimize the mass remaining after 20 years. Within 5, 10, 15 and 20 years it will remove 94.4, 98.5, and 99.4 and 99.7 percent of the total initial mass, respectively. These are improvements of 79.5, 82.8, 86.4 and 88.6 percent, respectively, over the results of continuing current pumping. Probably one should cease pumping long before twenty years.

Strategy USU1A is designed to minimize cost of achieving TNT and RDX Cleanup Levels (CLs). It costs $1,663,841, less than other strategies that achieve CLs within 4 years and pumping less than the allowable 1170 gpm. It can pump less because the second well is located closer to the RDX plume. The USU1A cost represents a 56.6 % reduction from the cost expected to result from continuing the current pumping strategy. Strategy USU1A is also the best strategy we obtained for Formulation 2.

Generic Strategy USU1B allows one to select a location for the second well that best satisfies considerations not included within the optimization problem formulation. USU1b pumps 1170 gpm and achieves CLs within four years. The total cost of USU1B differs slightly (up to several hundred dollars) depending on the location selected for the second new well. If USU1B employs the same well locations as USU1A, USU1B is a little more robust because it pumps more.

For Strategy USU1B, the location for the second new well should be selected based on robustness, constructability, and the likely management goal after CLs are achieved. A probable goal after achieving CLs is minimizing remaining contaminant mass. Our newly proposed Formulation 4 and Strategy USU4 address that situation.

USU4 is the best strategy among those discussed above. USU4 builds wells at (48,57) and (58,60). It uses the pumping rates of USU1B during the first five years and then different pumping rates for the next 15 years. It improves mass reduction by 72.9, 81.8, 86.3, and 88.7 percent over continuing current pumping. It costs the same to achieve CLs as USU1B, and is predicted to remove 2 grams more mass than USU3, after 20 years of pumping.

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TABLES AND FIGURES

Table 1. Executive summary of optimal strategies for Umatilla Chemical Depot formulations [1].

Formulation # (Strategy Name)	**1 (USU1A)**	**1 (USU1B)**	**2 (USU2)**	**3 (USU3)**	**4 (USU4)**
Objective Function Values [2] **- Cost to CL** **- Mass after 20 years**	**$1,663,841** **N/A**	**≅$1,664,200** **N/A**	**$1,663,841** **N/A**	**N/A** **0.2015 kg**	**$1,664,212** **0.1992 kg**
Number of New Extraction Wells Installed	**2**	**2**	**2**	**2**	**2**
Number of New Recharge Basins Installed	**0**	**0**	**0**	**0**	**0**
Number of New GAC Units Installed	**N/A**	**N/A**	**0**	**N/A**	**N/A**
Cleanup Time for RDX	**4**	**4**	**4**	**5**	**4**
Cleanup Time for TNT	**4**	**4**	**4**	**4**	**4**

1 Formulations 1-3 were addressed during the competition period. Formulation 4 was addressed after that period.

2 N/A means not applicable.

Table 2. Current, USU1A, & USU1B pumping strategies and results.

	Strategy Pumping Rates (GPM)			
Strategy Name		**CURRENT**	**USU1A**	**USU1B**
Well Name	**Well Location (K,I,J)**			
EW-1	**(1,60,65)**	**-128**	**-356**	**-358**
EW-2	**(1,83,84)**	**0**	**0**	**0**
EW-3	**(1,53,59)**	**-105**	**-351**	**-360**
EW-4	**(1,85,86)**	**-887**	**0**	**0**
IF-1	**4 cell total**	**233**	**0**	**0**
IF-2	**2 cell total**	**405**	**453**	**471**
IF-3	**4 cell total**	**482**	**701**	**699**
New U-1	**(1,48,57)**		**-360**	**-360**
New U-2	**(1,65,60)**		**-87**	
New U-2	**(1,58,60)**			**-92**
Total extraction (gpm)		**-1120**	**-1154**	**-1170**
Duration (yrs)		**17**	**4**	**4**
Total cost present value (M US dollars)		**3.836285**	**1.663841**	**1.664212**

Table 3. Twenty-year transient pumping Strategy USU3.

Well Name	**Location**	**Pumping Rates (GPM) per stress period (SP)**			
	(K,I,J)	**SP 1**	**SP 2**	**SP 3**	**SP 4**
EW-1	**(1,60,65)**	**-79**	**-7**	**-358**	**-153**
EW-2	**(1,83,84)**	**0**	**0**	**0**	**0**
EW-3	**(1,53,59)**	**-358**	**-234**	**-360**	**-66**
EW-4	**(1,85,86)**	**-13**	**-704**	**0**	**-800**
IF-1	**4 cell total**	**0**	**0**	**0**	**0**
IF-2	**2 cell total**	**454**	**377**	**943**	**535**
IF-3	**4 cell total**	**716**	**792**	**227**	**635**
New U-1	**(1,48,57)**	**-360**	**-225**	**-360**	**-152**
New U-3	**(1,49,62)**	**-360**	**0**	**-93**	**0**
Total extraction (gpm)		**-1170**	**-1170**	**-1170**	**-1170**

Table 4. Twenty-year transient pumping Strategy USU4.

Well Name	Location	Pumping Rates (GPM) per stress period (SP)			
	(K,I,J)	SP 1	SP 2	SP 3	SP 4
EW-1	(1,60,65)	-358	-33	-119	-39
EW-2	(1,83,84)	0	0	0	0
EW-3	(1,53,59)	-360	-190	-330	-18
EW-4	(1,85,86)	0	-567	0	-792
IF-1	4 cell total	0	0	0	0
IF-2	2 cell total	471	160	1043	554
IF-3	4 cell total	699	1009	127	616
New U-1	(1,48,57)	-360	-358	-360	-235
New U-2	(1,58, 60)	-92	-22	-360	-85
Total extraction (gpm)		-1170	-1170	-1169	-1169

Table 5. Representative example of GA input parameters.

total number of simulations	800
total number of generations	38
generation size (gen. 1)	60
generation size (later generations)	20
Penalty coefficient	100
crossover probability	0.85
mutation probability	0.04

Notes:

1. Total number of simulations performed by end of the number of generations specified in item 2.
2. Total number of generations used in a GA optimization.
3. The number of individuals in generation 1.
4. The number of individuals in all generations after generation 1.
5. Within the objective function, this is the coefficient used to weight unit violations of constraints. The resulting penalty makes the objective function less desirable proportionally with respect to the degree of constraint violation.
6. Probability that a pair of individuals will mate. Usually, one maintains a high probability (i.e. 0.7 ~ 0.9), since without mating, only mutation will change a strategy. Aly and Peralta (1999) report that a probability less than 0.7 produces inferior results.
7. Probability that each bit of a chromosome will mutate. The rate of mutation should generally be low (smaller than 0.1). Mutation is performed after crossover.

Table 6. Representative example of ANN-GA input parameters.

ANN input parameters	
1. number of cycles	8
2. min. no. of simulations per cycle	10
3. Number of ANN training sessions	2
4. Number of iterations per training session	10000
5. number of nodes in hidden layer	4
6. Kappa	0.1
7. Phi	0.5
8. Theta	0.7
9. Initial learning rate	0.15
GA input parameters	
10. population size	100
11. number of generations	1500
12. crossover probability	0.8
13. mutation probability	0.03
14. penalty coefficient	100

Notes:

1. The number of cycles. A cycle is one process of developing strategies, training ANNs and optimizing. The ANNs represent substitute simulators or response surfaces. The process is continued untill the total number of cycles are completed.
2. The minimum number of real model simulations per cycle. Included within these simulations is the best strategy from the previous cycle.
3. The number of training sessions usually is less than 10, but more is possible. A larger number will require more time to train the ANN, but might improve the training and yield a more accurate ANN.
4. The number of iterations for each ANN training session. This is usually between 500 and 10000.
5. The number of nodes (neurons) in the hidden layer. This number determines the number of weights between the input and hidden layer and hidden layer and output layer. Increasing the number of nodes causes the ANN architecture to become more complex, and increases run time. The more nodes, possibly the better the ANN-prediction abilities—up to a point. Too many nodes can cause an ANN to memorize all inputs and reduce its ability to recognize new patterns.
6. Kappa parameter. Used internally to determine a learning rate. Kappa should have a value between 0 and 1. Normally kappa is 0.1. ANN performance is not very sensitive to this.
7. Phi parameter. Used internally to help determine a learning rate. Phi should have a value between 0 and 1. Normally phi ranges from 0.5 to 0.7.
8. Theta parameter. Used in the adaptive learning algorithm. Theta should have a value between 0 and 1. Normally, we use a theta of 0.1.
9. The initial learning rate. This usually ranges from 0.15 to 0.5. A frequently used value is 0.5. Higher values could lead to oscillation or saturated processing elements (nodes).

10-14. See Notes of Table 5.

Fig. 1. Initial (Projected 1 Jan 2002) TNT concentrations exceeding 2.8 ppb, and part of finite difference grid with rows and columns numbered.

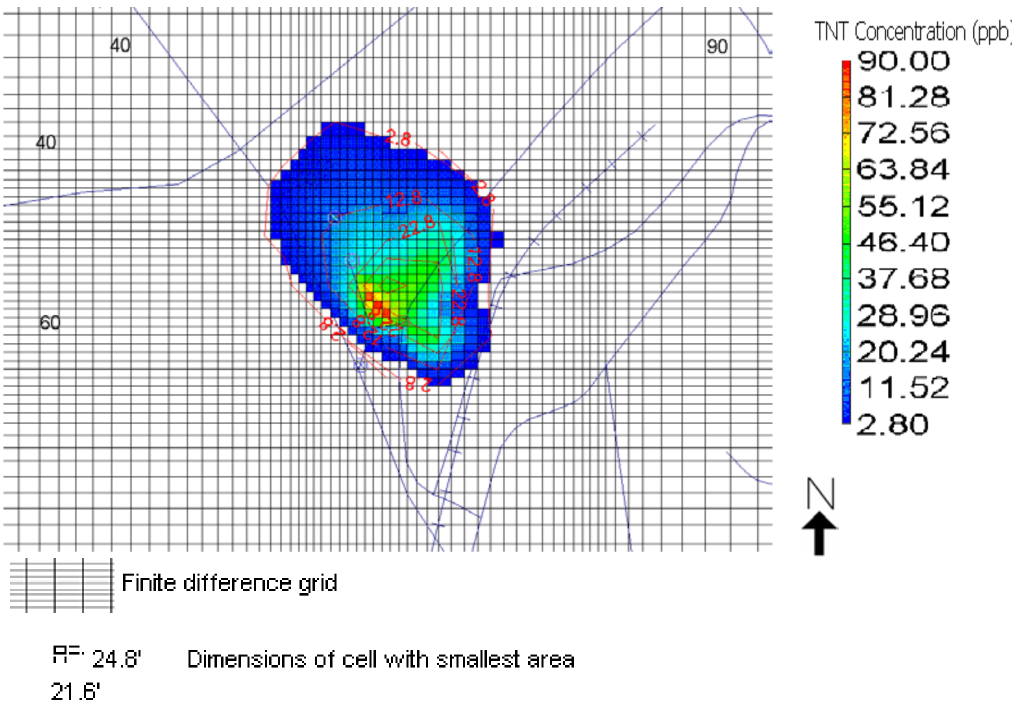


Fig. 2. Initial (Projected 1 Jan 2002) RDX concentrations exceeding 2.1 ppb, and part of finite difference grid.

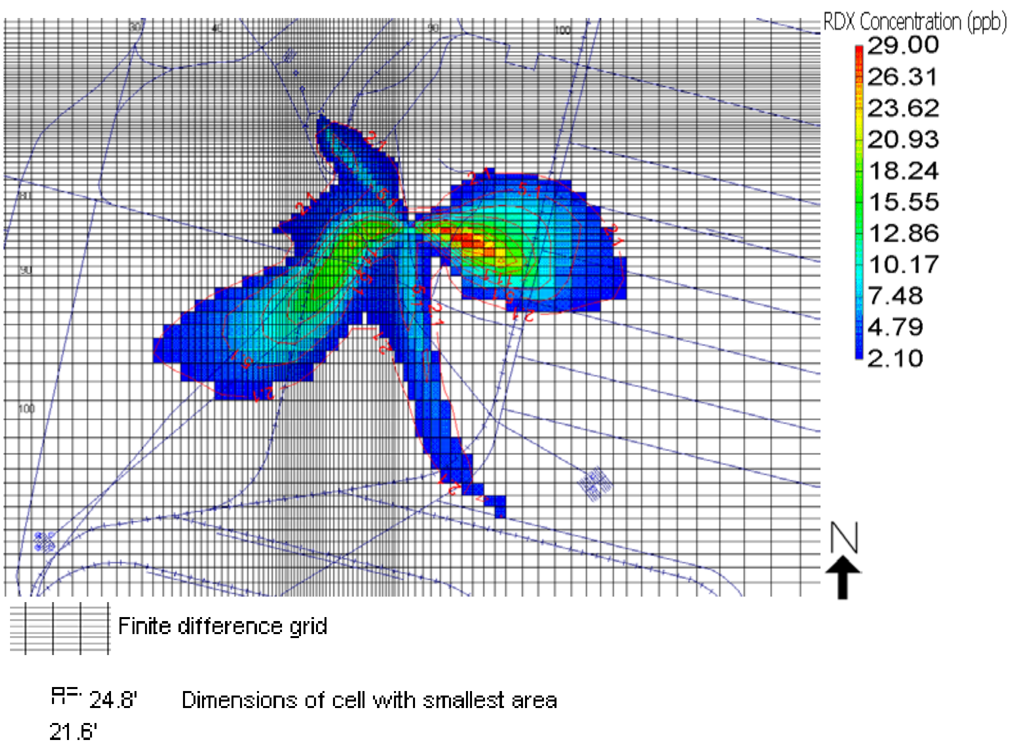


Fig. 3. Preliminary optimization problem: minimize mass remaining after 5 years.

MINIMIZE Total Adsorbed & Dissolved
RDX & TNT Mass After 5 Years

Subject to:

- Maximum RDX Forbidden Zone Conc.
  ≤ 2.1 ppb for each of 5 years
- Maximum TNT Forbidden Zone Conc.
  ≤ 2.8 ppb for each of 5 years
- Σ |Extraction| ≤ 1170 gpm
- Σ |Extraction| = Σ Injection
- Bounds on Pumping at Individual Wells
- Construct 1 or 2 New Wells

Fig. 4. Production functions for mass removal versus time for current strategy and strategies USU3 and USU4.

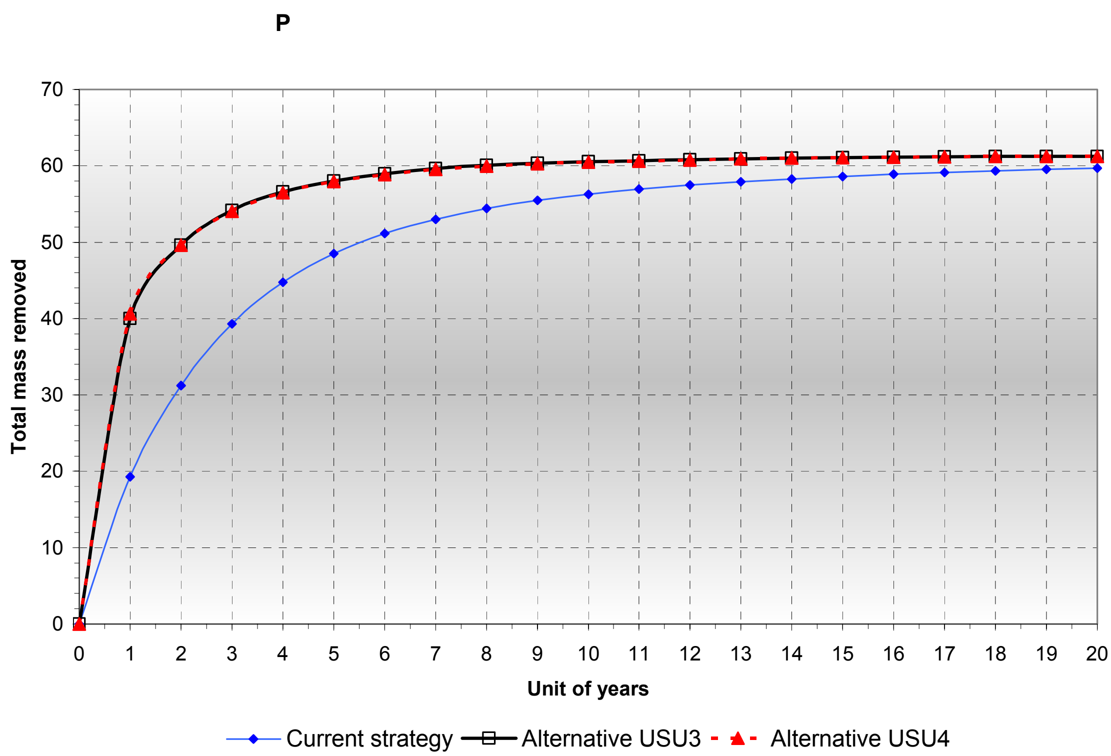


Fig. 5. Marginal functions for mass removal versus time for current strategy and strategies USU3 and USU4.

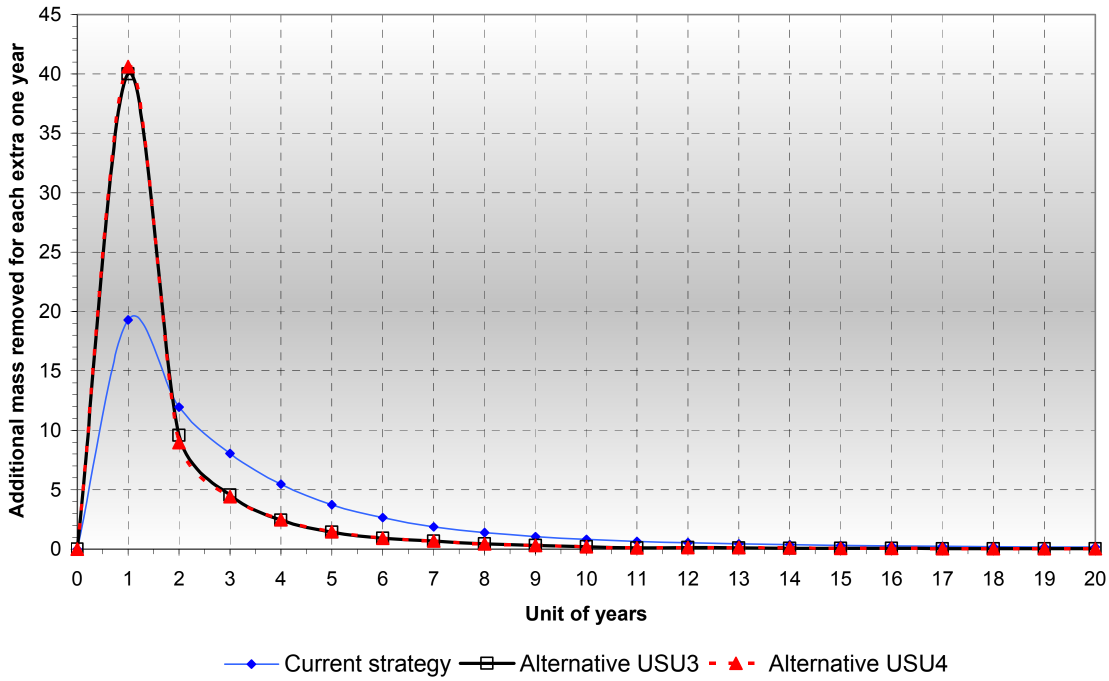


Fig. 6. Formulation 1 objective function: minimize present value of cost.

MINIMIZE (CCW + CCB + CCG + FCL + FCE + VCE + VCG + VCS)

Where all below costs need to be discounted:

CCW = New well capital cost ($75K)
CCB = New recharge basin capital cost ($25K)
CCG = New GAC unit capital cost ($150K)
FCL = Fixed annual labor cost ($237K)
FCE = Fixed annual electricity cost ($3.6K)
VCE = Variable annual electrical cost (>$11.7K for 1170gpm)
VCG = Variable GAC change cost (small)
VCS = Annual sampling cost ($150K, yrs 1-5)

Fig. 7. Formulation 1 surrogate optimization problem.

MINIMIZE |Total Extraction|

Subject to:

mum RDX Year-4 Cleanup Zone Conc.
2.1 ppb
mum TNT Year-4 Cleanup Zone Conc.
2.8 ppb
mum RDX Forbidden Zone Conc.
2.1 ppb for 20 years
mum TNT Forbidden Zone Conc.
2.8 ppb for 20 years
|Extraction| 1170 gpm
|Extraction| Σ Injection
ounds on Pumping at Individual Wells

Fig. 8. Strategy USU1A: Time series of resulting maximum concentrations.

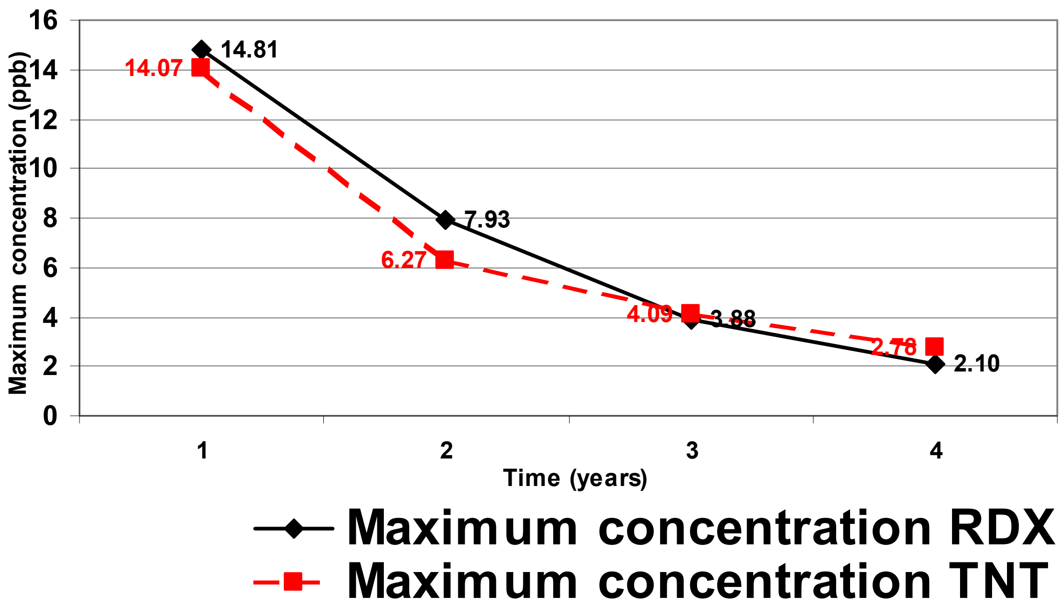


Fig. 9. Strategy USU1A: RDX concentrations ≥ 2.1 ppb after 1 year of pumping.

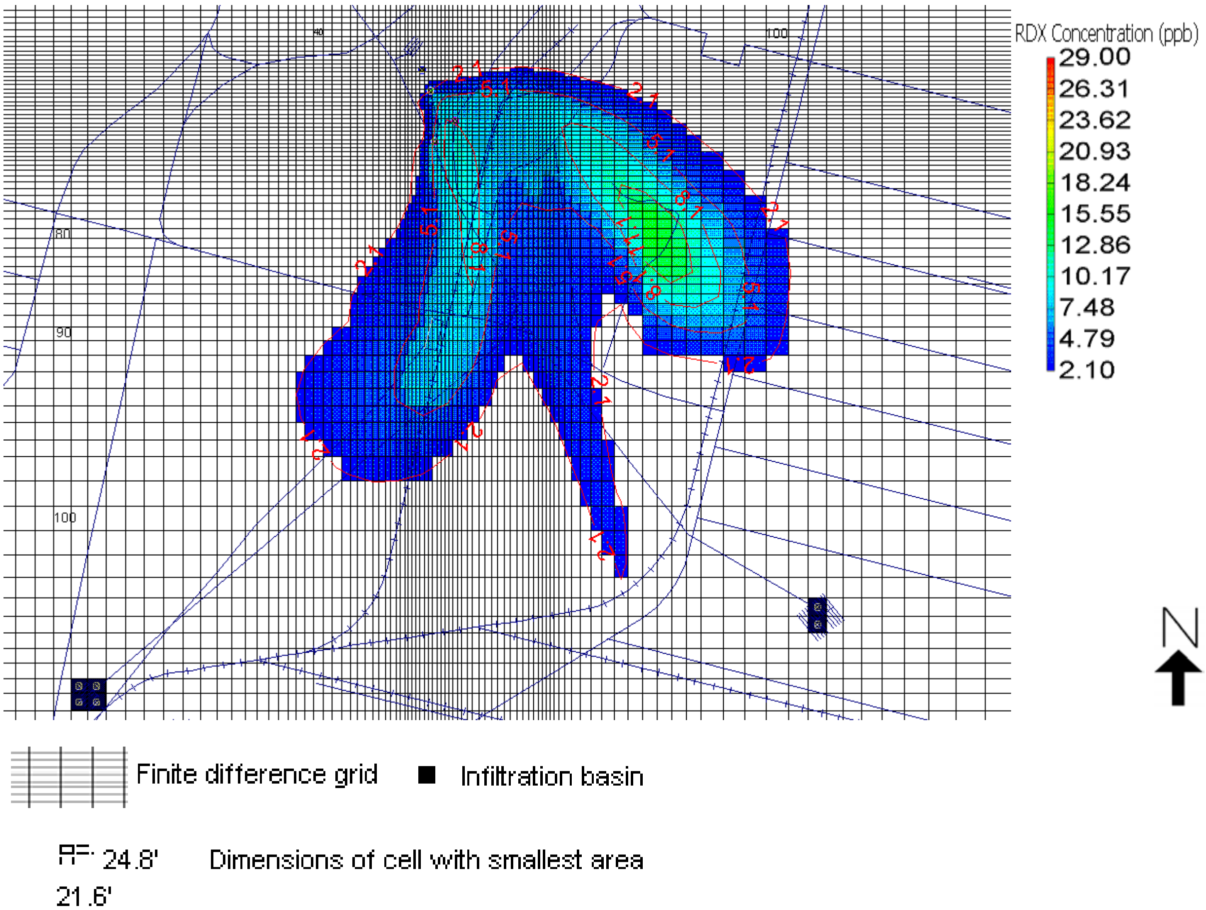


Fig. 10. Strategy USU1A: RDX concentrations ≥ 2.1 ppb after 2 years of pumping.

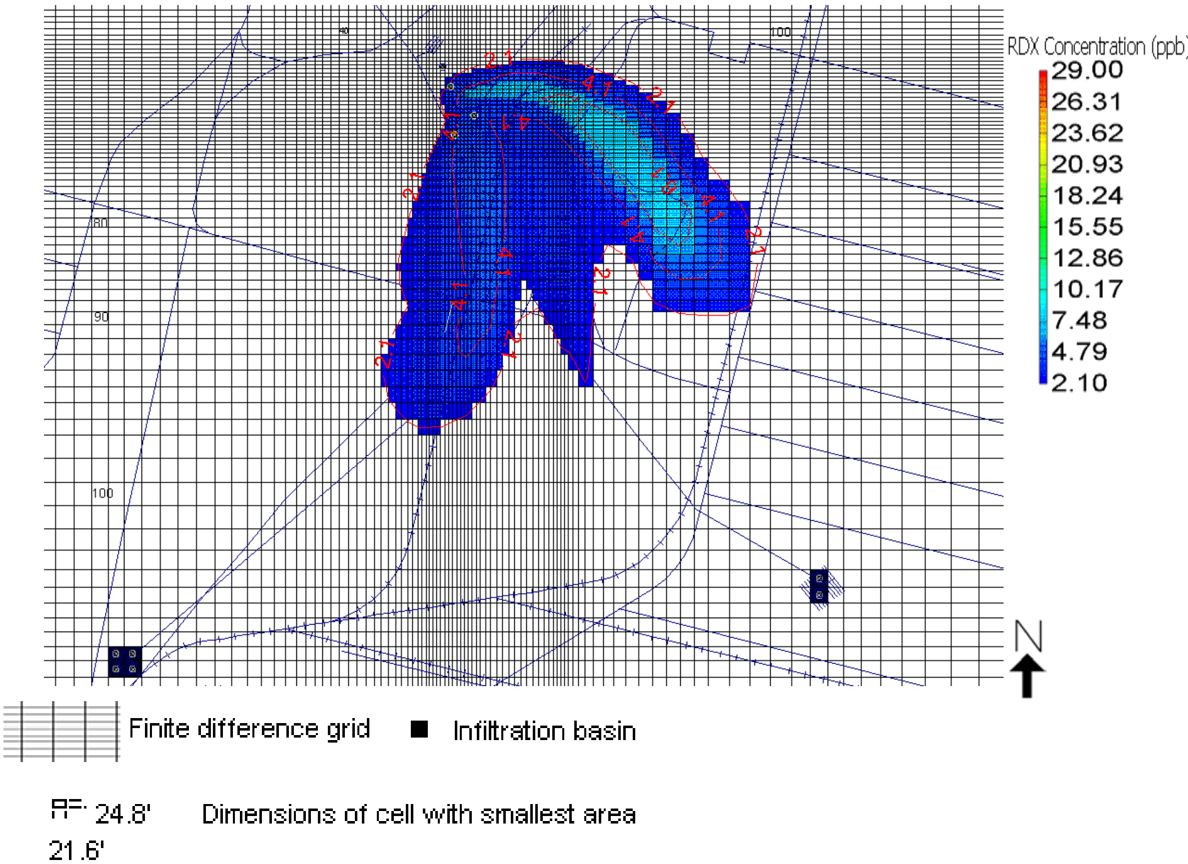


Fig. 11. Strategy USU1A: RDX concentrations ≥ 2.1 ppb after 3 years of pumping.

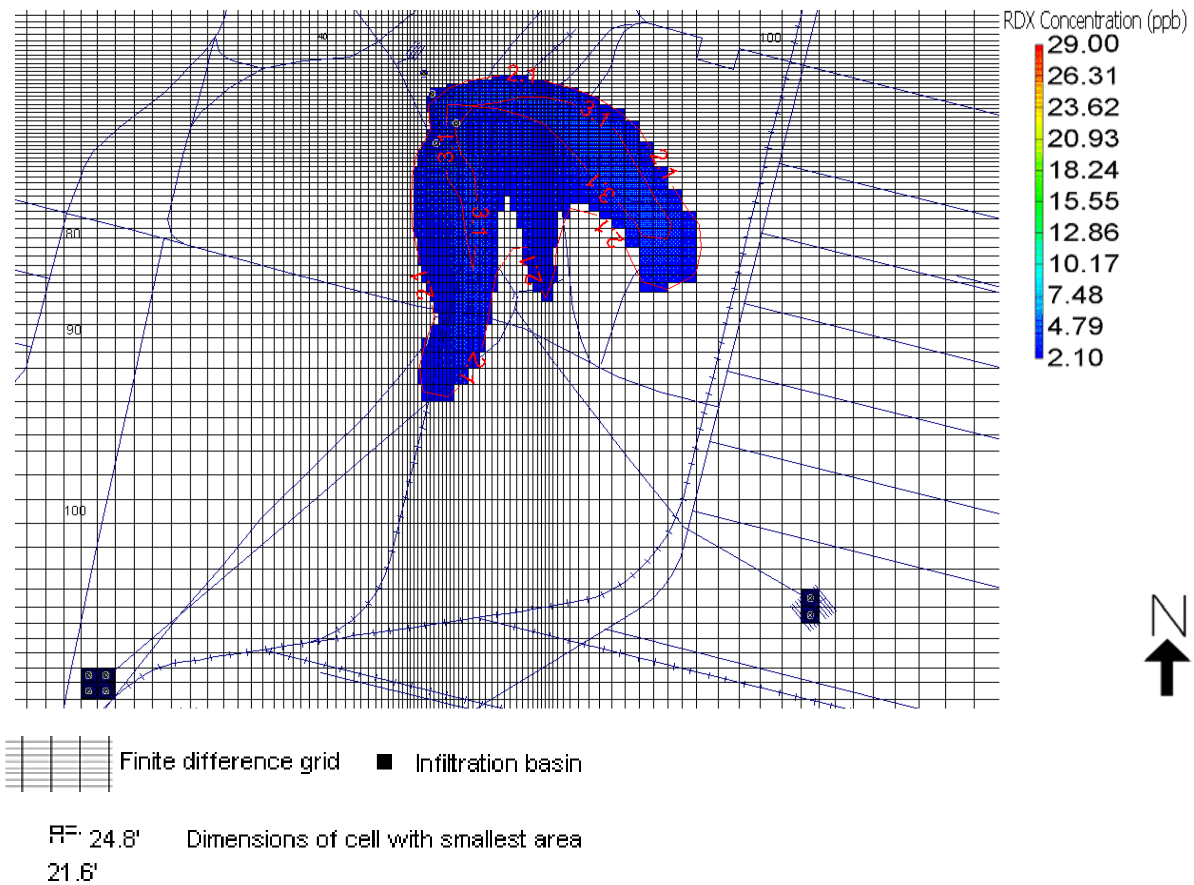


Fig. 12. Strategy USU1A: TNT concentrations ≥ 2.8 ppb after 1 year of pumping.

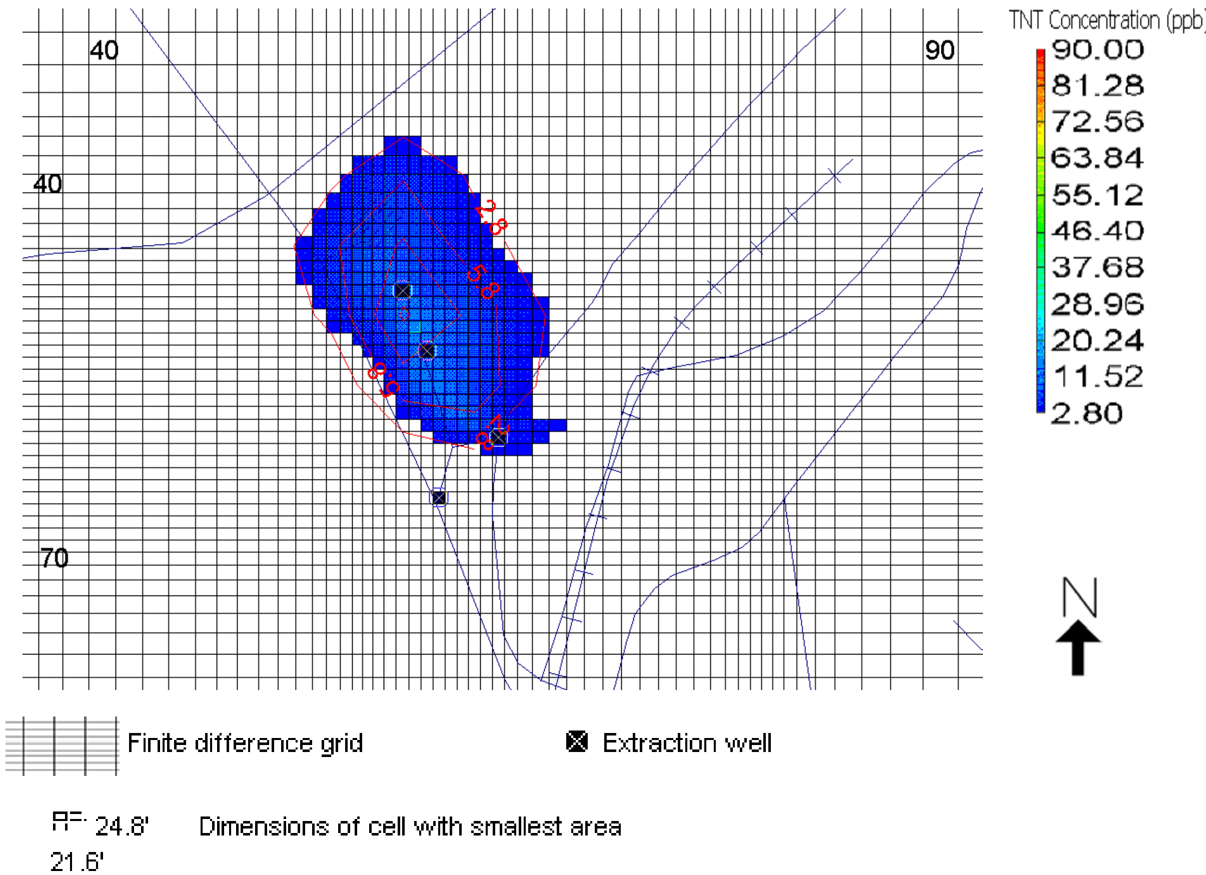


Fig. 13. Strategy USU1A: TNT concentrations ≥ 2.8 ppb after 2 years of pumping.

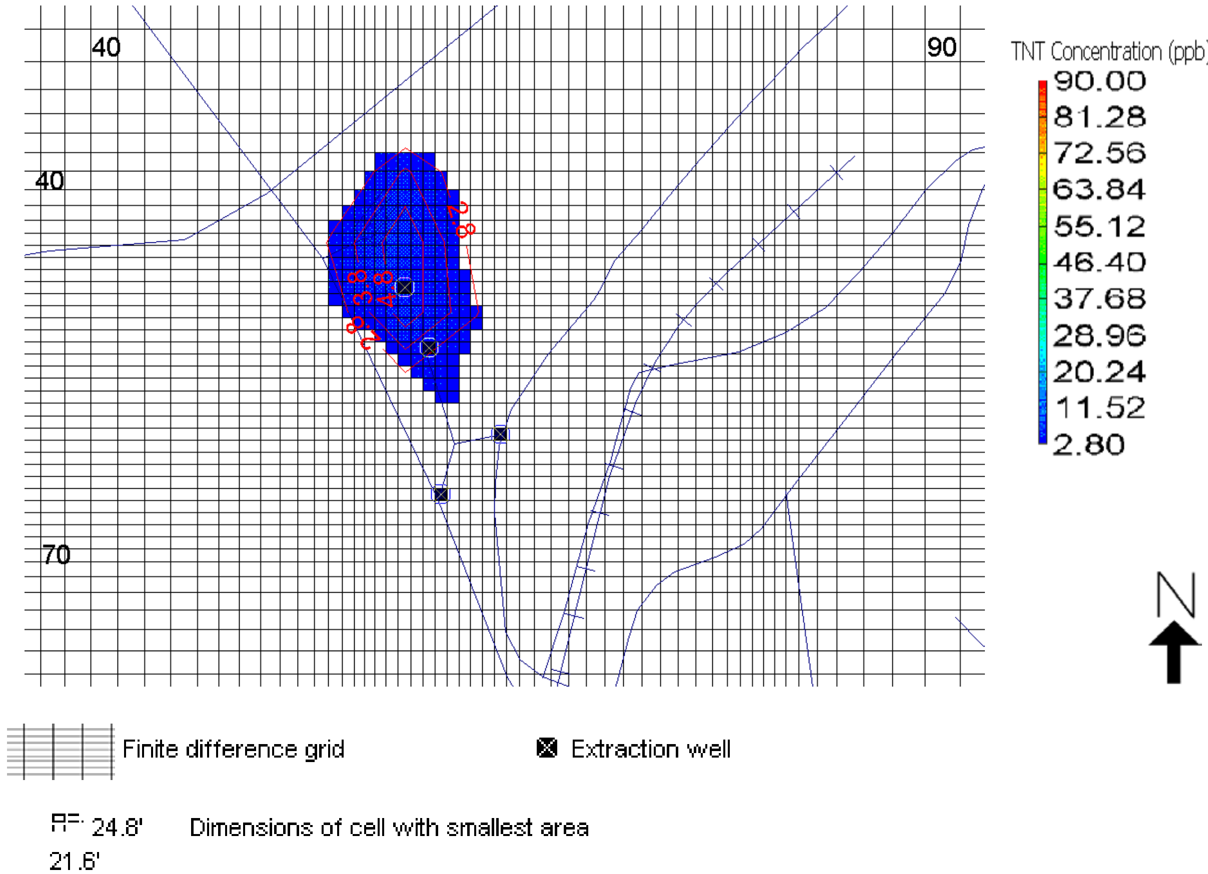


Fig. 14. Strategy USU1A: TNT concentrations ≥ 2.8 ppb after 3 years of pumping.

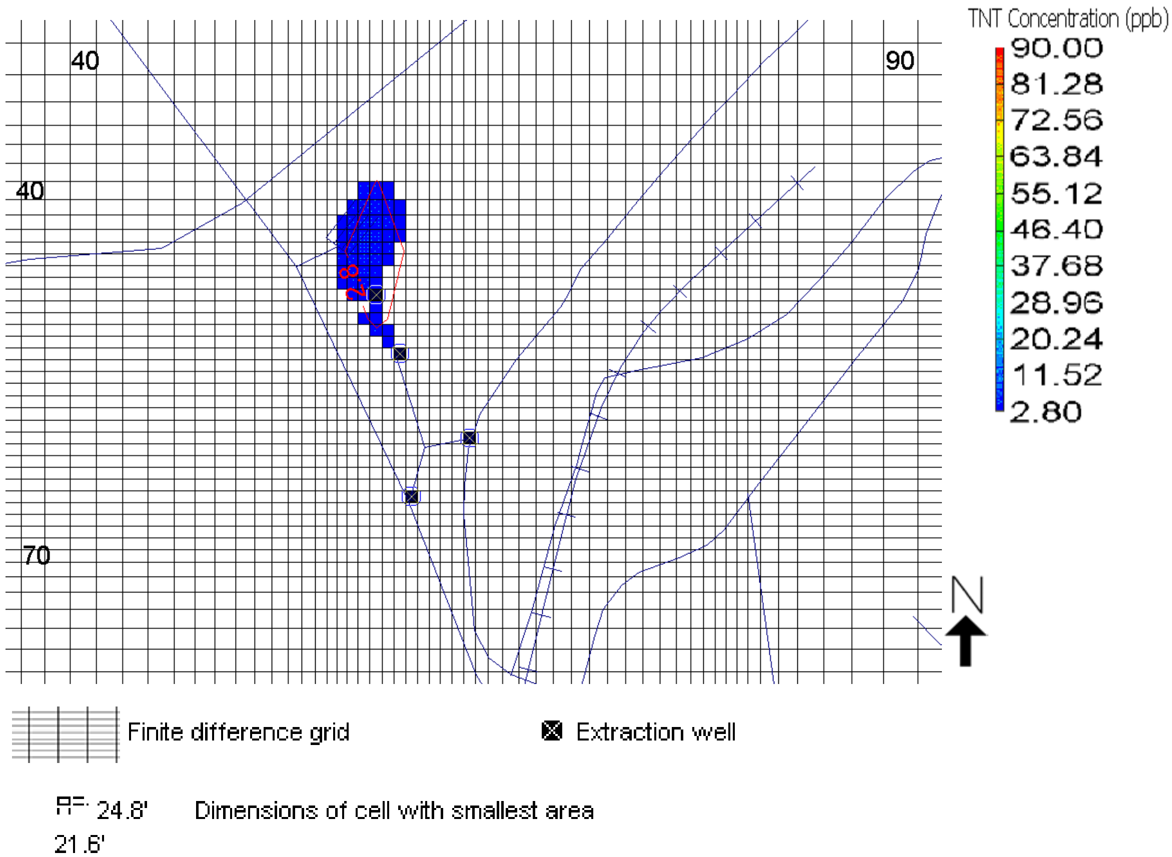


Fig. 15. Layer 1 hydraulic conductivity distribution (ft/day), and USU4 well locations.

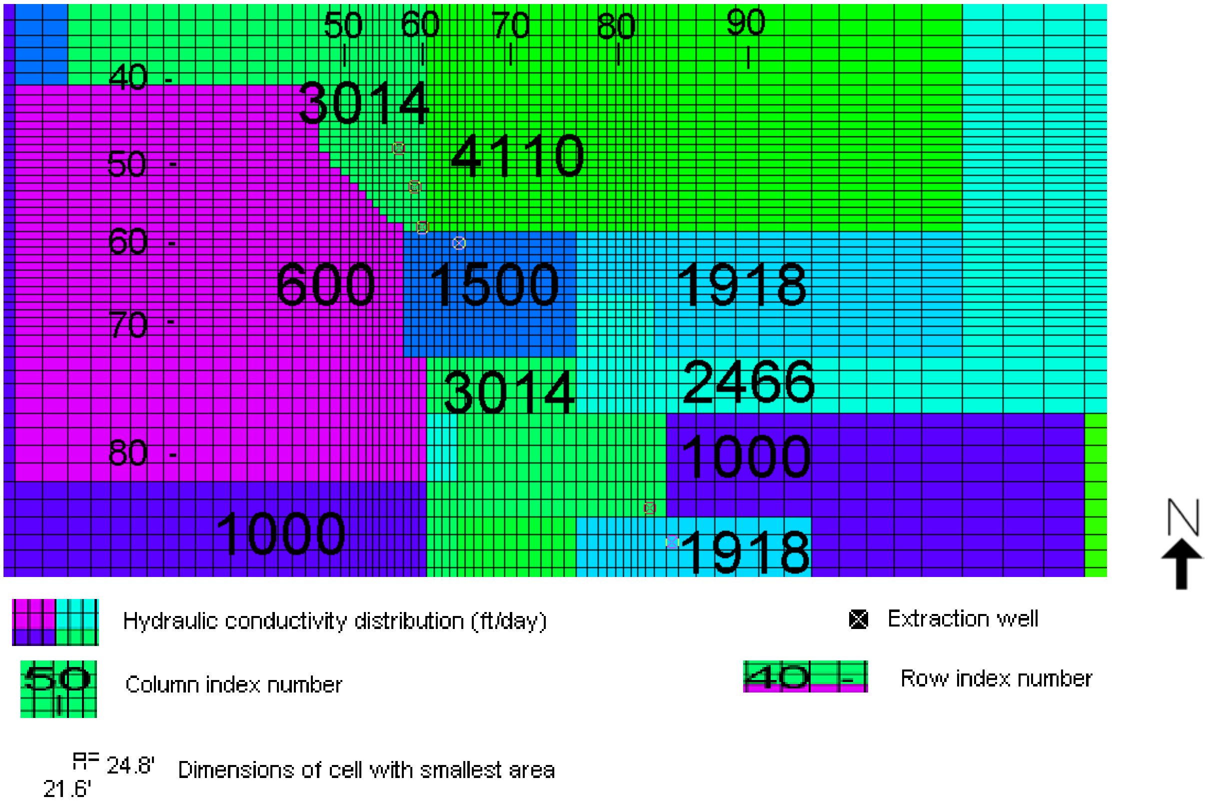


Fig. 16. Some feasible locations of well U-2 and selected robustness ranges.

Row \ Col	56	57	58	59	60	61	62	63	64	65
57										
58					0.84-1.07					
59		0.85-1.05								
60										well EW-1
61			0.88-1.08			0.87-1.08				
62										
63										
64										
65					0.9-1.17 well U2					

Note: Cleanup-in-4-years will be achieved if well U-2 is placed anywhere within this area, and pumped appropriately. Wavy lines indicate cells along existing pipelines.

Fig. 17. Optimization problem addressed by sequential optimization of four 5-year periods: minimize mass remaining after 20 years.

MINIMIZE Total Adsorbed & Dissolved RDX & TNT Mass After 20 Years

Subject to:

- Maximum RDX Forbidden Zone Conc. ≤ 2.1 ppb for 20 years
- Maximum TNT Forbidden Zone Conc. ≤ 2.8 ppb for 20 years
- Σ |Extraction| ≤ 1170 gpm
- Σ |Extraction| = Σ Injection
- Bounds on Pumping at Individual Wells

Fig. 18. USU3: heads after five years of pumping, and initial RDX ≥ 2.8 ppb.

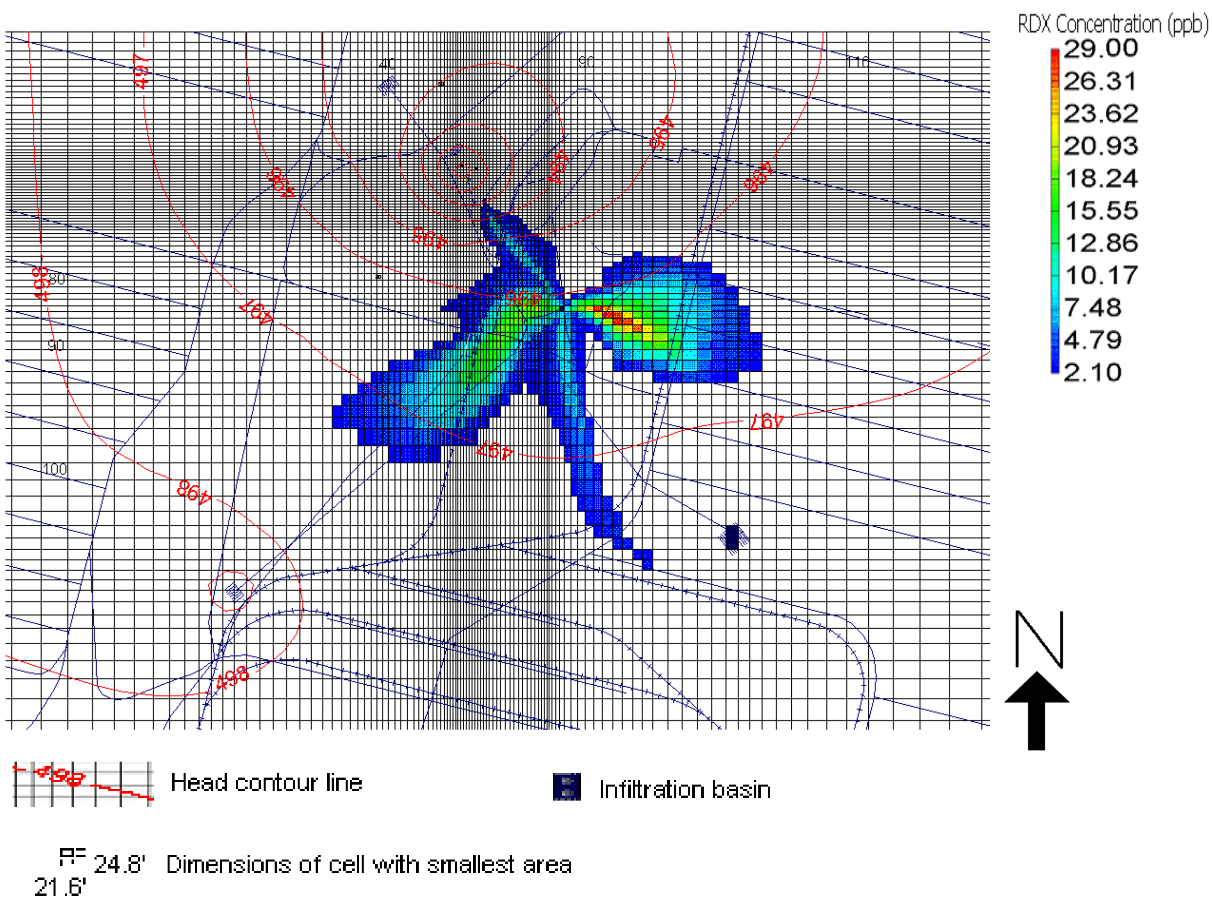


Fig. 19. Strategy USU3: time series of mass remaining.

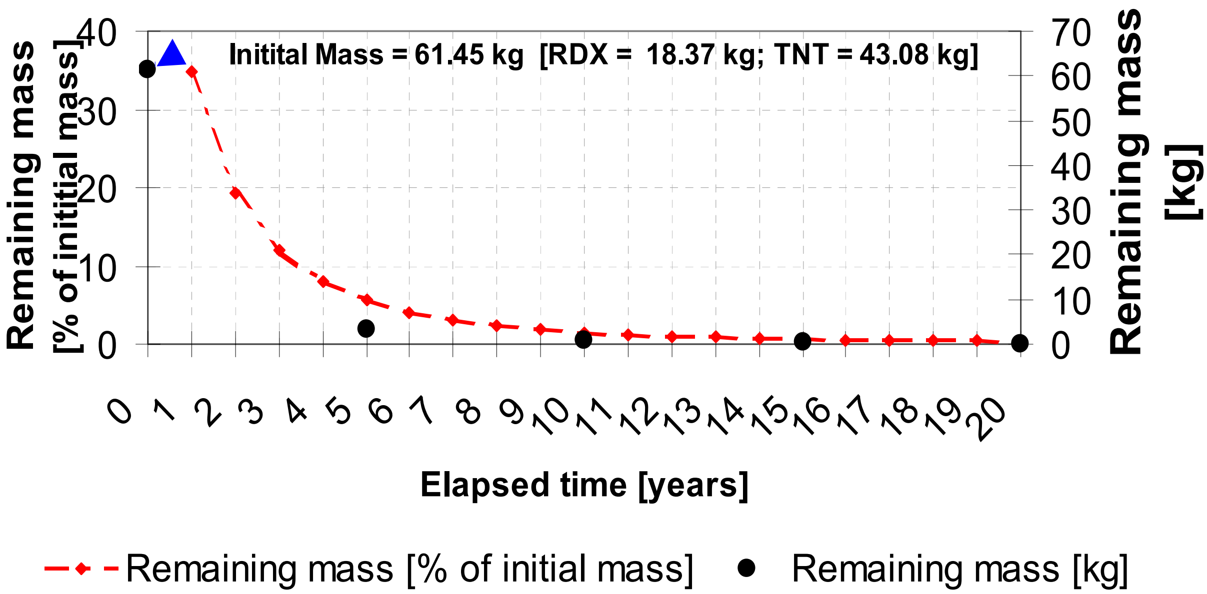


Fig. 20. Formulation 4 optimization problem (minimize cost to reach CL and continued pumping to minimize mass remaining).

MINIMIZE |Total Extraction|

Subject to:

- Maximum RDX Year-4 Cleanup Zone Conc.
  ≤ 2.1 ppb
- Maximum TNT Year-4 Cleanup Zone Conc.
  ≤ 2.8 ppb
- Maximum RDX Forbidden Zone Conc.
  ≤ 2.1 ppb for 20 years
- Maximum TNT Forbidden Zone Conc.
  ≤ 2.8 ppb for 20 years
- Σ |Extraction| ≤ 1170 gpm
- Σ |Extraction| = Σ Injection
- Bounds on Pumping at Individual Wells

Fig. 21. Modified USU4: cost to CLs versus conductivity multiplier.

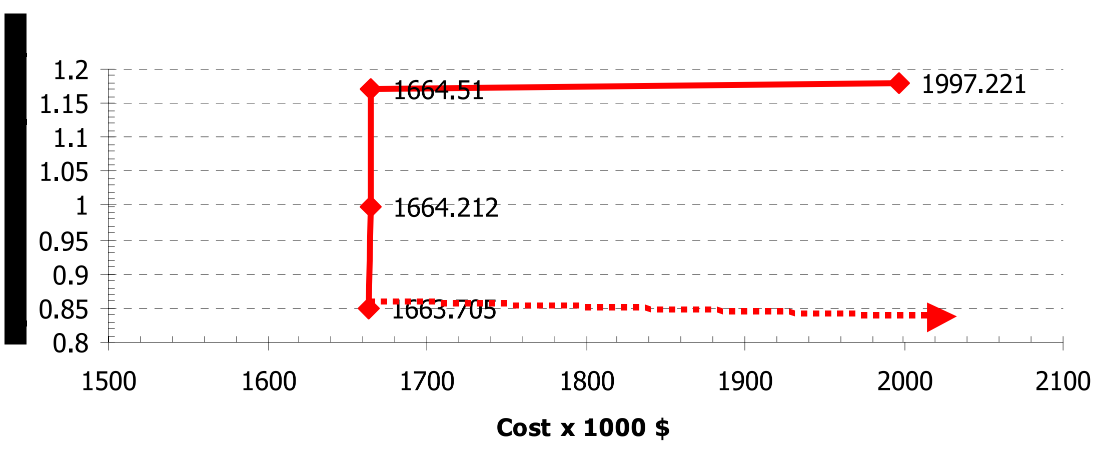


Fig. 22. Layer 1 bottom elevation and wells U-1, EW-3, and EW-1.

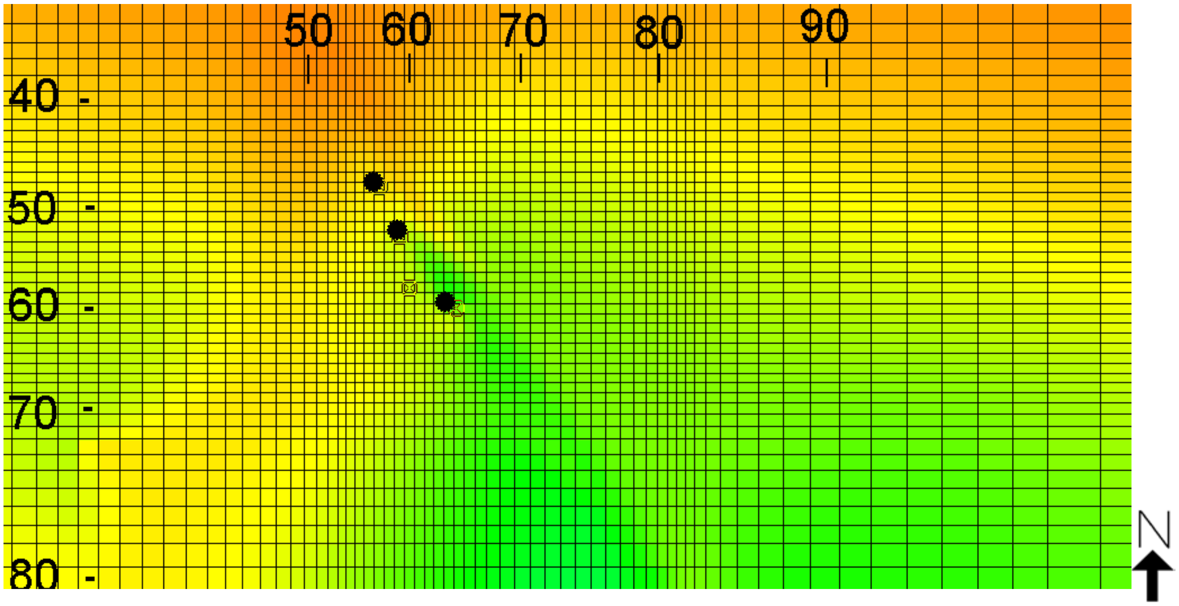


Fig. 23. Row 48, Layers 1-5 bottom elevations (ft MSL).

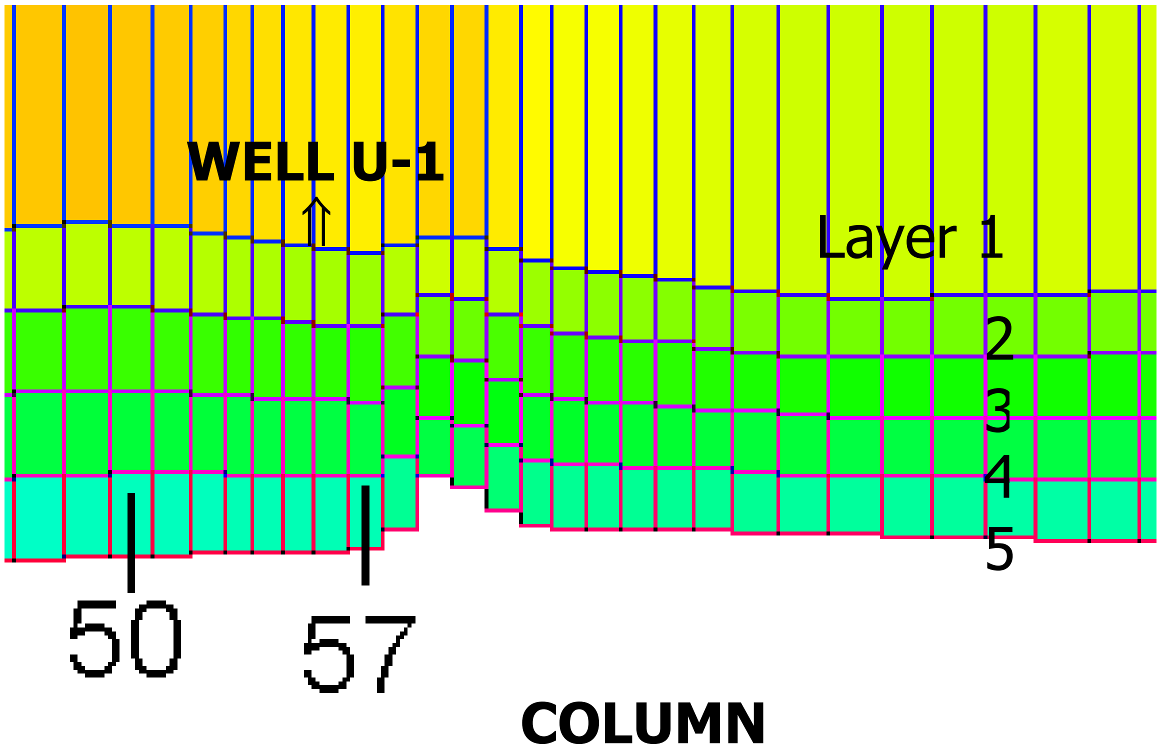
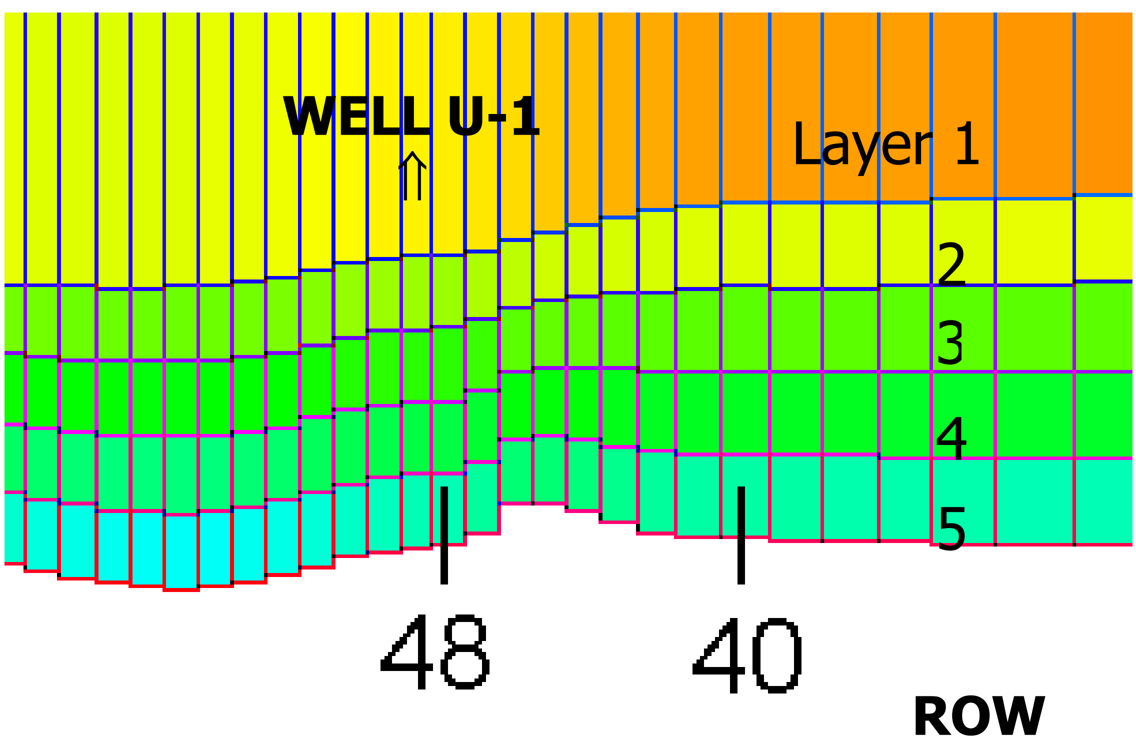


Fig. 24. Column 57, Layers 1-5, bottom elevations (ft MSL).



Appendix A. MODFLOW well package of Strategy USU1A.

```
10      0
10
 1     53      59 -24650000      1
 1     60      65 -25000000      2
 1    104     102  15903365      1
 1    105     102  15903365      1
 1    109      23  12312500      2
 1    109      24  12312500      2
 1    110      23  12312500      2
 1    110      24  12312500      2
 1     48      57 -25279700     13
 1     65      60  -6127030     69
 0
 0
 0
```

Appendix B. Post processor evaluation of Strategy USU1A.

Intermediate Variables Calculation

Cleanup Year for RDX
4
Cleanup Year for TNT
4
Cleanup Year for Formulation 1
4

Wells Used in Each Stress Period

Layer	Row	Column	Pumping Rate (gpm)	Concentration of RDX & TNT (ug/L) for Each Year					Zone #
Stress Period: 1									
1	53	59	350.770	15.867	7.692	4.416	2.706	1.780	1
1	60	65	355.750	11.781	5.457	3.327	2.207	1.530	1
1	48	57	359.730	10.702	5.494	3.191	1.963	1.265	1
1	65	60	87.188	7.015	4.861	3.100	1.938	1.218	1
Stress Period: 2									
Stress Period: 3									
Stress Period: 4									

Stress Period When EW-2 Starts
0

Number of New Wells in Each Stress Period
2
0
0
0

Number of New Recharge Basins in Each Stress Period
0
0
0
0

Total Pumping and Recharge Rates in Each Stress Period (gpm)

Pumping Rate	Recharge Rate
1153.437	1153.437
0.000	0.000
0.000	0.000
0.000	0.000

Number of GACs Installed in Each Stress Period
0
0
0

0

Plume Area at the Beginning of Each Stress Period

Stress Period	Plume Area (ft*ft)
1	0.399956E+07
2	0.000000E+00
3	0.000000E+00
4	0.000000E+00

Objective Function Calculation

The Capital Costs of New Wells (thousand of dollars)
150.000

The Capital Costs of New Recharge Basins (thousand of dollars)
0.000

The Capital Costs of New GAC Units (thousand of dollars)
0.000

The Fixed Costs of Labor (thousand of dollars)
882.410

The Fixed Costs of Electricity (thousand of dollars)
13.404

The Variable Costs of Electricity for Operating Wells (thousand of dollars)
47.717

The Variable Costs of Changing GAC Units (thousand of dollars)
11.824

The Variable Costs of Sampling (thousand of dollars)
558.487

The Objective Function Value (thousands of dollars) for Formulation # 1
1663.841

Constraints Check-Out

--- Cleanup Year Constraint ---

The Cleanup Year
4
The Cleanup Year Constraint Satisfied

--- Total Pumping Rate Constraint ---

Maximum Pumping Rate (gpm) After Ajustment
1281.597
The Total Pumping Rate Constraint Satisfied

--- Pumping Capacity Constraint ---

The Pumping Capacity Constraint Satisfied

--- Pumping-Recharge Balance Constraint ---

The Pumping-Recharge Balance Constraint Satisfied

--- Buffer Zone Constraint ---

The Buffer Zone Constraint Satisfied

Number of Constraints Not Satisfied
0

Appendix C. MODFLOW well package of Strategy USU1B.

```
10        0
        10
         1       53        59 -25298000       1
         1       60        65 -25130400       2
         1      104       102  16546100       1
         1      105       102  16546100       1
         1      109        23  12277350       2
         1      109        24  12277350       2
         1      110        23  12277350       2
         1      110        24  12277350       2
         1       48        57 -25298000      13
         1       58        60-6475175.1      69
         0
         0
         0
```

Appendix D. Post processor evaluation of Strategy USU1B and USU4 cost.

Intermediate Variables Calculation

Cleanup Year for RDX
4
Cleanup Year for TNT
4
Cleanup Year for Formulation 1
4

Wells Used in Each Stress Period

Layer	Row	Column	Pumping Rate (gpm)	Concentration of RDX & TNT (ug/L) for Each Year					Zone #
Stress Period: 1									
1	53	59	359.991	13.876	7.082	4.087	2.509	1.617	1
1	60	65	357.606	11.171	5.340	3.275	2.159	1.460	1
1	48	57	359.991	10.486	5.301	3.026	1.837	1.163	1
1	58	60	92.142	10.750	5.622	3.569	2.357	1.585	1
Stress Period: 2									
Stress Period: 3									
Stress Period: 4									

Stress Period When EW-2 Starts
0
0
0
0

Number of New Wells in Each Stress Period
2
0
0
0

Number of New Recharge Basins in Each Stress Period
0
0
0
0

Total Pumping and Recharge Rates in Each Stress Period (gpm)

Pumping Rate	Recharge Rate
1169.728	1169.729
0.000	0.000
0.000	0.000
0.000	0.000

Number of GACs Installed in Each Stress Period
0
0
0
0

Plume Area at the Beginning of Each Stress Period

Stress Period	Plume Area (ft*ft)
1	0.399956E+07
2	0.000000E+00
3	0.000000E+00
4	0.000000E+00

Objective Function Calculation

The Capital Costs of New Wells (thousand of dollars)
150.000

The Capital Costs of New Recharge Basins (thousand of dollars)
0.000

The Capital Costs of New GAC Units (thousand of dollars)
0.000

The Fixed Costs of Labor (thousand of dollars)
882.410

The Fixed Costs of Electricity (thousand of dollars)
13.404

The Variable Costs of Electricity for Operating Wells (thousand of dollars)
48.391

The Variable Costs of Changing GAC Units (thousand of dollars)
11.509

The Variable Costs of Sampling (thousand of dollars)
558.487

The Objective Function Value (thousands of dollars) for Formulation # 1
1664.201

Constraints Check-Out

--- Cleanup Year Constraint ---

The Cleanup Year
4
The Cleanup Year Constraint Satisfied

--- Total Pumping Rate Constraint ---

Maximum Pumping Rate (gpm) After Adjustment
1299.975
The Total Pumping Rate Constraint Satisfied

--- Pumping Capacity Constraint ---

The Pumping Capacity Constraint Satisfied

--- Pumping-Recharge Balance Constraint ---

The Pumping-Recharge Balance Constraint Satisfied

--- Buffer Zone Constraint ---

The Buffer Zone Constraint Satisfied

Number of Constraints Not Satisfied
0

Appendix E. MODFLOW well package of Strategy USU3.

```
        17         0
        17
         1        53        59 -25181100    0.0000         1
         1        60        65  -5517132    0.0000         2
         1        83        84         0    0.0000         3
         1        85        86   -925246    0.0000         4
         1        30        39         0    0.0000         5
         1        30        40         0    0.0000         5
         1        31        39         0    0.0000         5
         1        31        40         0    0.0000         5
         1       104       102  15934507    0.0000         6
         1       105       102  15934507    0.0000         6
         1       109        23  12586853    0.0000         7
         1       109        24  12586853    0.0000         7
         1       110        23  12586853    0.0000         7
         1       110        24  12586853    0.0000         7
         1        48        57 -25296471    0.0000         8
         1        49        62 -25296471    0.0000         9
         1        82        89         0    0.0000        10
        17
         1        53        59 -16459520    0.0000         1
         1        60        65   -487211    0.0000         2
         1        83        84         0    0.0000         3
         1        85        86 -49452169    0.0000         4
         1        30        39         0    0.0000         5
         1        30        40         0    0.0000         5
         1        31        39         0    0.0000         5
         1        31        40         0    0.0000         5
         1       104       102  13262863    0.0000         6
         1       105       102  13262863    0.0000         6
         1       109        23  13922388    0.0000         7
         1       109        24  13922388    0.0000         7
         1       110        23  13922388    0.0000         7
         1       110        24  13922388    0.0000         7
         1        48        57 -15816378    0.0000         8
         1        49        62         0    0.0000         9
         1        82        89         0    0.0000        10
        17
         1        53        59 -25267530    0.0000         1
         1        60        65 -25132710    0.0000         2
         1        83        84         0    0.0000         3
         1        85        86         0    0.0000         4
         1        30        39         0    0.0000         5
         1        30        40         0    0.0000         5
         1        31        39         0    0.0000         5
         1        31        40         0    0.0000         5
         1       104       102  33129873    0.0000         6
         1       105       102  33129873    0.0000         6
         1       109        23   3989583    0.0000         7
```

```
   1     109      24   3989583    0.0000       7
   1     110      23   3989583    0.0000       7
   1     110      24   3989583    0.0000       7
   1      48      57 -25297905    0.0000       8
   1      49      62  -6519932    0.0000       9
   1      82      89         0    0.0000      10
  17
   1      53      59  -4625600    0.0000       1
   1      60      65 -10727161    0.0000       2
   1      83      84         0    0.0000       3
   1      85      86 -56203029    0.0000       4
   1      30      39         0    0.0000       5
   1      30      40         0    0.0000       5
   1      31      39         0    0.0000       5
   1      31      40         0    0.0000       5
   1     104     102  18798593    0.0000       6
   1     105     102  18798593    0.0000       6
   1     109      23  11153818    0.0000       7
   1     109      24  11153818    0.0000       7
   1     110      23  11153818    0.0000       7
   1     110      24  11153818    0.0000       7
   1      48      57 -10656658    0.0000       8
   1      49      62         0    0.0000       9
   1      82      89         0    0.0000      10
   0
   0
   0
```

Appendix F. Post processor evaluation of Strategy USU3.

Intermediate Variables Calculation

Cleanup Year for RDX
5
Cleanup Year for TNT
4
Cleanup Year for Formulation 3
5

Wells Used in Each Stress Period

Layer	Row	Column	Pumping Rate (gpm)	Concentration of RDX & TNT (ug/L) for Each Year					Zone #
Stress Period: 1									
1	53	59	358.327	17.254	7.434	4.262	2.713	1.824	1
1	60	65	78.509	14.008	6.268	3.686	2.330	1.525	1
1	85	86	13.166	3.710	2.598	1.958	1.482	1.130	2
1	48	57	359.969	10.837	5.217	2.876	1.709	1.077	1
1	49	62	359.969	8.792	5.252	2.964	1.715	1.078	1
Stress Period: 2									
1	53	59	234.219	1.303	0.922	0.678	0.528	0.428	1
1	60	65	6.933	1.166	0.767	0.546	0.412	0.326	1
1	85	86	703.704	0.855	0.617	0.464	0.364	0.294	2
1	48	57	225.067	0.601	0.439	0.347	0.286	0.242	1
Stress Period: 3									
1	53	59	359.557	0.405	0.329	0.261	0.211	0.176	1
1	60	65	357.638	0.342	0.294	0.247	0.209	0.179	1
1	48	57	359.989	0.250	0.193	0.148	0.116	0.093	1
1	49	62	92.779	0.137	0.112	0.087	0.068	0.054	1
Stress Period: 4									
1	53	59	65.822	0.092	0.072	0.062	0.055	0.050	1
1	60	65	152.647	0.138	0.107	0.092	0.085	0.079	1
1	85	86	799.769	0.148	0.129	0.115	0.104	0.095	2
1	48	57	151.644	0.064	0.055	0.049	0.045	0.041	1

Stress Period When EW-2 Starts
0

Number of New Wells in Each Stress Period
2
0
0
0

Number of New Recharge Basins in Each Stress Period
0
0
0
0

Total Pumping and Recharge Rates in Each Stress Period (gpm)

Pumping Rate	Recharge Rate
1169.940	1169.940
1169.923	1169.923
1169.963	1169.963
1169.883	1169.883

Number of GACs Installed in Each Stress Period

0
0
0
0

Plume Area at the Beginning of Each Stress Period

Stress Period	Plume Area (ft*ft)
1	0.399956E+07
2	0.000000E+00
3	0.000000E+00
4	0.000000E+00

Objective Function Calculation

The Objective Function Value for Formulation 3

Modeling Year	Total Mass (kg)
1	0.214336E+02
2	0.118565E+02
3	0.730877E+01
4	0.485722E+01
5	0.342060E+01
6	0.250539E+01
7	0.182308E+01
8	0.139118E+01
9	0.109925E+01
10	0.890838E+00
11	0.779986E+00
12	0.644179E+00
13	0.533321E+00
14	0.450442E+00
15	0.387926E+00
16	0.324332E+00
17	0.275754E+00
18	0.244063E+00
19	0.220426E+00
20	0.201546E+00

Constraints Check-Out

--- Cleanup Year Constraint ---

The Cleanup Year
5
The Cleanup Year Constraint Satisfied

--- Total Pumping Rate Constraint ---

Maximum Pumping Rate (gpm) After Adjustment
1299.959
The Total Pumping Rate Constraint Satisfied

--- Pumping Capacity Constraint ---

The Pumping Capacity Constraint Satisfied

--- Pumping-Recharge Balance Constraint ---

The Pumping-Recharge Balance Constraint Satisfied

--- Buffer Zone Constraint ---

The Buffer Zone Constraint Satisfied

--- Maximum Number of New Wells Constraint ---

Total Number of New Wells Ever Installed
2

The Maximum Number of New Wells Constraint Satisfied

--- Maximum Number of New Recharge Basins Constraint ---

Total Number of New Recharge Basins Installed
0

The Maximum Number of New Recharge Basins Constraint Satisfied

Number of Constraints Not Satisfied
0

Appendix G. MODFLOW well package of Strategy USU4.

```
16         0
        10
         1        53        59 -25298000      1
         1        60        65 -25130400      2
         1       104       102  16546100      1
         1       105       102  16546100      1
         1       109        23  12277350      2
         1       109        24  12277350      2
         1       110        23  12277350      2
         1       110        24  12277350      2
         1        48        57 -25298000      1
         1        58        60 -6475175.1     1
        11
         1        53        59 -13340419             1
         1        60        65  -2316275             1
         1        85        86 -39845276             1
         1       104       102   5639126             1
         1       105       102   5639126             1
         1       109        23  17732957             1
         1       109        24  17732957             1
         1       110        23  17732957             1
         1       110        24  17732957             1
         1        48        57 -25151224             1
         1        58        60  -1556887             1
        10
         1        53        59 -23220650             1
         1        60        65  -8370832             1
         1       104       102  36644934             1
         1       105       102  36644934             1
         1       109        23   2232304             1
         1       109        24   2232304             1
         1       110        23   2232304             1
         1       110        24   2232304             1
         1        48        57 -25298000             1
         1        58        60 -25298000             1
        11
         1        53        59  -1258190             1
         1        60        65  -2779435             1
         1        85        86 -55685551             1
         1       104       102  19463667             1
         1       105       102  19463667             1
         1       109        23  10822937             1
         1       109        24  10822937             1
         1       110        23  10822937             1
         1       110        24  10822937             1
         1        48        57 -16502323             1
         1        58        60  -5993585             1
```

Appendix H. Post processor evaluation of Strategy USU4, mass remaining after 20 Years.

Intermediate Variables Calculation

Cleanup Year for RDX
4
Cleanup Year for TNT
4
Cleanup Year for Formulation 3
4

Wells Used in Each Stress Period

Layer	Row	Column	Pumping Rate (gpm)	Concentration of RDX & TNT (ug/L) for Each Year					Zone #
Stress Period: 1									
1	53	59	359.991	13.876	7.082	4.087	2.509	1.617	1
1	60	65	357.606	11.171	5.340	3.275	2.159	1.460	1
1	48	57	359.991	10.486	5.301	3.026	1.837	1.163	1
1	58	60	92.142	10.750	5.622	3.569	2.357	1.585	1
Stress Period: 2									
1	53	59	189.834	1.415	1.011	0.740	0.566	0.450	1
1	60	65	32.961	0.987	0.606	0.406	0.289	0.218	1
1	85	86	566.998	0.849	0.630	0.483	0.385	0.317	2
1	48	57	357.902	0.882	0.642	0.492	0.388	0.313	1
1	58	60	22.155	1.154	0.802	0.590	0.453	0.360	1
Stress Period: 3									
1	53	59	330.430	0.386	0.320	0.249	0.196	0.160	1
1	60	65	119.117	0.243	0.233	0.216	0.187	0.161	1
1	48	57	359.991	0.260	0.199	0.151	0.117	0.092	1
1	58	60	359.991	0.372	0.309	0.250	0.202	0.169	1
Stress Period: 4									
1	53	59	17.904	0.135	0.090	0.065	0.054	0.049	1
1	60	65	39.551	0.118	0.086	0.078	0.075	0.072	1
1	85	86	792.405	0.157	0.136	0.121	0.109	0.099	2
1	48	57	234.828	0.082	0.066	0.056	0.050	0.046	1
1	58	60	85.289	0.133	0.104	0.088	0.081	0.076	1

Stress Period When EW-2 Starts
0

Number of New Wells in Each Stress Period
2
0
0
0

Number of New Recharge Basins in Each Stress Period
0
0

0
0

Total Pumping and Recharge Rates in Each Stress Period (gpm)

Pumping Rate	Recharge Rate
1169.728	1169.729
1169.849	1169.849
1169.528	1169.977
1169.978	1169.978

Number of GACs Installed in Each Stress Period

0
0
0
0

Plume Area at the Beginning of Each Stress Period

Stress Period	Plume Area (ft*ft)
1	0.399956E+07
2	0.000000E+00
3	0.000000E+00
4	0.000000E+00

Objective Function Calculation

The Objective Function Value for Formulation 3

Modeling Year	Total Mass (kg)
1	0.208232E+02
2	0.118566E+02
3	0.742740E+01
4	0.496478E+01
5	0.350699E+01
6	0.258748E+01
7	0.190936E+01
8	0.146831E+01
9	0.116503E+01
10	0.945788E+00
11	0.829639E+00
12	0.679414E+00
13	0.549668E+00
14	0.456678E+00
15	0.390606E+00
16	0.324306E+00
17	0.273408E+00
18	0.241318E+00
19	0.217828E+00
20	0.199073E+00

Constraints Check-Out

--- Cleanup Year Constraint ---

The Cleanup Year
4
The Cleanup Year Constraint Satisfied

--- Total Pumping Rate Constraint ---

Maximum Pumping Rate (gpm) After Ajustment
1299.975
The Total Pumping Rate Constraint Satisfied

--- Pumping Capacity Constraint ---

The Pumping Capacity Constraint Satisfied

--- Pumping-Recharge Balance Constraint ---

The Pumping-Recharge Balance Constraint Satisfied

--- Buffer Zone Constraint ---

The Buffer Zone Constraint Satisfied

--- Maximum Number of New Wells Constraint ---

Total Number of New Wells Ever Installed
2

The Maximum Number of New Wells Constraint Satisfied

--- Maximum Number of New Recharge Basins Constraint ---

Total Number of New Recharge Basins Installed
0

The Maximum Number of New Recharge Basins Constraint Satisfied

Number of Constraints Not Satisfied
0

Appendix E: Formulation Document and Final Reports, Tooele

Formulation Document

Transport Optimization Tooele Army Depot
Draft Mathematical Formulations
10/31/01

INTRODUCTION

Tooele Army Depot (TEAD) was established in 1942 to provide storage, maintenance and demilitarization of troop support equipment especially wheeled vehicles and conventional weapons. From 1942-1966, large quantities of hazardous materials were used and generated in these operations in the industrial area. During this time period, the waste chemicals were piped through the industrial complex into a set of four unlined drainage ditches. These ditches ended at a set of natural depressions that were used as evaporation (and infiltration) ponds. These ponds have been called the Old Industrial Waste Lagoon (Old IWL). In 1966, a collector ditch was constructed to intercept the four existing ditches. This interceptor ditch ran north approximately 1.5 miles to an abandoned gravel pit, called the Industrial Wastewater Lagoon (IWL), which was used as an evaporation pond until its closure in 1988 when an industrial wastewater plant was brought on line. The primary contaminant of concern was TCE used as a solvent in the repair operations of military equipment.

In 1983, the Army began investigating sources of contamination contributing to a plume of TCE (the “Main Plume”) that originated in the southeast portion of the Industrial Area and extends approximately 3.3 miles to the northwest. This plume was believed to have originated in the wastewater discharge through the unlined ditches to the original and then new evaporation ponds. A groundwater pump and treat system was put in place to treat this plume and prevent TCE concentrations greater than MCLs from crossing the property boundary. By the mid-1990’s however it became apparent that there was contamination associated with the Main Plume that could not have originated in the IWL system and must therefore have originated somewhere in the industrial area or perhaps in the Defense Reutilization ad Marketing Office (DRMO) yard. Therefore, The Main Plume originates from several source areas within the industrial area and the IWL.

More recently, an additional plume (the “Northeast Plume”) has also been identified. The Northeast Plume is originating from a recently identified point source in the industrial area, the oil/water separator at Building 679. The Northeast Plume extends beyond the property boundary, and the offsite extent is not fully characterized.

Groundwater flow trends in a northwest direction across TEAD. Uplifted, fractured bedrock in the central area of the Depot is a controlling hydrogeological feature. In general, the Depot can be divided into three separate hydrogeologic regimes, 1) the steep flow gradients of the fractured bedrock and adjoining low conductive alluvium in the central area of TEAD; 2) the highly transmissive alluvium in the northern part of the Depot and 3) the shallow alluvium at the southern upgradient end of the site. The uplifted bedrock block and adjoining low conductive alluvium are the hydraulically controlling features of the study area due to the steep gradients required for flow across this area. The uplifted bedrock block strikes roughly east-northeast and dips north–northwest. On the local scale the bedrock block exhibits strongly heterogeneous hydrogeology typical of fractured flow environments. Flow through the bedrock block consists of a steep gradient when entering the bedrock, a flatter gradient through the bedrock core and a steep gradient when exiting the bedrock.

A recent Independent Technical Review (ITR), Final Draft dated December 2000, at TEAD suggests that a risk-based approach be implemented. According to the ITR, the reissued Postclosure Permit (the principal legal driver for the site) will allow for the application of alternate concentration limits (ACL) via petition if:

> "The corrective action described … fails to meet the groundwater protection standard… and after the Permittee has demonstrated that all other feasible methods have been used to meet the groundwater protection standard, or (emphasis added) if in accordance with R315-101, a risk assessment concludes that a contaminant concentration greater than the concentration limits specified … poses no unacceptable risk to human health or the environment".

According to the ITR, the Utah RCRA Regulations at R315 also known as "the Risk Rule", upon which the Postclosure Permit is based, will also be legally applicable requirements for remediation. Under the Risk Rule, the magnitude of the level of risk present at a site determines the degree to which actions must be taken (i.e., no further action versus institutional controls versus active remediation). Two separate requirements are set out in the Risk Rule, which apply regardless of the presence or absence of risk at the site. First, the Risk Rule requires the responsible party to "take appropriate action to stabilize the site either through source removal or source control" [R315-101-2]. Referred to as stabilization, the agency will require in part that, all continuing sources be removed or contained as a part of remediation. Secondly, the Risk Rule requires "when closing or managing a contaminated site, the responsible party shall not allow levels of contamination in groundwater, surface water, soils, and air to increase beyond the existing levels of contamination at a site when site management commences" (referred to as the principle of non-degradation) [R315-101-3].

The ITR recommends that, for the Main Plume, the IWL and the industrial area should be considered one waste management area with the circumscribing line as the Point of Compliance (POC), and the downgradient property boundary considered as the Point of Exposure (POE). Using this approach, an Alternate Concentration Limit (ACL) is determined by establishing a contaminant concentration at the POC that will attain a concentration at the POE that is protective of human health and the environment taking into consideration the attenuation of contaminants between the POC and the POE. For the IWL/Industrial waste management area, the ACL would be the concentration of TCE at the POC that will result in a concentration of 5 ug/l of TCE at the POE.

Based on the ESTCP site visit at Tooele on May 31, 2001, the Northeast Plume is not well-defined, and for the purpose of our study, all formulations will include a specified well in the NE plume @ 1500 gpm (implemented as 1425 gpm in the well package to account for downtime of 5%, discussed later), to represent a general containment solution in that area.

DEFINITIONS SPECIFIC TO TOOELE FORMULATIONS

POE-MP — "Point of Exposure-Main Plume": TCE concentrations cannot exceed 5 ug/L for TCE at the POE-MP, evaluated in all model layers. POE-MP will be the property boundary, specifically at the cells in Table 1 (located at end of the formulation document).

POC-MPx — "Point of Compliance – Main Plume": POC-MP1 is defined as the southern boundary of the displaced sediments near Well P-3. It is in row106 and extends between model columns 25 and 36. POC-MP2 is defined as the boundary along the upstream edge of the low permeability gouge surrounding the bedrock, beginning at r106, c37 and ending at r103, c55 *with exception of three model cells which are one source cell and two adjacent cells*. These evaluations will be made in model layers 1 and 2. Specific cells for POC-MP1 and POC-MP2 are listed in Table 2 (located at the end of the formulation document).

PROPOSED FORMULATIONS

Each formulation consists of an objective function (to be maximized or minimized) and a set of constraints that must be satisfied. The formulations are provided in detail in the following pages and can be summarized as follows:

<u>Formulation 1</u>: Seven management periods, each 3 years. The objective function is to minimize a cost function, subject to: 1) POE-MP of 5ppb is achieved at the end of 1st management period (3 yrs) and all years thereafter; 2) a specified well location and pumping rate for addressing the NE plume is included; and 3) current capacity of the treatment plant is held constant and includes the specified pumping for the NE plume.

<u>Formulation 2</u>: Same as Formulation 1 (including the POE-MP constraint), but also add POC constraints: 1) POC-MP1 is 50% of the initial concentrations or ≤ 20 ug/l at the end of 1st management period (year 3) and thereafter; (2) POC-MP2 is 50ppb at the end of the 1st management period (3 yrs), and 20ppb at the end of 3rd management period (9 yrs) and thereafter.

<u>Formulation 3</u>: Same as Formulation 2 but with the following changes/additions: 1) source concentrations decline 25% each management period (i.e., source term in period 2 is 25% less than source term in period 1, source term in period 3 is 25% less than source term in period 2, etc.); 2) in addition to point-of-exposure and point-of-compliance constraints, cleanup (TCE ≤ 50 ppb) must also be achieved at a specified group of cells associated with the main plume in layers 1 to 4 within 3 management periods (9 yrs); and 3) maximum of 4 new extraction wells and 4 new injection wells can be installed for Main Plume not including the specified new well used for the NE Plume.

SPECIAL NOTES

<u>Fixed Well, NE Plume</u>

All formulations include a specified well in the NE plume @ 1500 gpm (implemented as 1425 gpm in the well package to account for downtime of 5%, discussed later). The fixed pumping for the NE plume will be implemented at one well location (row117, column 68, apportioned between layers 1 and 2 as weighted by transmissivity), to represent a generalized containment solution in that area without specifically developing an "optimal management solution" for the NE plume. *The fixed NE well will be counted towards total plant capacity, and included in the constraint balancing extraction and injection, but will not be included in any objective function terms based on number of wells and/or pumping rate (CCE, VCE, VCC) because it is common to all solutions. This new well for NE plume will also not be subject to the maximum well rate limit for new wells, since it is conceptual and not part of the management solution*.

<u>Treatment of Multi-Aquifer Wells</u>

Many of the existing wells in the model are "multi-aquifer", i.e., they screened in multiple model layers and therefore have multiple entries in the MODFLOW well package (one per model layer screened by the well). This is often done in models, and the rate specified in each model layer for a multi-aquifer well is usually calculated according to the weighted average of transmissivity in each layer.

For new wells in our study this becomes quite complicated, because new wells specified in the same row and column, but different layers, can represent either of the following two cases:

- Case 1: the multiple wells specified in the same cell but different layers represent one multi-aquifer well (i.e., capital cost is for only one well, limit on the maximum well rate applies to the combined well, and the ratio of rates between model layers must be consistent with the transmissivity of each layer).

  Since layer 1 in the model is defined as an unconfined aquifer, thus the transmissivity in layer 1 is calculated as a multiplier of hydraulic conductivity and saturated thickness that varies with time. The saturated thickness ranges 49.1-52.2ft based on simulated heads at the beginning of optimization simulation, i.e., 1/1/2003. To simplify the calculation, 50ft saturated thickness is used to calculate the transmissivity in layer 1 for the purpose of establishing ratios for multi-aquifer wells.

- Case 2: the multiple wells specified in the same cell but different layers represents a different new well in each layer (i.e., capital cost are incurred for more than one well, the limit on maximum rate applies separately to each well, and the well rate in each layer need not conform to transmissivity ratios between layers).

Our optimization problem allows for either type of new well (if not, the formulation would be unrealistically restrictive). However, the user will need to keep track of which case is being employed for situations where new wells are specified in the same row and column, but different layers, so that the objective function and constraints can be properly evaluated.

Well Numbers Must Be Specified in Well Package

To differentiate between Case 1 and Case 2 described above, an additional column (after layer, row, column, and rate) is needed in the WEL package for each cell to indicate well number for extraction wells or injection wells. There are 16 extraction wells and 13 injection wells in the current system, and the fixed NE plume well is counted as extraction well #17, thus any new extraction well has to start at number 18 and in ascending order thereafter, e.g., 18, 19, 20, ……, and any new injection well has to start at number 14 and in ascending order thereafter, e.g., 14, 15, 16, ……Use the same number more than once to indicate a multi-aquifer well.

The FORTRAN postprocessor being provided by GeoTrans will calculate the number of new extraction wells and number of new injection wells based on well numbers assigned by users. The FORTRAN postprocessor will also check the transmissivity ratios for multi-aquifer wells and output the error messages if the rates don't obey the transmissivity ratio rule.

Different MT3D Model for Formulation 3

Note that formulation 3 has a different source term than the other formulations to account for declining source strength over time. Therefore, two versions of the MT3d source/sink file will be distributed, one for the first two formulations, and the other for the third formulation.

Feasible Solutions

GeoTrans has determined feasible (though certainly sub-optimal) solutions for formulations 1 and 2. Each involves a large number of new extraction and injection wells (there is no specific limits on new wells in Formulations 1 and 2, although it is likely sub-optimal to have so many new wells). Well packages for those runs will be provided to each modeling group. For formulation 3, there is a limit of 4 new extraction wells and 4 new injection wells, plus a constraint on cleanup. GeoTrans found a solution that satisfies the cleanup constraints, but does not satisfy the constraint on # of new wells (that well package will also be provided to each modeling group). If a modeling group feels Formulation 3 as stated is infeasible after trying to solve it, they report that result. Additionally, if they choose to (but not required) they can determine and report the minimum number of new wells (extraction and injection) they determine is necessary to meet all the other constraints including the cleanup constraint (i.e., by relaxing the limits on number of new extraction and injection wells).

Formulation #1

This formulation includes

- 7 management period of 3 years, total 21 years
- POE-MP = 5 ppb at end of 1st management period
- Specified well location and rate to address NE Plume (detailed earlier)
- No capital cost limits
- Continuous source
- Existing limits on existing extraction well rates and treatment plant rates (no limit on # added extraction/injection wells as long treatment plant capacity not exceeded)
- Limit of 400 gpm on new pumping wells, 600 gpm on new injection wells

Formulation 1 -- Definitions

year – the modeling year defined by

$$year = \text{Roundup}(elapsed\ modeling\ years)$$

- January 1, 2003 corresponds to zero elapsed modeling years
- 2003 corresponds to *year* =1
- The end of June 2004 corresponds to about 1.5 elapsed modeling years and *year* =2
- **Roundup**() is a function to convert a real number into an integer by rounding up (i.e., 1.0 → 1 but 1.1 → 2).

d – use 5%, this represents the conversion of capital and annual costs incurred to present value (i.e., discounted) with the following discount function:

$$PV = \frac{cost}{(1+rate)^{year-1}}$$

- PV is the present value of a *cost* incurred in *year* with a discount rate of *rate*
- No discounting is done for all costs for *year*=1(i.e., 2003)
- All costs in subsequent years are discounted at the ends of those years
- Example 1: Assuming a discount rate of 5% and a $1000 cost incurred at any time during 2003 (*year*=1) the present value of the cost is $1000
- Example 2: Assuming a discount rate of 5% and a $1000 cost incurred in 2004 (*year*=2), the present value of that cost is $1000/1.05=$952.38.

management period – 3-year periods during which the pumping rates cannot be modified. Modifications may only be made during the initial time step of each management period.

Formulation 1-- Objective Function

This function minimizes total cost over 21 years. This function must be evaluated at the end of every year, rather than after every management period, to properly account for discounting of annual costs. All costs are in thousands of dollars.

MINIMIZE (CCE + CCI + FCO + VCE + VCS + VCC)

CCE: Capital costs of new extraction wells (does not include fixed well in NE plume)

$$\text{CCE} = \sum_{i=1}^{ny} (307 \times NW_i)^d$$

ny is total number of the modeling years, i.e., 21 years
NW_i is the total number of new extraction wells installed in year *i*. New wells may only be installed in years corresponding to the beginning of a 3-yr management period. Capital costs are not incurred for operating a well that previously has been in service (i.e., already installed).
$307K is cost of installing a new extraction well.
d indicates application of the discount function to yield Net Present Value (NPV).

****note: see discussion regarding "Treatment of Multi-Aquifer Wells" with respect to how the number of new wells is determined*

CCI: Capital costs of new injection wells

$$\text{CCI} = \sum_{i=1}^{ny} (223 \times NIW_i)^d$$

ny is total number of the modeling years, i.e., 21 years
NIW_i is the total number of new injection wells installed in year *i*. New wells may only be installed in years corresponding to the beginning of a 3-yr management period. Capital costs are not incurred for operating a well that previously has been in service (i.e., already installed).
$223K is cost of installing a new injection well.
d indicates application of the discount function to yield Net Present Value (NPV).

****note: see discussion regarding "Treatment of Multi-Aquifer Wells" with respect to how the number of new wells is determined*

FCO: Fixed cost of O&M any year system operates

$$\text{FCO} = \sum_{i=1}^{ny} (525)^d$$

ny is total number of the modeling years, i.e., 21 years
\$525K is the fixed annual O&M cost.
d indicates application of the discount function to yield Net Present Value (NPV).

VCE: Variable electrical costs of operating wells (based on fixed electric cost per well, does not include fixed well in NE plume)

$$VCE = \sum_{i=1}^{ny} \sum_{j=1}^{nwel} \left(34.5 \times IW_{ij}\right)^d$$

ny is total number of the modeling years, i.e., 21 years
nwel is the total number of extraction wells.
\$34.5K is the electrical cost operating an extraction well
IW_{ij} is a flag indicator; 1 if the extraction well *j* is on in year *I* (do not include fixed well in NE plume), 0 otherwise.
d indicates application of the discount function to yield Net Present Value (NPV).

VCS: Variable cost of sampling

$$VCS = \sum_{i=1}^{ny} \left[208 \times (A_i / IA)\right]^d$$

ny is total number of the modeling years, i.e., 21 years
IA is the initial plume area (118,720,000 sq. ft.) as determined from the model in January 2003, based on TCE > 5.0 µg/l in any of the model layers, within the property boundary (calculated this way based on installation request, so that future sampling off the base property will account for scaled up costs relative to current sampling appropriately)
\$208K is the sampling cost (as of January 2001) and considers both labor and analysis.
d indicates application of the discount function to yield Net Present Value (NPV).
A_i is the plume area during year *I*, including on-site and off-site. The plume area is only measured at the beginning of a management period; therefore, A_i can only change during years corresponding to the beginning of a management period. A_i is measured as the composite summed area of all model grid cells in all four layers that are not "clean" at the beginning of the management period, where "clean" is less than or equal to 5.0 µg/l.

$$A_i = \sum_{j=1}^{m} \sum_{k=1}^{n} \left[\Delta x_j \Delta y_k \times IC_{jk}\right]$$

m is the number of grid cells in the *x* direction
n is the number of grid cells in the *y* direction
Δx_j is length of the *j*th grid space in the *x* direction.
Δy_k is the length of the *k*th grid space in the *y* direction.

IC_{jk} is a flag

$$\begin{aligned} &If\ (C_{jk}^{l} > 5.0 \text{ ug/L}, \quad l = 1,2,3, \text{or } 4) \\ &\text{then } IC_{jk} = 1, \\ &\text{else } IC_{jk} = 0 \end{aligned}$$

C_{jk}^{l} is the concentration of TCE of layer l in the grid cell with indices j and k.

VCC: Variable cost of chemicals (does not include fixed well in NE plume)

$$\text{VCC} = \sum_{i=1}^{ny} (0.02 \times Q_i)^d$$

ny is total number of the modeling years, i.e., 21 years
Q_i is the total pumping rate in year *I (not including fixed well in NE plume)*.
$0.02K is unit cost of chemical per pumping rate, based on $109K/yr.
d indicates application of the discount function to yield Net Present Value (NPV).

Formulation 1 – Constraints

1) Modifications to the system may only occur at the beginning of each management period (i.e., the beginning of modeling years 1, 4, 7, 10, 13, 16, and 19).

2) The total modeled pumping rate (including fixed well for NE Plume), when adjusted for the average amount of uptime, cannot exceed 8000gpm, the current maximum treatment capacity of the plant.

$$Q^* / \alpha \leq 8000 \text{ gpm}$$

α: 0.95, a coefficient that accounts for the amount of average amount of uptime (i.e., model assumes up-time of 95% with α=0.95).
Q^*: the modeled flow rate in the well package (including 1425 gpm for NE plume).

When Evaluated: The beginning of each 3-year management period

3) POE-MP = 5ppb in each layer at the end of 1st management period and thereafter

At $year \geq 3$, and for each POE-MP location,

$$C_k \leq 5\,ppb$$

C_k : the TCE concentration at the *k*th POE-MP cell

When Evaluated: End of each year beginning with end of year 3.

4) Individual limits on rate at each extraction/injection well, as follows:

$$Q_i / \alpha \leq L_i$$

Q_i: Extraction or injection rate at well *i*
α: 0.95, a coefficient that accounts for the amount of average amount of uptime (i.e., model assumes up-time of 95% with α=0.95).
L_i: Limit on extraction/injection rate at well *i*

Extraction Well	*Limit L_i (gpm)*	*Well Number*	*Layers*	*Injection Well*	*Limit L_i (gpm)*	*Well Number*	*Layers*
E-1	*220*	*1*	*2*	*I-1*	*204*	*1*	*2*
E-2-1	*310*	*2*	*2*	*I-2*	*95*	*2*	*2,3*
E-2-2	*520*	*3*	*3*	*I-3*	*653*	*3*	*2*
E-3-1	*450*	*4*	*1,2*	*I-4*	*804*	*4*	*2*
E-3-2	*500*	*5*	*3*	*I-5*	*963*	*5*	*2*
E-4	*800*	*6*	*2*	*I-6*	*413*	*6*	*2,3*
E-5	*690*	*7*	*2*	*I-7*	*1188*	*7*	*2,3*
E-6	*320*	*8*	*2,3*	*I-8*	*786*	*8*	*2*
E-8	*220*	*9*	*2,3*	*I-9*	*739*	*9*	*2,3*
E-9	*850*	*10*	*2,3,4*	*I-10*	*728*	*10*	*2,3*
E-10	*850*	*11*	*3*	*I-11*	*603*	*11*	*2*
E-11	*650*	*12*	*2*	*I-12*	*402*	*12*	*2*
E-12	*211*	*13*	*2*	*I-13*	*229*	*13*	*2,3*
E-13	*580*	*14*	*2*				
E-14	*530*	*15*	*2,3*				
E-15	*640*	*16*	*2,3*				

The maximum extraction rate for new wells is 400 gpm. The maximum injection well flow rate for new injection wells is 600 gpm.

When Evaluated: The beginning of each 3-year management period

5) To balance pumping and reinjection (including pumping for NE plume):

ABS(Total simulated pumping - total simulated injection) ≤ 1 gpm

When Evaluated: The beginning of each 3-year management period

Formulation #2

This formulation includes

- 7 management period of 3 years, total 21 years
- POE-MP = 5 ppb at end of 1st management period
- Concentrations at POC-MP1 (Table 2) are 50% of initial concentrations or ≤ 20 ug/l at end of 1st management period (3 yrs).
- Concentrations at POC-MP2 (table 2) are reduced to 50 ppb by end of 1st management period (3 yrs) and further reduced to 20ppb by end of 3rd management period (9 yrs).
- Specified well location and rate to address NE Plume (discussed earlier)
- No capital cost limits
- Continuous source
- Existing limits on existing extraction well rates and treatment plant rates (no limit on # added extraction/injection wells as long treatment plant capacity not exceeded)
- Limit of 400 gpm on new pumping wells, 600 gpm on new injection wells

Formulation 2-- Definitions

Same as Formulation 1

Formulation 2-- Objective Function

Same as Formulation 1

Formulation 2 – Constraints

Same as Formulation 1 (five constraints), plus:

6) Concentrations at POC-MP1 in layers 1 & 2 are either 50% of initial concentrations or ≤ 20ppb at end of 1st management period (3 yrs) and thereafter.

   At $year \geq 3$, and for each POC-MP1 location,

$$CC_k \leq MAX\,(\,(SC_k/2),\ 20\,ppb)$$

   CC_k : the TCE concentration at the kth POC-MP1 cell
   SC_k : the TCE initial concentration at the kth POC-MP1 cell

   When Evaluated: End of each year beginning with end of year 3.

7) Concentrations at POC-MP2 in layers 1 & 2 are reduced to 50 ppb by end of 1st management period and further reduced to 20ppb by end of 3rd management period.

At $year \geq 3$, and for each POC-MP2 location,

$$CC_k \leq 50\,ppb$$

CC_k : the TCE concentration at the *k*th POC-MP2 cell

When Evaluated: End of each year beginning with end of year 3

At $year \geq 9$, and for each POC-MP2 location,

$$CC_k \leq 20\,ppb$$

CC_k : the TCE concentration at the *k*th POC-MP2 cell

When Evaluated: End of each year beginning with end of year 9

Formulation #3

This formulation includes elements of formulation 2:

- 7 management period of 3 years, total 21 years
- POE-MP = 5 ppb at end of 1st management period
- Concentrations at POC-MP1 (Table 2) are 50% of initial concentrations or ≤ 20 ug/l at end of 1st management period (3 yrs).
- Concentrations at POC-MP2 (Table 2) are reduced to 50 ppb by end of 1st management period (3 yrs) and further reduced to 20ppb by end of 3rd management period (9 yrs).
- Specified well location and rate to address NE Plume (discussed earlier)
- Existing limits on existing extraction and treatment plant rates
- Limit of 400 gpm on new pumping wells, 600 gpm on new injection wells

The following additions/modifications also apply

- Only up to 4 new extraction wells are allowed to be installed for the Main Plume (in addition to the new well specified for NE Plume)
- Only up to 4 new injection wells are allowed to be installed for the Main Plume
- Cleanup, defined as all specified cells (exempted cells from this constraint are specified in the FORTRAN postprocessor input file, and illustrated on Figure 2 and 3) must have TCE ≤ 50 ppb achieved within 9 years in layers 1-4
- Source reduction with 25% decline each management period relative to the previous period

Note that formulation 3 has a different source term than the other formulations. Therefore, two versions of the MT3d source/sink file will be distributed, one for the first two formulations, and the other for the third formulation.

Formulation 3-- Definitions

Same as Formulation 1, except the definition for *CLEANUP locations:*

CLEANUP locations - located in columns 1-55 (at request of installation, to represent main plume but not NE plume), and excepting specific locations immediately adjacent to source areas (see Figures 2 and 3 for exempted cells), these locations in layers 1-4 must be cleaned up (i.e., $TCE \leq 50\, ppb$) within 9 years

EXECEPTED locations - exempted cells are all locations in columns 56 and higher (layers 1-4), plus cells where the bedrock low-K zone is located (layers 1-4), plus cells where the source strength exceeds 50 ug/l at the end of year 9 (layer1 only), plus additional cells (layer 1 only) surrounding several high-concentration source cells (exempted cells from this constraint are specified in the FORTRAN postprocessor input file, and illustrated on Figures 2 & 3)

Formulation 3-- Objective Function

Same as Formulation 1

Formulation 3 – Constraints

Same as formulation 2 (seven constraints), plus:

8) Limit on number of new extraction wells is 4, at request of installation (in addition to the new well specified for NE Plume)

$$NEW \leq 4$$

NEW is the total number of new extraction wells (not including the NE plume well) installed over the entire management period of 21 years.

When Evaluated: The beginning of each 3-year management period

9) Limit on number of new injection wells is 4, at request of installation

$$NIW \leq 4$$

NIW is the total number of new injection installed over the entire management period of 21 years.

When Evaluated: The beginning of each 3-year management period

10) Cleanup constraints for the main plume.

At $year \geq 9$, and for each CLEANUP location (in each model layer),

$$C_k \leq 50\,ppb$$

C_k : the TCE concentration at the kth CLEANUP cell

When Evaluated: End of each year beginning with end of year 9.

Table 1. Cell Locations for POE-MP:

ROW	COL
41	30
42	31
43	32
44	33
45	34
45	35
46	36
47	37
48	38
49	39
49	40
50	41
51	42
52	43
53	44
54	45
54	46
55	47
56	48
57	49
58	50
58	51
59	52
60	53
61	54
62	55

Table 2. Locations for POC-MP1 and POC-MP2

POC-MP1:

ROW	COL
106	25
106	26
106	27
106	28
106	29
106	30
106	31
106	32
106	33
106	34
106	35

POC-MP2:

ROW	COL
106	36
106	37
107	38
107	39
108	40
108	41
108	42
{gap for source cell and two adjacent cells}	
108	46
108	47
108	48
108	49
108	50
108	51
108	52
108	53
108	54
108	55

Figure 1. Location of POE-MP, POC-MP1, and POC-MP2

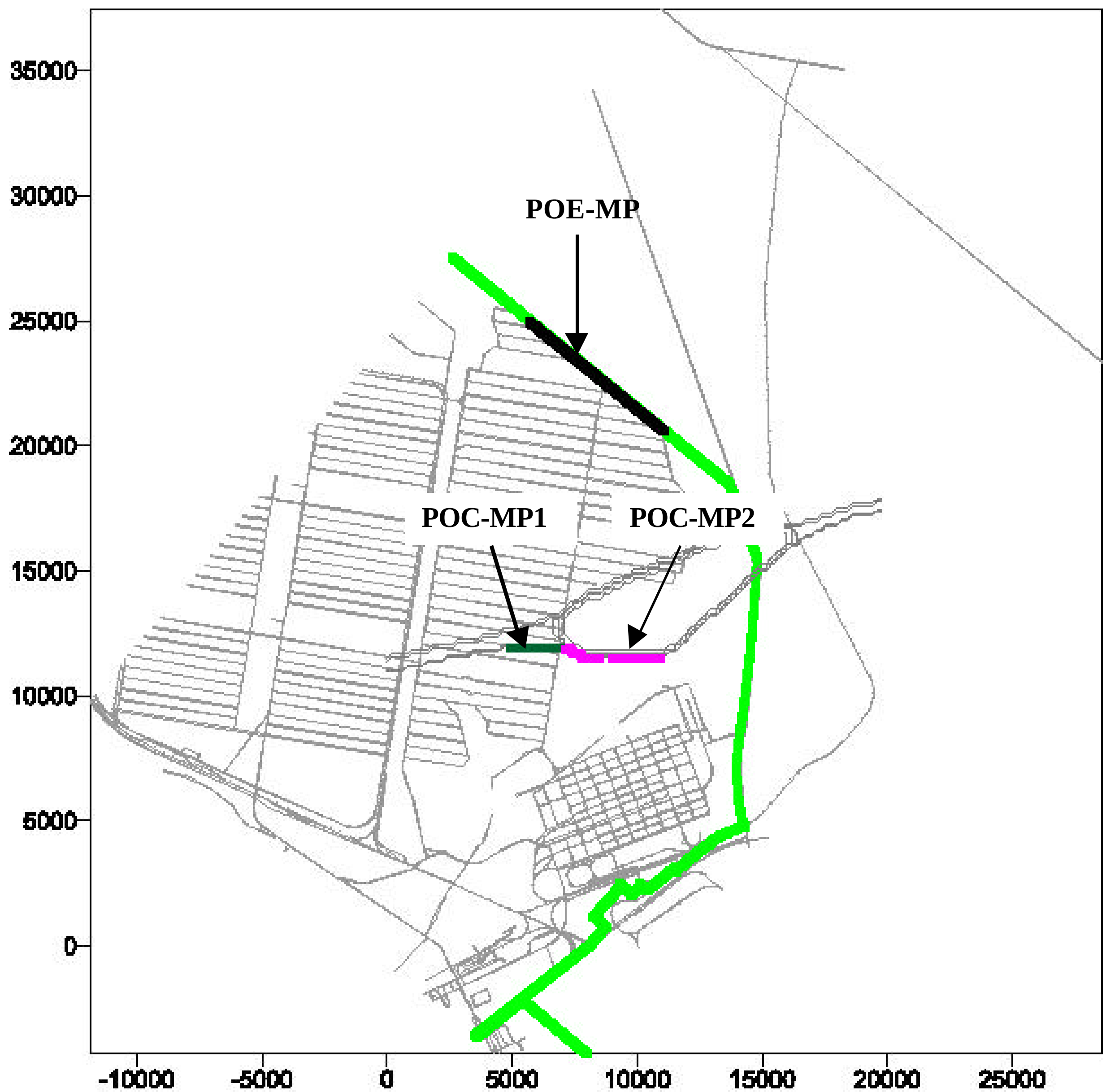


Figure 2. Location of Cells Exempted From Cleanup Constraint in Layer 1, Used in Formulation #3

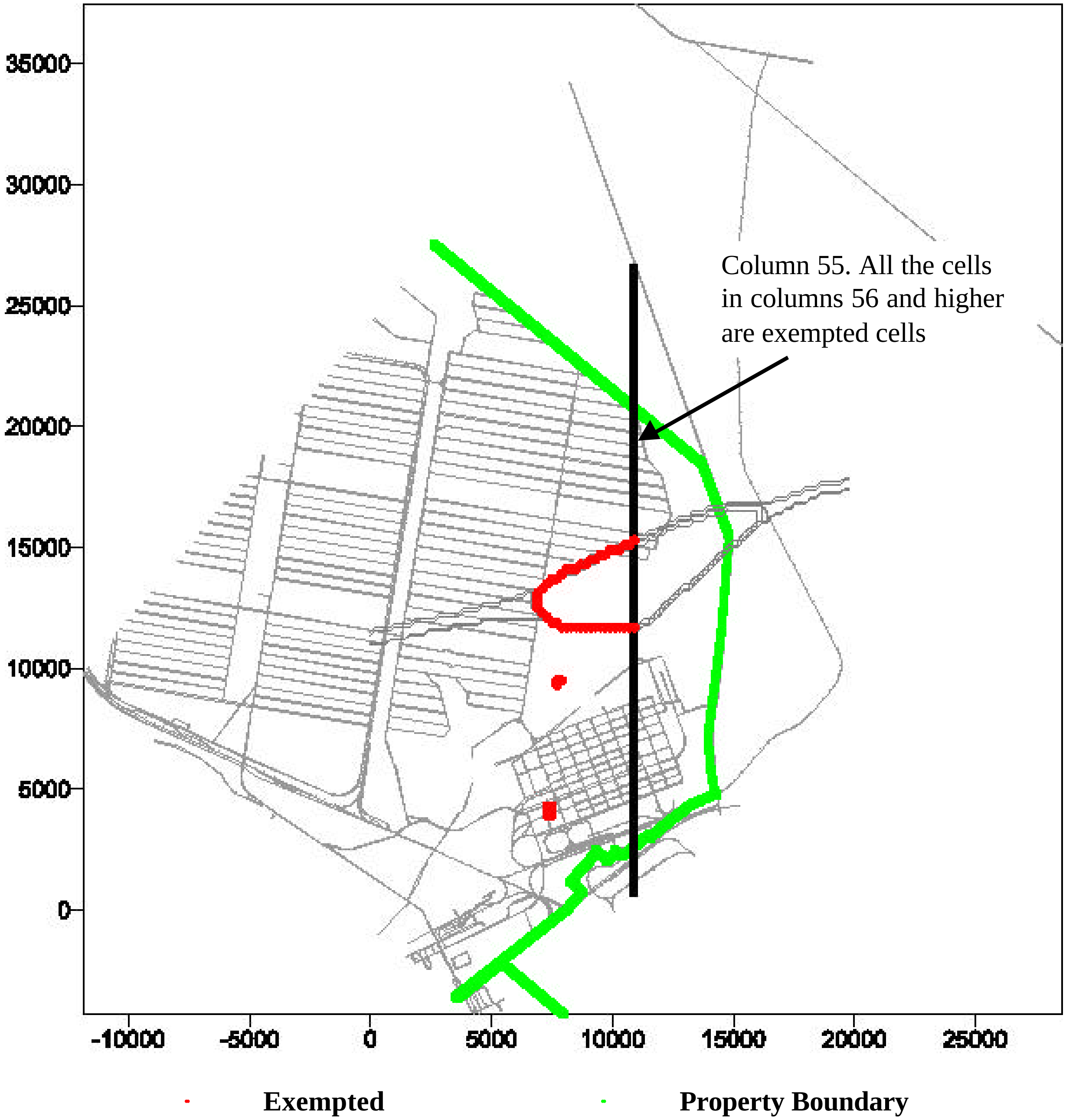
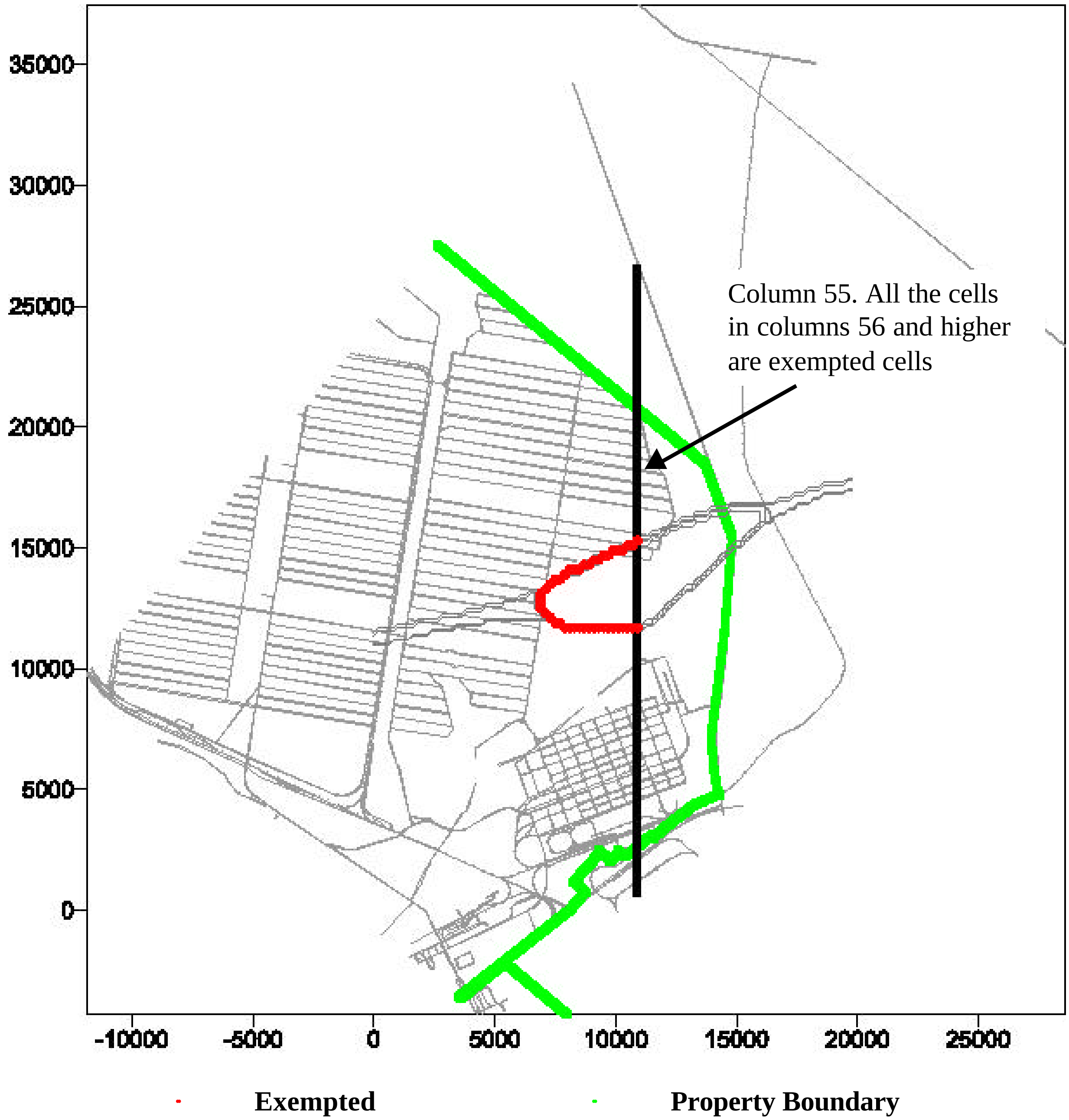


Figure 3. Location of Cells Exempted From Cleanup Constraint in Layers 2-4, Used in Formulation #3



GeoTrans Report on Tooele

OPTIMIZATION RESULTS: GEOTRANS

ESTCP TRANSPORT OPTIMIZATION PROJECT
SITE #2: TOOELE ARMY DEPOT

Prepared By:

Yan Zhang and Rob Greenwald
GeoTrans, Inc.
2 Paragon Way
Freehold, New Jersey 07728

NOTICE

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PREFACE

The goal of the ESTCP Transport Optimization project (“the project”) is to evaluate the effectiveness and cost/benefit of transport optimization software for pump-and-treat (P&T) system optimization. When coupled with a site-specific solute transport model, transport optimization software implements complex mathematical algorithms to determine optimal site-specific well locations and pumping rates. This demonstration project is intended to address the following scientific questions:

1) Do the results obtained from these optimization software packages (e.g. recommended optimal P&T scenarios) differ substantially from the optimal solutions determined by traditional "trial-and-error" optimization methods?

2) Do the results obtained from these optimization software packages warrant the additional effort and costs when compared to traditional "trial-and-error" optimization methods?

The project involves the determination of optimal extraction and pumping well scenarios at three Department of Defense (DoD) P&T systems. The installations are encouraged (but not required) to implement optimization suggestions resulting from the demonstration.

For each of the three sites, three site-specific optimization problems (“formulations”) will be defined. Each of three modeling groups will independently attempt to determine the optimal solution for each of the optimization formulations. Two of the modeling groups will use their own independently developed transport optimization software, and the other group (GeoTrans) will use a traditional "trial-and-error" optimization method as a control. Thus, the optimization recommendations from two separate transport optimization software programs will be compared to each other and to the recommendations from the trial-and-error control.

This report presents the “trial-and-error” results determined by GeoTrans for Site #2, which is the Tooele Army Depot in Tooele Valley in Tooele County, Utah. The three formulations for this site are described in detail in a separate document.

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1.0 OPTIMIZATION TECHNIQUE

GeoTrans applied “trial-and-error” optimization for each of the three formulations. The management horizon associated with each formulation consisted of seven 3-year management periods (21 years total), beginning January 2003. Each trial-and-error simulation involved modifying pumping wells (locations and rates) and injection wells (locations and rates) in the MODFLOW/MT3D well package. Pumping and recharge could be modified at the beginning of each of the 3-year management periods within a specific simulation.

The simulations discussed in this report were performed by GeoTrans between November 1, 2001 to February 28, 2002. The general optimization approach utilized by GeoTrans is described below.

<u>Step 1: Program FORTRAN Postprocessor</u>

For each simulation, it was necessary to evaluate the objective function value, and to determine if that simulation produced an improved solution relative to previous simulations. For each simulation it was also necessary to determine if all constraints were satisfied. For “trial-and-error” optimization, it was essential that the evaluation of objective function and constraints be done efficiently. Therefore, GeoTrans coded a FORTRAN program to read specific components of model input and output, and then print out the objective function value (broken into individual components) and all constraints that were violated. GeoTrans provided this FORTRAN code to the other modeling groups, to allow those groups to check their solutions (i.e., to make sure they had not made any errors in programming associated with their methods that would invalidate their results).

<u>Step 2: Develop “Animation” Approach</u>

The purpose of the animations was to clearly illustrate the plume movement over time based on simulation results. The animations were developed by creating a concentration contour map for model layers at the end of each year in the simulation, using SURFER, and then compiling those into a Microsoft PowerPoint file to allow the plume movement over time to be displayed as an “animation”. It is time consuming updating SURFER files manually and simply using copy-and-paste command since the components of the optimization formulations apply to all 4 model layers. Thus, a 3 part procedure was developed: 1) updating SURFER grid files automatically using SURFER script (22 files per layer, total 88 files); 2) exporting as image files automatically using SURFER script; and 3) importing the image files into Microsoft PowerPoint files automatically using MS macro.

<u>Step 3: Modify Pumping/Recharge, Run FORTRAN Code, and Create/Evaluate Animation</u>

This is the classic “trial-and-error” method. After each simulation, the FORTRAN code allowed immediate determination regarding the objective function value, and whether or not the run was feasible (i.e., all constraints satisfied). Based on evaluation of the animations for TCE, modified pumping/recharge strategies were selected for one or more subsequent simulations, to better address areas of relatively high concentrations and/or areas where cleanup was not progressing fast enough.

2.0 OPTIMIZATION RESULTS

2.1 Current System

2.1.1 Layout of Wells for Current System

The Main Plume sources were identified during 1980's to mid-1990's. A groundwater pump-and-treat (P&T) system was put in place for the Main Plume. The concentration distribution for TCE used as the initial condition for the optimization simulations (simulated concentrations at the end of 2002) is illustrated for model layer 1 on Figure 2-1, to provide an illustration of plume extent. The remedial design configuration for the current system is also shown in Figure 2-1. The current P&T system has 16 extraction wells and 13 injection wells. Well rates for the current system, as implemented in the model provided by the Installation, are listed below.

Well Rates, Current System

Extraction Well	Model Layer	Rate (gpm)	Injection Well	Model Layer	Rate (gpm)
E-1	2	313	I-1	2	89
E-2-1	2	74	I-2	2,3	85
E-2-2	3	306	I-3	2	364
E-3-1	1,2	254	I-4	2	511
E-3-2	3	271	I-5	2	557
E-4	2	269	I-6	2,3	422
E-5	2	565	I-7	2,3	858
E-6	2,3	382	I-8	2	383
E-8	2,3	157	I-9	2,3	501
E-9	2,3,4	463	I-10	2,3	539
E-10	3	519	I-11	2	403
E-11	2	354	I-12	2	259
E-12	2	0	I-13	2,3	212
E-13	2	431			
E-14	2,3	686			
E-15	1,2	418			
		Total Extraction: 5462			*Total Injection: 5183*

More recently, an additional plume, i.e., the Northeast Plume, has also been identified. The Northeast Plume extends beyond the property boundary, and the offsite extent is not fully characterized. Thus, for the purpose of the optimization formulations, a specified well with 1500 gpm pumping is implemented to represent a generalized containment solution in that area without specifically developing an "optimal management solution" for the Northeast Plume (detailed discussion on this is provided in the formulation document).

2.1.2 Constraint Evaluations for Current System

In the optimization formulations, the POE (Point of Exposure) boundary is defined as specific cells along the property boundary for the Main Plume (see formulation document for details). There are two POC (Point of Compliance) boundaries defined in formulations. The POC-MP1 is defined as specific cells at the southern boundary of the displaced sediments near Well P-3. The POC-MP2 is defined as specific cells at the boundary along the upstream edge of the lower permeability gouge surrounding the bedrock. Again, full details are included in the formulation document. The current system does not satisfy either of the POE, POC-MP1, and POC-MP2 constraints. Additionally, the formulations require balance between total pumping and total injection, and that constraint is not satisfied by the current system as represented by the model provided by the installation.

2.1.3 Costs for Current System

For three formulations, a cost function to be minimized was developed (in conjunction with the installation) that combines the "Up-Front Costs" with the "Total of Annual Costs" over a 21 year time frame, beginning January 2003, assuming a discount rate of 5%. The components of cost are:

MINIMIZE (CCE + CCI + FCO + VCE + VCS + VCC)

where

CCE: Capital costs of new extraction wells
CCI: Capital costs of new injection wells
FCO: Fixed cost of O&M
VCE: Variable electrical costs of operating wells
VCS: Variable costs of sampling
VCC: Variable cost of chemicals

The specifics of the cost function are provided in the detailed problem formulation (separate document). All costs are in thousands of dollars. Based on the modeling results, the value of the cost function for the current system (over a 21 year simulation period) is $19,364K.

2.2 Formulation 1: Minimize Cost, POE Constraint

2.2.1 Objective Function and Constraints

The objective function is to minimize the cost function over a 21 year time frame (see Section 2.1.3), subject to the following constraints:

- The modeling period consists of seven 3-year management periods (21 years total) beginning January 2003;

- Modifications to the system may only occur at the beginning of each management period;

- The total modeled pumping rate, when adjusted for the average amount of uptime, cannot exceed 8000gpm, the current maximum treatment capacity of the plant;

- The POE constraint, i.e., 5ppb, has to be met in each layer at the end of 1st three-year management period and thereafter;

- The extraction and injection wells cannot exceed the rate limits;

- The total pumping rate and total recharge rate have to be balanced.

The specifics of the cost function and detail of the constraints are provided in the detailed problem formulation (separate document).

2.2.2 Optimal Solution

For Formulation 1, a total of 21 major runs were performed, consisting of a total of 60 simulations (i.e., some major runs included a series of sub-runs). The best solution was found in major simulation 19 (total simulation 47), and has the following details:

Results, Formulation 1

	Current System	Optimal Solution
Objective Function (Total)	$19,364.303K	$14,628.049K
Number of New Extraction Wells	NA	4
Number of New Injection Wells	NA	0
Objective Function (Components)		
CCE: Capital costs of new extraction wells	0	1,228K
CCI: Capital costs of new injection wells	0	0
FCO: Fixed cost of O&M	7,067.663K	7,067.663K
VCE: Variable electrical costs of operating wells	6,966.696K	2,006.951K
VCS: Variable costs of sampling	3,859.485K	3,918.745K
VCC: Variable cost of chemicals	1,470.459K	406.69K

There are total four new extraction wells are included in the optimal solution. No new injection wells are included. Extraction rates and recharge rates, by management period, are listed below:

Optimal Rates, Formulation 1

Well	New or Existing	Location (Row,Col)	Layer	Period 1 (gpm)	Period 2-3 (gpm)	Period 4-7 (gpm)
E-2-1	Existing	(76,41)	2	294.5	294.5	0
E-11	Existing	(57,45)	2	323	323	0
NE Well	Fixed NE well	(118,69)	1,2	1425	1425	1425
NEW-1	New	(49,37)	1	250	0	0

Well	New or Existing	Location (Row,Col)	Layer	Period 1 (gpm)	Period 2-3 (gpm)	Period 4-7 (gpm)
NEW-2	New	(51,39)	1	355	355	355
NEW-3	New	(53,41)	1,2	380	380	380
NEW-4	New	(51,38)	2	380	380	380
Total Extraction				**3407.5**	**3157.5**	**2540**
I-1	Existing	(72,65)	2	193.8	193.8	193.8
I-2	Existing	(62,61)	2,3	90.3	90.3	90.3
I-3	Existing	(58,60)	2	620.4	620.4	620.4
I-4	Existing	(53,58)	2	763.8	763.8	763.8
I-5	Existing	(45,56)	2	324.3	434.3	16.8
I-6	Existing	(40,54)	2,3	355.0	355.0	355.0
I-9	Existing	(31,37)	2,3	500.0	700.0	500.0
I-10	Existing	(37,33)	2,3	560.0	0	0
Total Injection				**3407.6**	**3157.6**	**2540.1**

Locations of extraction wells and injection wells are presented in Figure 2-2. A chart illustrating objective function value versus simulation number is provided in Figure 2-3. A chart illustrating mass remaining after each year for this solution versus the current system is provided in Figure 2-4.

Note from Figure 2-4 that more mass remains in the system for this solution than for the current system. This is true for the both the main plume area and the area associated with the NE plume. This makes sense, since total pumping rate is reduced relative to the current system, and is also concentrated in downgradient portions of the plume. Note that total mass in the entire system actually goes up over time according to this solution (due to continuing sources and inefficient mass removal).

2.2.3 General Approach to Determining the Optimal Solution

It was evident from the cost function that total cost is impacted significantly by installation of new wells, so first priority was placed on minimizing the number of new wells. Once that was accomplished, attention was placed on lowering the pumping rate. The general approach used to determine the optimal solution for Formulation 1, via trial-and-error, can be summarized as follows (all simulation numbers refer to “major simulations”):

<u>Major Simulation 1</u>

In addition to current system, 4 new pumping wells were installed along the POE boundary with continuous pumping for 21 years. All the constraints were achieved and the total cost was $20,416K.

Major Simulation 2

To meet the POE constraint, not all the current wells were necessary. Thus, the existing wells except E-1 and E-11 were turned off, and. 4 new pumping wells and 1 new injection well were installed. The POE constraint wasn't achieved because one POE cell was barely above 5ppb. The total cost was $15,841K.

Major Simulations 3-4

Try to push the plume towards the pumping wells by shifting the injection rates among the injection wells. No feasible solution was found.

Major Simulation 5

Combine simulations 1 and 2, i.e., same 4 new pumping wells as Simulation 1 but keep only existing wells E-1 and E-11 on. All the wells were pumping continuously for 21 years. The POE constraint were achieved and the total cost was $15,623K.

Major Simulations 6-11

To reduce the total cost, attempt to decrease VCE and VCC terms in the cost function by shutting off some pumping wells and/or lowering the pumping rates of some wells. The changes made were: turn off existing well E-1 and new well NEW-1 in sp 2 and lower the pumping rate of existing well E-11. The POE constraint was achieved and the total cost was $14,723K.

Major Simulations 12-14

To prevent the NE plume migrating to the Main Plume area north of the bedrock block (i.e., to reduce the VCS term in the cost function), one or more pumping wells were installed. Even though the POE constraint was still met, the total cost was much higher at $15,278K, which indicated the savings on VCS can't compensate for the capital cost for installing new wells and the cost for operating the wells.

Major Simulations 15-17

The previous simulations indicated that no less than 4 new pumping wells could achieve the POE constraint. Thus, focus was directed towards reducing the pumping rates. Turning on E-2-1 to replace E-1 and lowering the rate of E-11 and NEW-1 made the total cost drop to $14,633K.

Major Simulation 18

Further attempt was made to install only 3 new pumping wells instead of 4 pumping wells. No feasible solution was found.

Major Simulations 19-21 (***Optimal Solution was Major Simulation 19, Total Simulation 47***)

Further reduced the pumping rates of new pumping wells in different periods to reduce the total cost. The total cost of the optimal solution was $14,628K. There were 4 new pumping wells installed and no injection wells.

2.3 Formulation 2: Minimize Cost, POE and POC Constraints

2.3.1 Objective Function and Constraints

The objective function is to minimize the cost function over a 21 year time frame (see Section 2.1.3), subject to the same constraints as Formulation 1, except with additional POC constraints

- POC-MP1 must be 50% of the initial concentrations or < 20 ug/l at the end of 1st management period (year 3) and thereafter; and

- POC-MP2 must be 50ppb at the end of the 1st management period (3 yrs), and 20ppb at the end of 3rd management period (9 yrs) and thereafter.

2.3.2 Optimal Solution

For Formulation 2, a total of 43 major runs were performed, consisting of a total of 72 simulations (i.e., some major runs included a series of sub-runs). The best solution was found in major simulation 43 (total simulation 72), and has the following details:

Results, Formulation 2

	Current System	Optimal Solution
Objective Function (Total)	$19,364.303K	$16,321.579K
Number of New Extraction Wells	NA	5
Number of New Injection Wells	NA	3
Objective Function (Components)		
CCE: Capital costs of new extraction wells	0	1,535K
CCI: Capital costs of new injection wells	0	669K
FCO: Fixed cost of O&M	7,067.663K	7,067.663K
VCE: Variable electrical costs of operating wells	6,966.696K	2,534.988K
VCS: Variable costs of sampling	3,859.485K	3,988.346K
VCC: Variable cost of chemicals	1,470.459K	526.595K

Five new extraction wells and three new injection wells are included in the optimal solution. Extraction rates and recharge rates are listed below:

Optimal Rates, Formulation 2

Well	New or Existing	Location (Row,Col)	Layer	Period 1 (gpm)	Period 2-3 (gpm)	Period 4 (gpm)	Period 5-7 (gpm)
E-2-1	Existing	(76,41)	2	294.5	294.5	294.5	0
E-11	Existing	(57,45)	2	323	323	0	0
NE Well	Fixed NE well	(118,69)	1,2	1425	1425	1425	1425
NEW-1	New	(49,37)	1	250	0	0	0

Well	New or Existing	Location (Row,Col)	Layer	Period 1 (gpm)	Period 2-3 (gpm)	Period 4 (gpm)	Period 5-7 (gpm)
NEW-2	New	(51,39)	1	380	380	380	380
NEW-3	New	(53,41)	1,2	380	380	380	380
NEW-4	New	(51,39)	2	380	380	380	380
NEW-5	New	(108,27)	1	380	380	380	380
Total Extraction				**3812.5**	**3562.5**	**3239.5**	**2945**
I-1	Existing	(72,65)	2	193.8	193.8	193.8	193.8
I-3	Existing	(58,60)	2	500.0	500.0	374.5	330.0
I-4	Existing	(53,58)	2	763.8	763.8	625.6	625.6
I-5	Existing	(45,56)	2	574.9	324.9	335.6	335.6
I-6	Existing	(40,54)	2,3	390.0	390.0	390.0	390.0
I-7	Existing	(35,49)	2,3	0	0	500.0	250.0
I-10	Existing	(37,33)	2,3	0	0	40.0	40.0
NIW-1	New	(106,31)	1	570	570	570	570
NIW-2	New	(107,39)	1	570	570	40	40
NIW-3	New	(108,46)	1,2	250	250	170	170
Total Injection				**3812.5**	**3562.5**	**3239.5**	**2945**

Locations of extraction wells and injection wells are presented in Figure 2-5. A chart illustrating objective function value versus simulation number is provided in Figure 2-6. A chart illustrating mass remaining after each year for this solution versus the current system is provided in Figure 2-7.

This solution costs approximately $1.5M more than the solution for Formulation 1, over 21 years, due to more wells and slightly higher pumping rates. As with Formulation 1, the solution for Formulation 2 leaves more mass within the aquifer than does the current system, in both the main plume area and the NE plume area. The solution for Formulation 2 does remove more mass than the solution for Formulation 1 from the main plume area. However, the solution for Formulation 2 leads to more mass left in place in the NE plume area compared to Formulation 1. This is because the injection near the POCs associated with the solution causes TCE in the main plume to be pushed to the northeast (groundwater flow is already to the northeast, the injection increases the driving force). As discussed in Section 2.3.3, reinjection near the POC boundaries was found to be the best way to meet the POC constraints within the context of the mathematical formulation.

It is important to note that the intent behind the POC approach is that, ultimately, achieving the POC should allow the POE to also be met without additional pumping near the POE boundary. It is obvious from the results after 21 years, for layers 1 and 2, that achieving the POC constraints does not achieve this larger goal (for instance, see left side of Figure 11). When coupled with the increase in mass pushed to the northeast associated with this strategy, the POC approach as represented by this formulation does not seem to provide much advantage.

2.3.3 General Approach to Determining the Optimal Solution

The general approach was to achieve the POC1 constraint first, then focus on the POC2 constraint. Once an improved feasible solution was found, the next priority was to reduce the number of new wells and/or lower the pumping rates. The general approach used to determine the optimal solution for Formulation 2, via trial-and-error, can be summarized as follows (all simulation numbers refer to "major simulations"):

<u>Major Simulations 1-2</u>

Based on a feasible solution of Formulation 1 (but not the final one, since Formulation 2 work was initiated prior to determining the final solution for Formulation 1), 3 new pumping wells were installed south of POC1 in an attempt to meet the POC1 constraint, but a feasible solution was not achieved. Because of the 400gpm limit at individual wells, each new well had little impact on the plume capture.

<u>Major Simulations 3-8</u>

Because the impact of pumping wells on POC1 was limited, an attempt was made to use injection wells. Two new injection wells were installed along the POC1 in addition to 4 new pumping wells along the POE boundary. Several minor changes were made to make both the POC1 and POE constraints feasible.

<u>Major Simulations 9-12</u>

Several test runs were performed to demonstrate the relative impact of pumping wells versus injection wells along the POC boundaries. The results indicated that as much as 3000 gpm pumping still couldn't achieve the POC1 constraint, and the injection wells were effective primarily because they cause dilution of the plume at the POCs.

<u>Major Simulations 13-15</u>

Since there is a small continuous source just upgradient of POC1, it might be more practical to put a pumping well to contain that source. Attempt was made to install one pumping well and one injection well. The POC1 constraint was met.

<u>Major Simulations 16-26, 39-40</u>

Two injection wells and two pumping wells were installed along POC2. Two pumping wells were located near the continuous source south of POC2. A feasible solution was found. There were seven new pumping wells and 3 new injection wells installed. The total cost was $17,962K.

<u>Major Simulation 41</u>

To reduce the total cost, turn off one new pumping wells south of the POC2. The solution was feasible with the total cost of $17,766K. There were total of 6 new pumping wells and 3 new injection wells installed.

Major Simulations 27-38, 42

Attempt was made to use only 2 injection wells to achieve the POC2 constraint (in addition to one injection well for POC1), without some of the pumping wells previously used along POC2. Feasible solution was ultimately found with the total cost of $16,928K. Total of 5 new pumping wells and 3 injection wells were installed.

Major Simulation 43 (***Optimal Solution was Major Simulation 43, Total Simulation 72***)

To further reduce the total cost, several changes were made consistent with final result for Formulation 1 (determined after work on Formulation 2 was underway): turn off E-1; turn off E-11 in later sp; and lower the pumping rates. Feasible solution was found with the total cost of $16,322K. Total of 5 new pumping wells and 3 injection wells were installed.

2.4 Formulation 3: Minimize Cost, Cleanup Constraint, Reduced Source Term

2.4.1 Objective Function and Constraints

The objective function is to minimize the total cost over a 21 year time frame. The constraints are the same as Formulation 2, except that cleanup (defined as TCE <50ppb) for the Main Plume (except specifically excluded areas) must be met at the end of the 3rd management period, the maximum number of new extraction wells cannot exceed 4, and the maximum number of new injection wells cannot exceed 4. This Formulation also includes a source term that declines over time, unlike the first two formulations. Full details are provided in the formulation document.

A feasible problem could not be found for the problem as stated. As per instructions in the formulation document, the modelers could at their discretion relax one or more constraints and solve that new problem. A modified formulation was created and solved by relaxing constraints on the number of new wells allowed to as many as desired. All discussion in this report regarding Formulation 3 pertains to this modified form of the problem formulation.

2.4.2 Optimal Solution

For Formulation 3, a total of 21 major runs were performed, consisting of a total of 67 simulations (i.e., some major runs included a series of sub-runs). The best solution was found in major simulation 21 (total simulation 67), and has the following details:

Results, Formulation 3

	Current System	Optimal Solution
Objective Function (Total)	$19,364.303K	$18,572.715K
Number of New Extraction Wells	NA	9
Number of New Injection Wells	NA	4

	Current System	Optimal Solution
Objective Function (Components)		
CCE: Capital costs of new extraction wells	0	2,763K
CCI: Capital costs of new injection wells	0	892K
FCO: Fixed cost of O&M	7,067.663K	7,067.663K
VCE: Variable electrical costs of operating wells	6,966.696K	3,229.01K
VCS: Variable costs of sampling	3,859.485K	3,906.652K
VCC: Variable cost of chemicals	1,470.459K	714.39K

Nine new extraction wells and four new injection wells are included in the optimal solution. Extraction rates and recharge rates are listed below:

Optimal Rates, Formulation 3

Well	New or Existing	Location (Row,Col)	Layer	Period 1 (gpm)	Period 2 (gpm)	Period 3 (gpm)	Period 4-5 (gpm)	Period 6-7 (gpm)
E-4	Existing	(102,37)	2	0	0	600	0	0
E-11	Existing	(57,45)	2	617.5	617.5	617.5	0	0
NE Well	Fixed NE Well	(118,69)	1,2	1425	1425	1425	1425	1425
NEW-1	New	(49,37)	1	380	0	0	0	0
NEW-2	New	(51,39)	1	380	380	380	380	380
NEW-3	New	(53,41)	1,2	380	380	380	380	380
NEW-4	New	(51,38)	2	380	380	380	380	380
NEW-5	New	(108,27)	1	380	380	380	0	0
NEW-6	New	(144,38)	1,2	380	380	380	380	0
NEW-7	New	(117,38)	1	180	180	180	0	0
NEW-8	New	(72,40)	1	380	380	380	0	0
NEW-9	New	(115,52)	1,2	300	300	300	0	0
Total Extraction				**5182.5**	**4802.5**	**5402.5**	**2945**	**2565**
I-1	Existing	(72,65)	2	193.8	193.8	193.8	193.8	193.8
I-2	Existing	(62,61)	2,3	90.3	90.3	90.3	90.3	90.3
I-3	Existing	(58,60)	2	620.4	620.4	620.4	620.4	620.4
I-4	Existing	(53,58)	2	763.8	763.8	763.8	419.3	419.3
I-5	Existing	(45,56)	2	271.1	124.3	344.3	0	0
I-7	Existing	(40,54)	2,3	450.0	450.0	450.0	0	0

Well	New or Existing	Location (Row,Col)	Layer	Period 1 (gpm)	Period 2 (gpm)	Period 3 (gpm)	Period 4-5 (gpm)	Period 6-7 (gpm)
I-9	Existing	(35,49)	2,3	233.2	0	380.0	380.0	0
I-10	Existing	(37,33)	2,3	350.0	350.0	350.0	350.0	350.0
NIW-1	New	(106,31)	1	570	570	570	570	570
NIW-2	New	(107,39)	1	570	570	570	71.3	71.3
NIW-3	New	(108,46)	1,2	570	570	570	250	250
NIW-4	New	(105,52)	1,2	500	500	500	0	0
Total Injection				**5182.6**	**4802.6**	**5402.6**	**2945.1**	**2565.1**

Locations of extraction wells and injection wells are presented in Figure 2-8. A chart illustrating objective function value versus simulation number is provided in Figure 2-9. A chart illustrating mass remaining after each year for this solution versus the current system is provided in Figure 2-10.

The optimal solution for this problem costs approximately $4M more than the solution for Formulation 1 and approximately $2.3M more than the solution for Formulation 2, over 21 years. This is due to more wells and higher pumping rates. It is important to note that, although the solution satisfies the “cleanup” constraint of 50 ppb TCE, there are still substantial portions of the plume with concentrations between 20 and 50 ppb TCE after 21 years.

The mass remaining plot (Figure 2-10) cannot be compared directly to the similar plot for other formulations (Figure 2-4 and 2-7), because this formulation includes a declining source term whereas Formulation 1 and Formulation 2 do not. Interestingly, the optimal solution determined for this formulation is also not as effective as the current system with respect to mass remaining in place, in either the main plume or the NE plume area.

2.4.3 General Approach to Determining the Optimal Solution

The general approach was to achieve a feasible solution. The next priority was to reduce the number of new wells and/or lower the pumping rates. The general approach used to determine the optimal solution for Formulation 3, via trial-and-error, can be summarized as follows (all simulation numbers refer to “major simulations”):

<u>Major Simulations 1-2</u>

Start with a feasible solutions of Formulation 2 (major simulation 40), and couple that with the reduced source. No cleanup can be achieved without more than 4 new extraction wells. The conclusion was that no feasible solution could be found for the problem as stated. It was decided to remove the constraint on number of new wells allowed.

<u>Major Simulations 3-9</u>

Install more pumping wells in plume hot-spots. Feasible solution was found with total of 11 new extraction wells and 4 new injection wells. The total cost was $20,898K.

Major Simulation 10

To lower the cost, an existing well E-4 was turned on to replace a new pumping well. The solution was feasible with 10 new extraction wells and 4 new injection wells installed. The total cost was $20,669K.

Major Simulations 11-19

To further reduce the total cost, turn off some wells in the later stress periods and lower the pumping rates. The cleanup constraint was met with the total cost of $19,103K. There were total of 10 new extraction wells and 4 new injection wells installed.

Major Simulation 20

One new injection well was turned off to lower the total cost. Thus, there were total of 10 new extraction wells and 3 new injection wells installed. The cleanup constraint was satisfied with the total cost of $18,914K.

Major Simulations 21 (***Optimal Solution was Major Simulation 21, Total Simulation 67***)

Since capital cost of a new injection well is lower than a new extraction well, replace the new extraction well installed within the bedrock block with a new injection well. The cleanup constraint was satisfied. The total cost was $18,573K with total of 9 new extraction wells and 4 new injection wells installed.

3.0 ADDITIONAL SIMULATIONS

GeoTrans still had budget remaining after the solution of all three formulations, and did not feel that significantly improved solutions to those already found could be determined for the three formulations with additional trial-and-error.

Therefore, GeoTrans performed an additional 26 simulations that were variations on Formulation 2, in an attempt to provide a better management solution for the Installation while deviating from the stated management formulations. These simulations were all performed within the project budget, and within the pre-specified period for performing simulations (i.e., completed prior to February 28, 2002).

The three major classes of additional simulations were:

(A) try to achieve cleanup to 5 ppb between the bedrock block and POE within 21 years at little additional cost (solution need not achieve POC or POE constraints)

(B) try to remove more mass with little additional cost relative to Formulation 2 (while still satisfying all constraints of Formulation 2) by adding one pumping well in a source area with very high concentrations

(C) try to prevent mass transfer to the Northeast, in the area south of the bedrock block (while still satisfying all constraints of Formulation 2), by adding one or more additional pumping wells.

The results of these additional simulations are discussed below.

3.1 Additional Simulations A: Attempt Cleanup Beyond Bedrock Block

The POE constraint in the three formulations does not lead to solutions that more aggressively address cleanup north of the bedrock block. For these additional simulations, an attempt was made to add pumping wells between the bedrock block and the POE wells used in Formulations 1 and 2. The goal was to cleanup the area between the bedrock block and the POE boundary within 21 years, to 5 ppb if possible, without incurring too much additional cost (a subjective constraint). The solutions were compared to Formulation 2, since it was assumed that some pumping associated with containment near the bedrock block would be required (which is closer in spirit to Formulation 2 than Formulation 1).

The best solution found is summarized below:

Results, Additional Simulations A

	Formulation 2	Additional Simulations A
Objective Function (Total)	$16,322K	$19,334K
Number of New Extraction Wells	5	7
Number of New Injection Wells	3	3

	Formulation 2	Additional Simulations A
Objective Function (Components)		
CCE: Capital costs of new extraction wells	1,535K	2,149K
CCI: Capital costs of new injection wells	669K	669K
FCO: Fixed cost of O&M	7,067.663K	7,067.663K
VCE: Variable electrical costs of operating wells	2,534.988K	4,485.633K
VCS: Variable costs of sampling	3,988.346K	3,962.494K
VCC: Variable cost of chemicals	526.595K	1,000.045K

Seven new extraction wells and three new injection wells are included in the best solution found. Extraction rates and recharge rates are listed below:

Well Rates, Additional Simulations A

Well	New or Existing	Location (Row,Col)	Layer	Period 1 (gpm)	Period 2-3 (gpm)	Period 4-7 (gpm)
E-1	Existing	(63,48)	2	209	0	0
E-2-1	Existing	(76,41)	2	295	295	295
E-2-2	Existing	(77,41)	3	0	0	209
E-9	Existing	(94,48)	1,2,3	0	0	808
E-11	Existing	(57,45)	2	617	617	0
NE Well	Fixed NE well	(118,69)	1,2	1425	1425	1425
NEW-1	New	(108,27)	1	380	380	380
NEW-2	New	(115,43)	1	380	380	380
NEW-3	New	(113,52)	1,2	300	300	300
NEW-4	New	(70,40)	1	380	380	380
NEW-5	New	(84,38)	1	380	380	380
NEW-6	New	(60,39)	1,2	380	380	380
NEW-7	New	(92,40)	1,2	380	380	380
Total Extraction				**5126**	**4917**	**5317**
I-1	Existing	(72,65)	2	194	194	194
I-2	Existing	(62,61)	2,3	90	90	90
I-3	Existing	(58,60)	2	620	620	620
I-4	Existing	(53,58)	2	764	764	764
I-5	Existing	(45,56)	2	343	134	134
I-6	Existing	(40,54)	2,3	380	380	380

Well	New or Existing	Location (Row,Col)	Layer	Period 1 (gpm)	Period 2-3 (gpm)	Period 4-7 (gpm)
I-7	Existing	(35,49)	2,3	1025	1025	1129
I-8	Existing	(32,43)	2	0	0	295
NIW-1	New	(106,31)	1	570	570	570
NIW-2	New	(107,39)	1	570	570	570
NIW-3	New	(108,46)	1,2	570	570	570
Total Injection				**5126**	**4917**	**5316**

A comparison of TCE distributions in model layers 1 and 2, at the end of the 21-year period, is provided in Figure 2-11. A chart illustrating mass remaining after each year for this solution versus the solution for Formulation 2 is provided in Figure 2-12.

From Figure 2-11, it is observed that the solution for Simulation A does not meet the POE constraints, but does substantially reduce plume area and/or concentrations between the bedrock block and the POE boundary. Based on Figure 2-12, approximately 25% less mass remains in the main plume after 21 years, relative to the solution for Formulation 2. However, cleanup north of the bedrock block is not achieved to either the 5 ppb or 20 ppb level in either layer 1 or layer 2, after 21 years. This solution costs approximately $3M more than the solution to Formulation 2 over 21 years. It is not clear that this solution represents a preferred management strategy.

3.2 Additional Simulations B: Attempt to Improve Mass Removal in the Main Plume

The purpose of this set of simulations was to maintain all constraints associated with Formulation 2, and also to add a well in the area of highest source concentrations (south of the bedrock block) to improve mass removal.

The best solution found is summarized below:

Results, Additional Simulations B

	Formulation 2	Additional Simulations B
Objective Function (Total)	$16,322K	$17,768K
Number of New Extraction Wells	5	6
Number of New Injection Wells	3	3

	Formulation 2	Additional Simulations B
Objective Function (Components) CCE: Capital costs of new extraction wells CCI: Capital costs of new injection wells FCO: Fixed cost of O&M VCE: Variable electrical costs of operating wells VCS: Variable costs of sampling VCC: Variable cost of chemicals	 1,535K 669K 7,067.663K 2,534.988K 3,988.346K 526.595K	 1,842K 669K 7,067.663K 3,448.424K 3,949.658K 790.828K

Six new extraction wells and three new injection wells are included in this solution. Extraction rates and recharge rates are listed below:

Well Rates, Additional Simulations B

Well	New or Existing	Location (Row,Col)	Layer	Period 1 (gpm)	Period 2-7 (gpm)
E-1	Existing	(63,48)	2	209	0
E-2-1	Existing	(76,41)	2	295	295
E-11	Existing	(57,45)	2	617	617
NE Well	Fixed NE well	(118,69)	1,2	1425	1425
NEW-1	New	(47,37)	1	380	0
NEW-2	New	(51,39)	1	380	380
NEW-3	New	(53,41)	1,2	380	380
NEW-4	New	(51,39)	2	380	380
NEW-5	New	(108,27)	1	380	380
NEW-6	New	(144,38)	1,2	380	380
Total Extraction				**4826**	**4237**
I-1	Existing	(72,65)	2	194	194
I-2	Existing	(62,61)	2,3	90	90
I-3	Existing	(58,60)	2	620	620
I-4	Existing	(53,58)	2	764	764
I-5	Existing	(45,56)	2	911	799
I-6	Existing	(40,54)	2,3	380	380
I-7	Existing	(35,49)	2,3	477	0
NIW-1	New	(106,31)	1	570	570
NIW-2	New	(107,39)	1	570	570

Well	New or Existing	Location (Row,Col)	Layer	Period 1 (gpm)	Period 2-7 (gpm)
NIW-3	New	(108,46)	1,2	250	250
Total Injection				**4826**	**4237**

A comparison of TCE distributions in model layers 1 and 2, at the end of the 21-year period, is provided in Figure 2-13. A chart illustrating mass remaining after each year for this solution versus the solution for Formulation 2 is provided in Figure 2-14.

This solution costs approximately $1.5M more than the solution for Formulation 2, over 21 years. Based on Figure 2-13, this solution does lead to improvement south of the bedrock block, especially in layer 2, after 21 years. Looking at Figure 2-14, mass in place in the main plume after 21 years is reduced a little less than 10% relative to the solution for Formulation 2, and the mass left in place in the NE plume area is not significantly impacted. This reduction in mass near the source area may be a reasonable component of a future management strategy and intuitively makes some sense, although it does not fully achieve any specific objective and does lead to increased cost.

3.3 Additional Simulations C: Attempt to Prevent Mass Transfer to Northeast, South of Bedrock

The results from Formulation 2 indicate that the POC constraints are best met by using injection wells near the POCs, which serve to dilute concentrations at the POCs. However, this injection also pushes mass to the northeast, especially in the area south of the bedrock block. The purpose of this set of simulations was to attempt to continue to meet the constraints of Formulation 2, but also add one or more wells south of the bedrock block, at the eastern edge of the main plume, to prevent mass transfer to the northeast.

The best solution found is summarized below:

Results, Additional Simulations C

	Formulation 2	Additional Simulations B
Objective Function (Total)	$16,322K	$19,455K
Number of New Extraction Wells	5	8
Number of New Injection Wells	3	3
Objective Function (Components)		
CCE: Capital costs of new extraction wells	1,535K	2,456K
CCI: Capital costs of new injection wells	669K	669K
FCO: Fixed cost of O&M	7,067.663K	7,067.663K
VCE: Variable electrical costs of operating wells	2,534.988K	4,377.317K
VCS: Variable costs of sampling	3,988.346K	3,889.937K
VCC: Variable cost of chemicals	526.595K	995.462K

Eight new extraction wells and three new injection wells are included in this solution. Extraction rates and recharge rates are listed below:

Well Rates, Additional Simulations C

Well	New or Existing	Location (Row,Col)	Layer	Period 1 (gpm)	Period 2-3 (gpm)
E-1	Existing	(63,48)	2	209	0
E-2-1	Existing	(76,41)	2	295	295
E-11	Existing	(57,45)	2	617	617
NE Well	Fixed NE well	(118,69)	1,2	1425	1425
NEW-1	New	(47,37)	1	380	0
NEW-2	New	(51,39)	1	380	380
NEW-3	New	(53,41)	1,2	380	380
NEW-4	New	(51,39)	2	380	380
NEW-5	New	(108,27)	1	380	380
NEW-6	New	(115,52)	1,2	380	380
NEW-7	New	(105,52)	1,2,3	380	380
NEW-8	New	(120,52)	1,2	380	380
Total Extraction				**5586**	**4997**
I-1	Existing	(72,65)	2	194	194
I-2	Existing	(62,61)	2,3	90	90
I-3	Existing	(58,60)	2	620	620
I-4	Existing	(53,58)	2	764	764
I-5	Existing	(45,56)	2	915	679
I-6	Existing	(40,54)	2,3	380	380
I-7	Existing	(35,49)	2,3	500	500
I-8	Existing	(32,43)	2	733	380
NIW-1	New	(106,31)	1	570	570
NIW-2	New	(107,39)	1	570	570
NIW-3	New	(108,46)	1,2	250	250
Total Injection				**5586**	**4997**

A comparison of TCE distributions in model layers 1 and 2, at the end of the 21-year period, is provided in Figure 2-15. A chart illustrating mass remaining after each year for this solution versus the solution for Formulation 2 is provided in Figure 2-16.

This solution cost approximately $3M more than the solution to Formulation 2. Based on Figure 2-15, little improvement is noted in plume extent or peak concentrations after 21 years. Based on Figure 2-16, there is some improvement with respect to mass left in place relative to Formulation 2, for both the main plume and the NE plume area. However, it is not clear that the improved mass removal is worth the extra cost.

4.0 COMPUTATIONAL PERFORMANCE

Preliminary Items

Development of the three formulations, and development of the FORTRAN postprocessing code, were considered separate tasks from the actual solution of the problems, and are not described herein (since each of the other optimization groups started after the formulations and FORTRAN postprocessor were provided to them). However, those costs (approximately $12K) should be accounted for when evaluating the cost of the overall optimization process.

Solution of the Three Formulations

GeoTrans worked within a pre-specified budget of approximately $34,000 for developing optimal solutions for each of the three formulations. Development of the SURFER/PowerPoint animation technique accounted for approximately $3,000 of this $34,000, and the remaining $31,000 went towards solving the problems.

Each flow and transport simulation required approximately 10 minutes on a Pentium IV, 1.8 GHZ computer. Running the FORTRAN code required less than one minute. Creating the SURFER grid files, contour maps, and subsequent animations for all 4 layers required approximately 0.5 hours (average) per simulation. The remaining time was spent reviewing the results, deciding what modifications to make to pumping/recharge, and modifying the well package for the subsequent run.

GeoTrans ultimately made 111 “major simulations”, consisting of 235 total simulations (i.e., some major runs included a series of sub-runs), as follows:

formulation 1:	21 major simulations, 60 total simulations
formulation 2:	43 major simulations, 72 total simulations
formulation 3:	21 major simulations, 67 total simulations
additional:	26 total simulations

Based on a cost of approximately $31,000 allocated towards solving the problems, this represents a cost of approximately $132 per simulation. That represents approximately 1.5 hours for project level staff (Yan Zhang) and approximately 0.2 hours for senior level staff (Rob Greenwald) for each simulation, associated with setting up, running, and postprocessing the simulation, and determining what to implement for the subsequent simulation.

As noted in Section 2, determining feasible solutions is not straightforward for this site. A large amount of time was spent trying to find improved solutions that were feasible. For Formulation 3, no feasible solution could be found, and a modified formulation was generated by removing the constraint on number of new wells.

GeoTrans would likely not have performed as many trial-and-error simulations if work was not being performed within the context of this project.

5.0 SENSITIVITY ANALYSIS (IF PERFORMED)

Sensitivity analysis, as it relates to optimization, refers to the extent to which the optimal solution changes with respect to specific changes in the optimization formulation. GeoTrans did not attempt to solve any problems other than the three that were specified. Therefore, sensitivity analysis was not performed. The "trial-and-error" methodology is poorly suited for performing that type of sensitivity analysis, because the solution method is not automated.

6.0 SUMMARY, SITE-SPECIFIC ITEMS, AND LESSONS LEARNED

Formulations Fixed at the Beginning of the Simulation Period

For this project, the three formulations had to be "locked in" prior to the simulation period. This is not typical for optimization projects. In most cases it would be beneficial to start with one formulation, and based on those results develop different formulations, based on interaction with the Installation on an ongoing basis.

Costs of Optimal Solutions Versus Current System

Comparisons between the optimal solution for each formulation versus the performance of the current system must be made with caution. The current system was not designed with the current flow and transport models, and was not designed based on the mathematical formulations considered herein. Additionally, calculations of percentage reduction in cost between the current system and the optimal solution for each problem, if made, must further recognize that a substantial portion of total cost in each simulation was fixed (i.e., $7.068M) and could not be reduced, making percentage changes due to management decisions appear less impressive on a percentage basis when the fixed costs are included. Such calculations were not included in this report. The more meaningful comparison is to compare solutions obtained via trial-and-error (GeoTrans) versus solutions obtained with optimization algorithms.

Preferred Management Strategy

It is not clear that a preferred management strategy stands out. The POE strategy (Formulation 1) costs the least, and with respect to the POE boundary as specified, is protective. All of the other strategies attempt more aggressive pumping to reduce mass and/or cleanup time, but do not successfully remove the need for a P&T system within 21 years (and in fact do not allow even for discontinued pumping near the POE boundary after 21 years). Furthermore, the model indicates interaction between the main plume and NE plume, including transfer of mass from the main plume to the NE plume, and that should be addressed by the overall management strategy. No solution presented herein fully addresses that issue. At the same time, it intuitively makes some sense to remove mass and/or contain groundwater flow near source areas where concentrations are highest, and that is not a component of the solution for Formulation 1 (which is the least costly approach).

Impact of Extraction Wells and Injection Wells

Because of the low pumping limit at individual wells, the large extent of contamination, and the amount of water moving through the system, an individual new well pumping the maximum 370gpm (accounting 5% downtime) does not have a noticeable impact on the groundwater flow field. Thus, it is hard to use extraction wells to effectively contain groundwater near the POC boundaries. Injection has to be included to reduce the concentrations at the POC boundaries (via dilution), even though the re-injection of treated water can spread the plume over a larger area. In other words, injection near the POC was the best approach to optimize with respect to the mathematical formulations, but reinjecting water inside the plume may not ultimately be an acceptable management approach.

Containment and Cleanup

The original concept of the POC constraints is to turn off the pumping wells along the POE boundary when the POC constraints are met. However, the way the POC constraints are set up does not ensure containment so that the wells along the POE boundary can be turned off. GeoTrans did some test runs to try to contain the plume at the POC and also clean up the plume between the bedrock and the POE boundary. The results indicate that the plume between the bedrock and the POE boundary could not be cleaned up within 21 years even with significant amount of pumping added between the POC and POE. It may be possible to achieve that goal (i.e., cleanup to 5 ppb north of bedrock block in 25 years), but it will require even greater cost.

Mass Transfer to Northeast

The eastern part of the main plume, south of the bedrock block, migrates to the Northeast Plume area due to the groundwater flow direction in that area. Re-injection along the POC boundaries (Formulation 2) pushes the plume further towards the Northeast Plume area. To prevent plume migration to the Northeast Plume area, and to reduce the total remaining mass in the aquifers, GeoTrans performed additional test runs (Addition Runs C). Unfortunately, no solution was found that completely addresses this issue, and to do so would require significant additional cost.

Figure 2-1 System Configuration and simulated TCE plume in Layer 1, End of Year 2002 (Initial Condition for Optimization Runs)

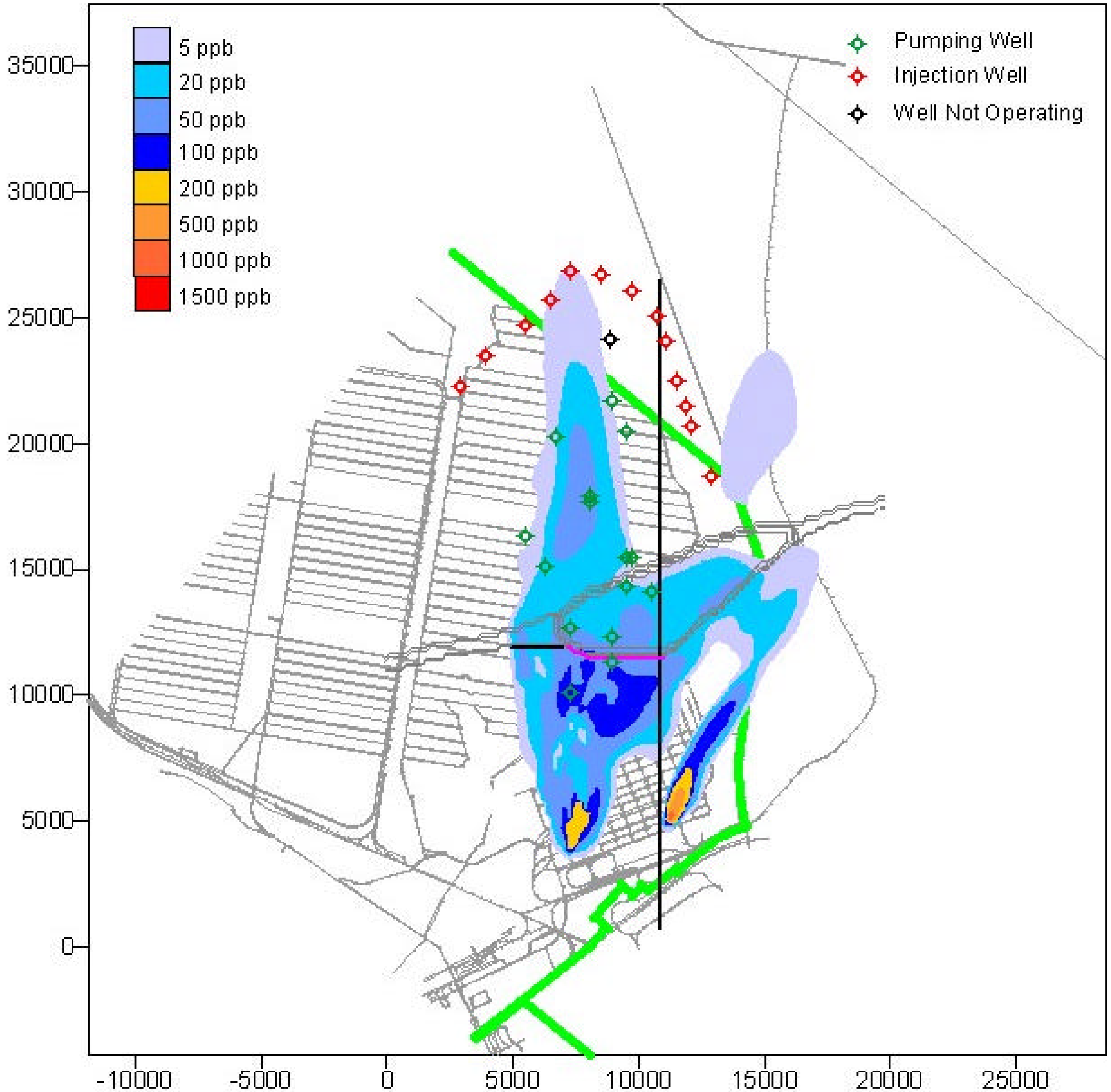


Figure 2-2 Locations of Wells in Optimal Solution, Formulation 1

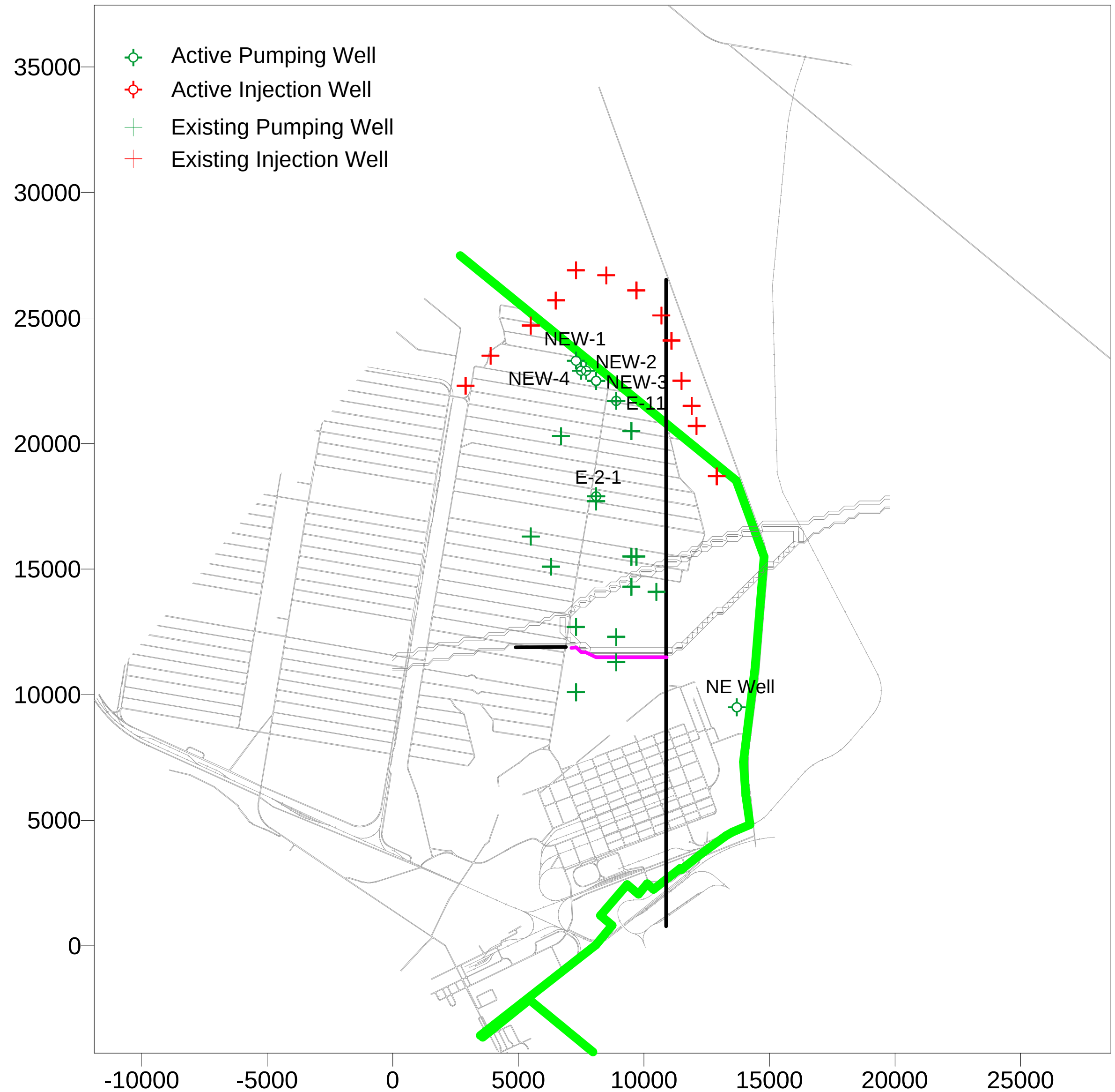


Figure 2-3 Objective Function Value by Major Runs, Formulation 1

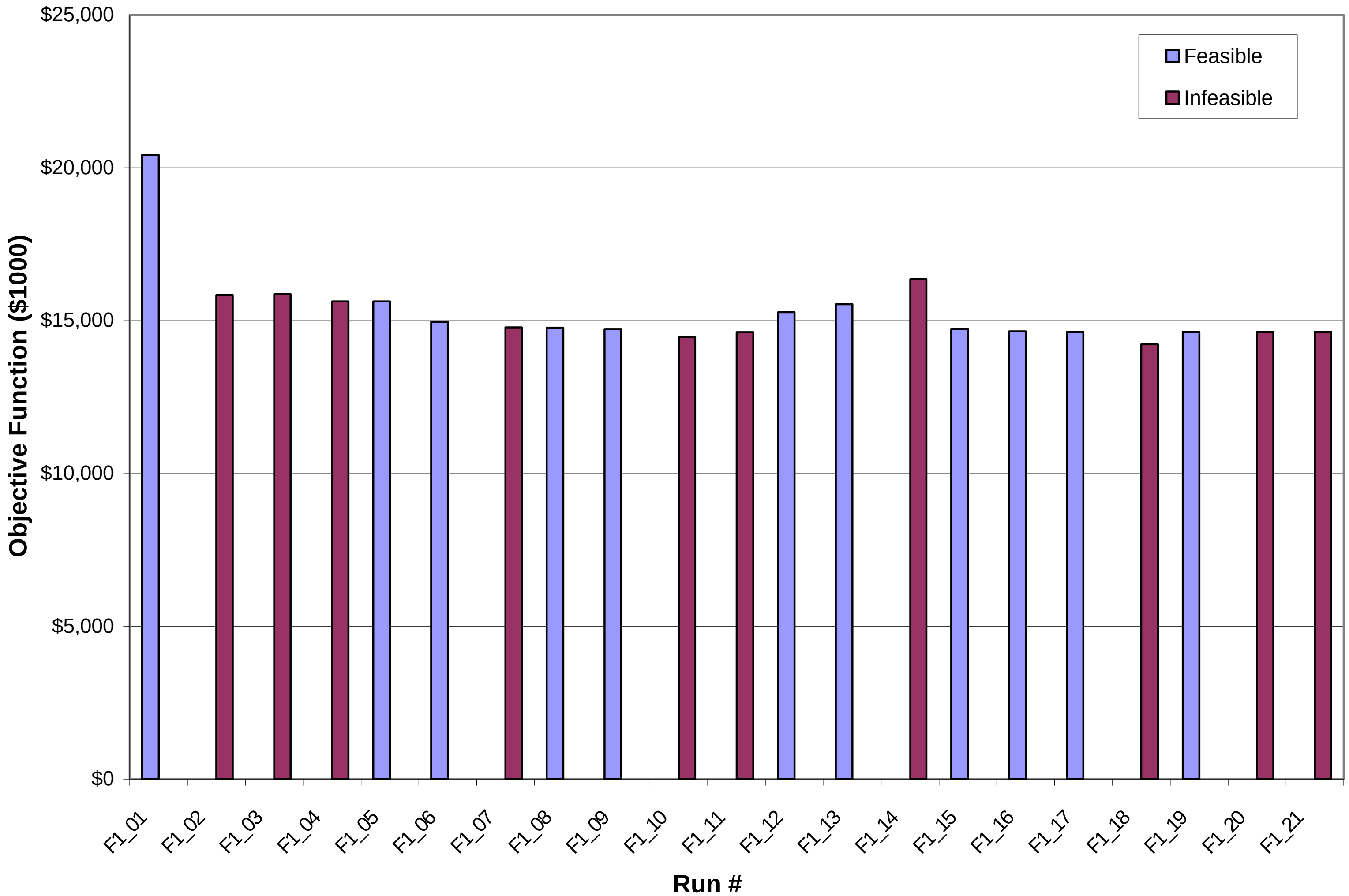


Figure 2-4 Mass Remaining After Each Year, Formulation 1

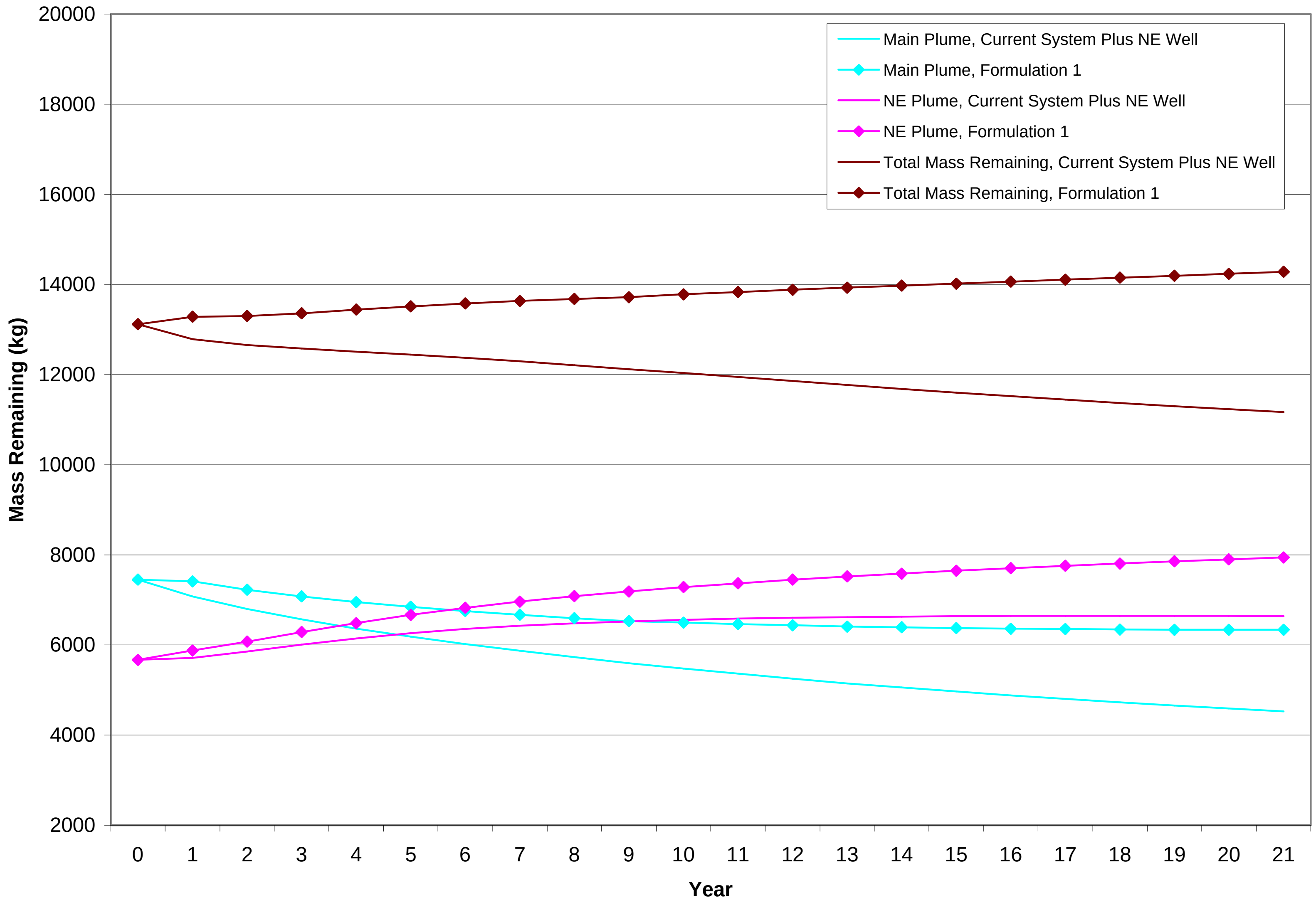


Figure 2-5 Location of Wells in Optimal Solution, Formulation 2

Figure 2-6 Objective Function Value by Major Runs, Formulation 2

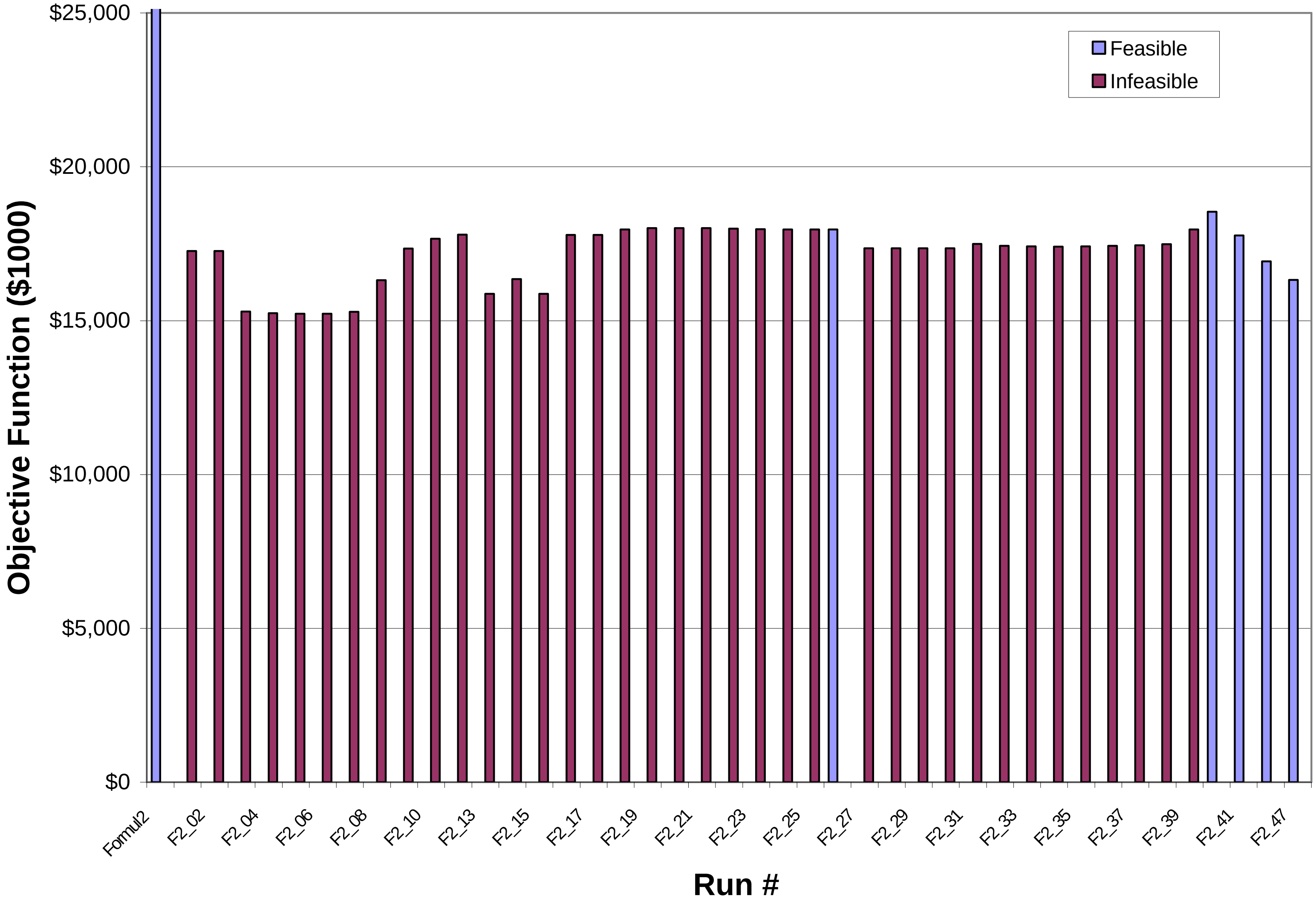


Figure 2-7 Mass Remaining After Each Year, Formulation 2

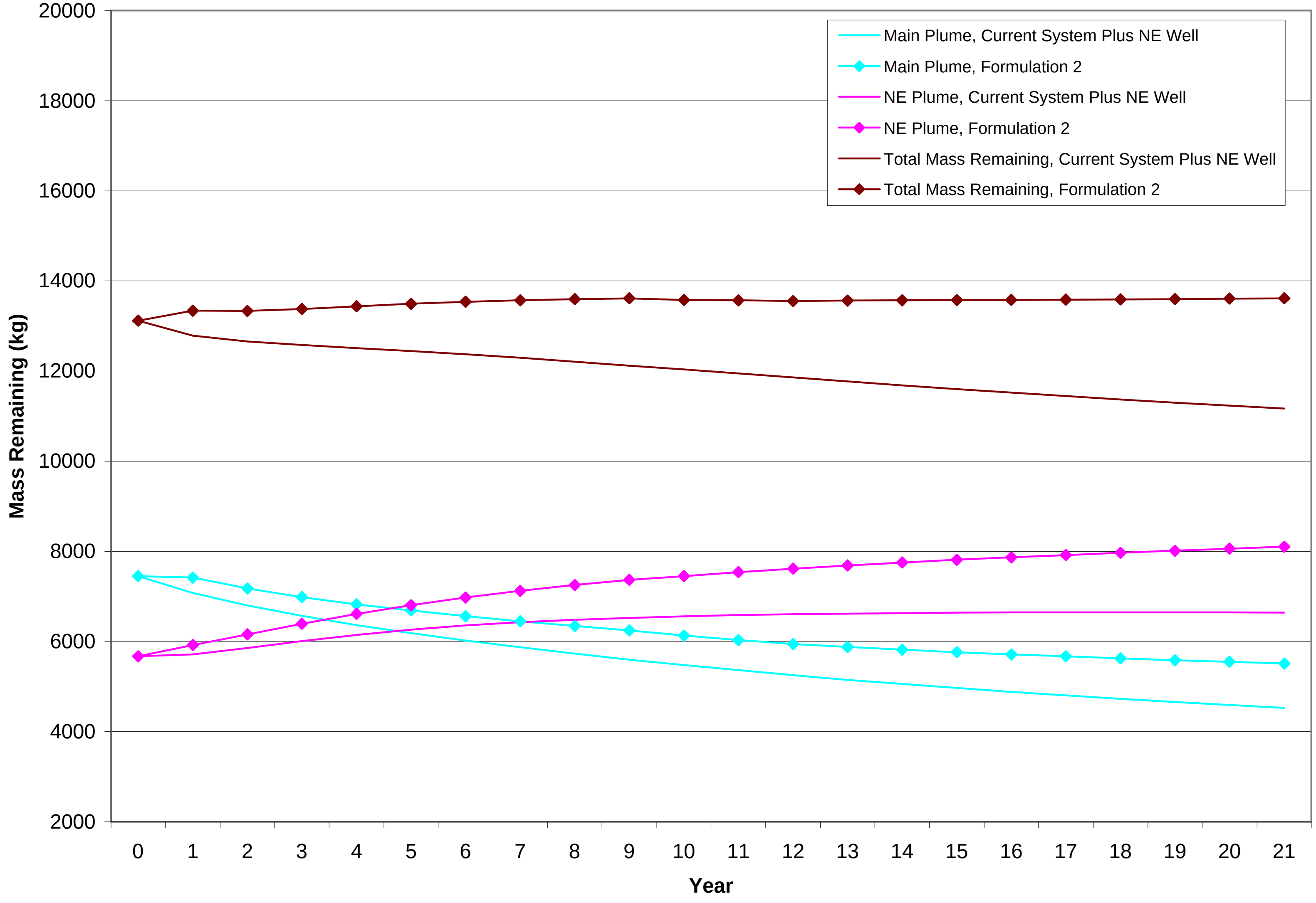


Figure 2-8   Locations of Wells in Optimal Solution, Formulation 3

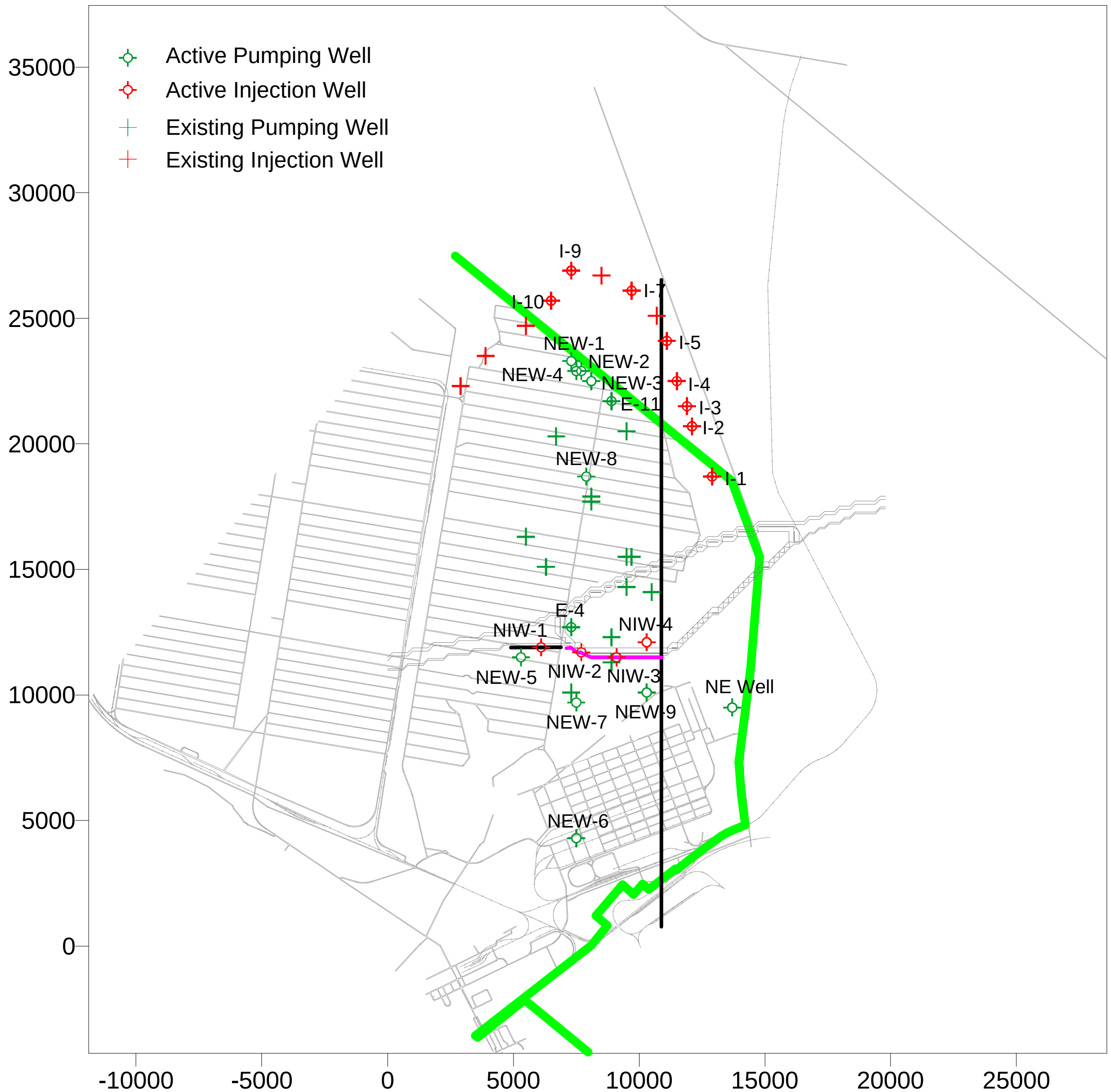


Figure 2-9   Objective Function Value by Major Runs, Formulation 3

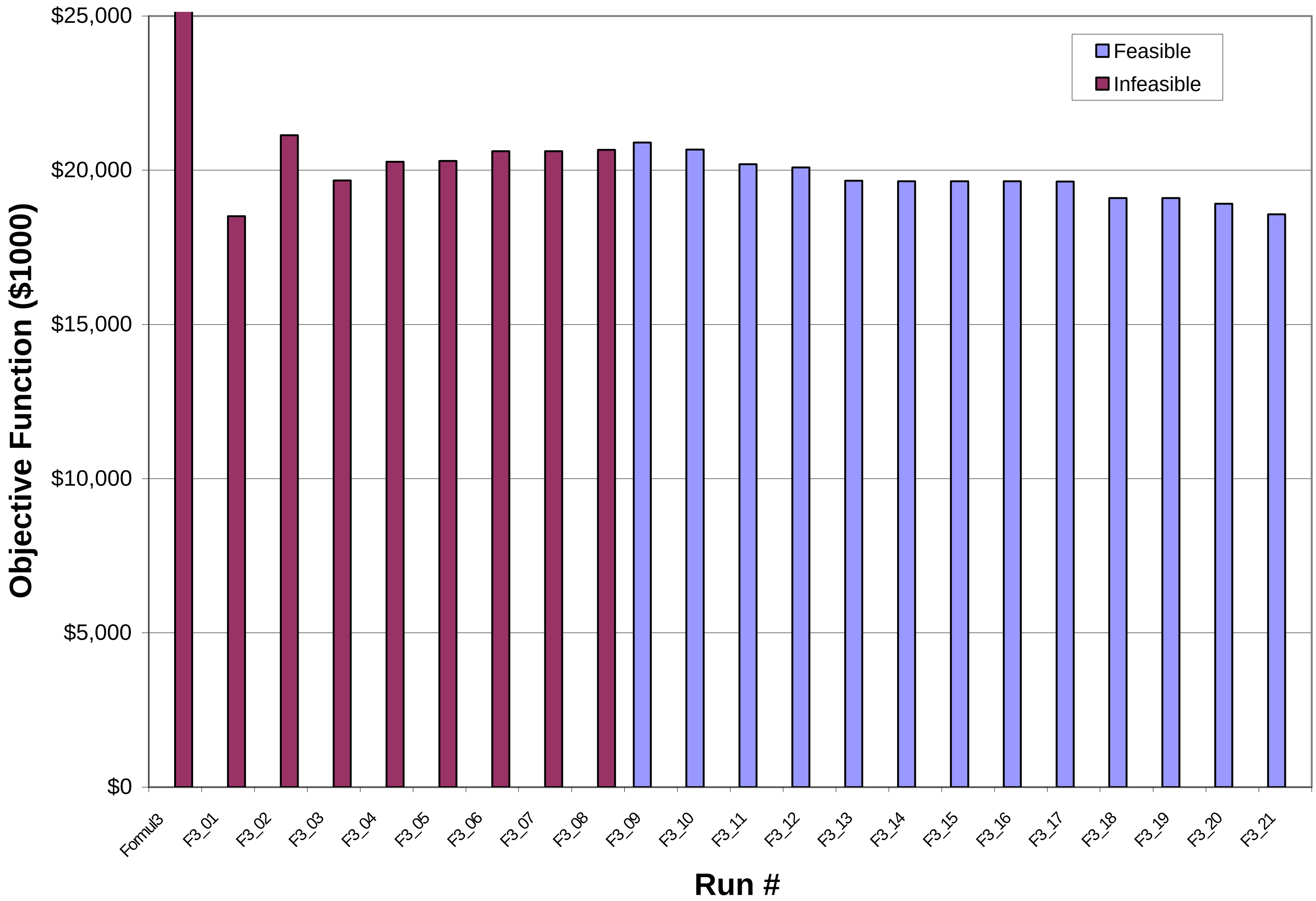


Figure 2-10   Mass Remaining After Each Year, Formulation 3

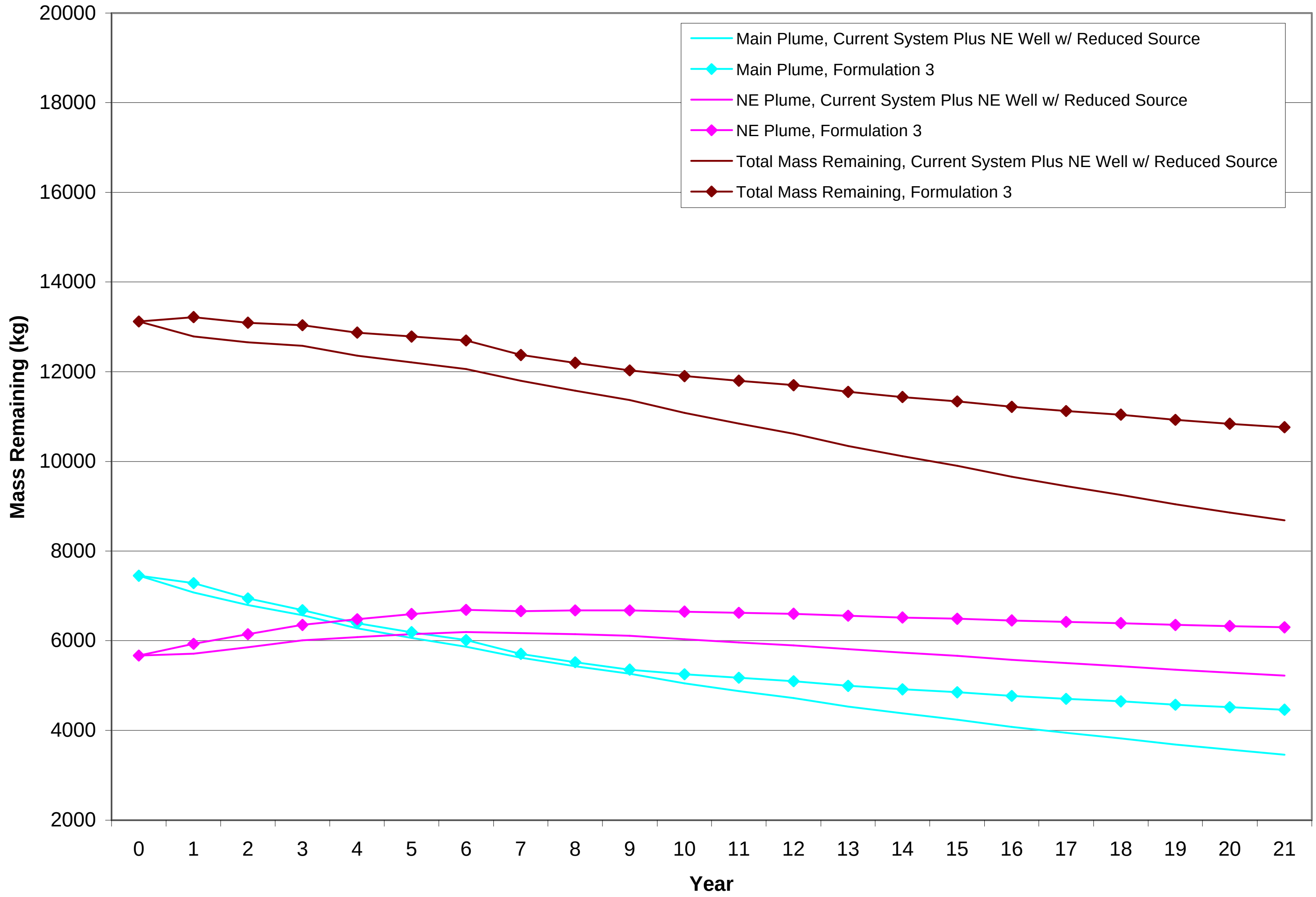


Figure 2-11 TCE Distributions After 21 Years, Model Layers 1 and 2, Additional Simulations A

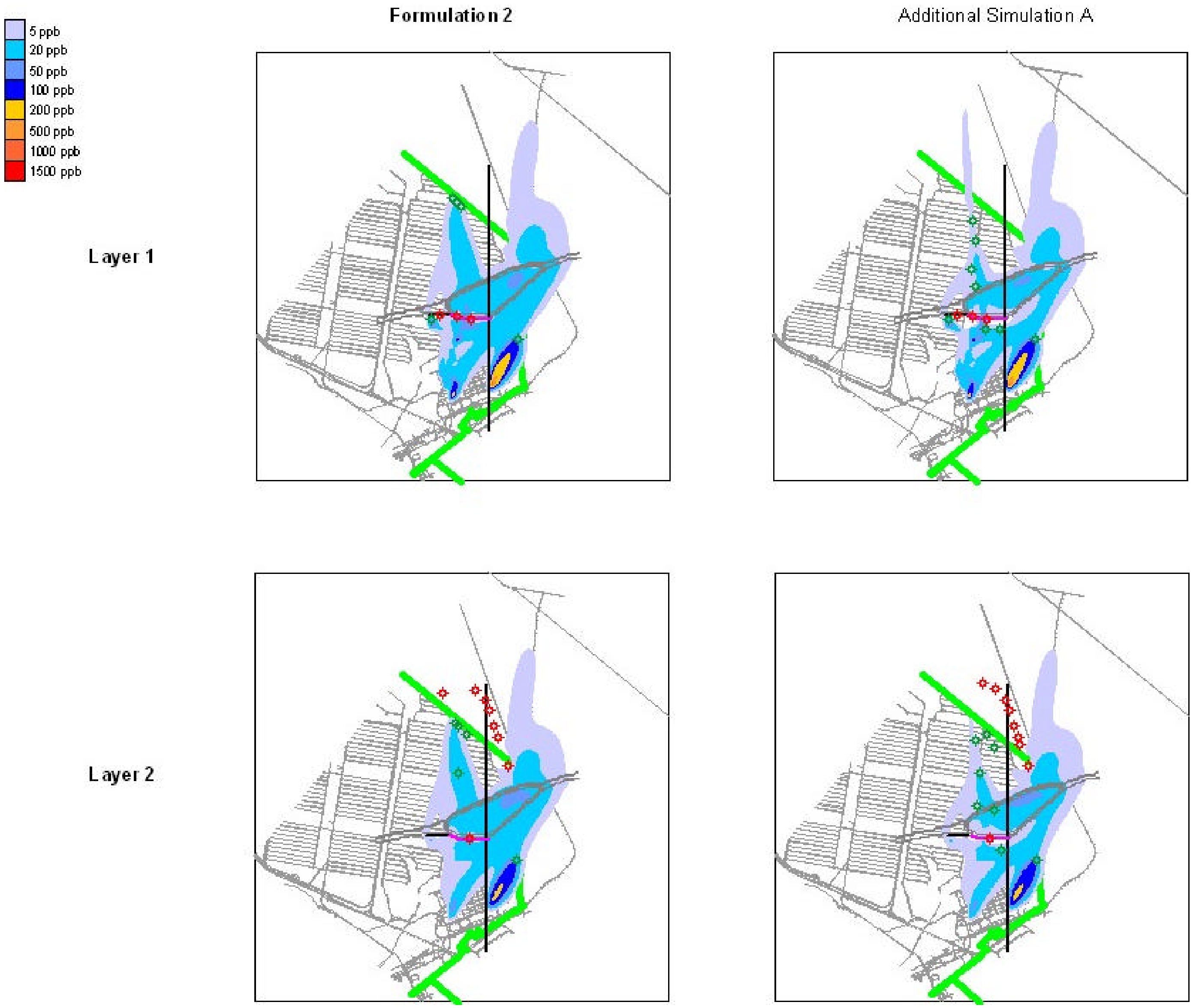


Figure 2-12 Mass Remaining After Each Year, Additional Simulations A

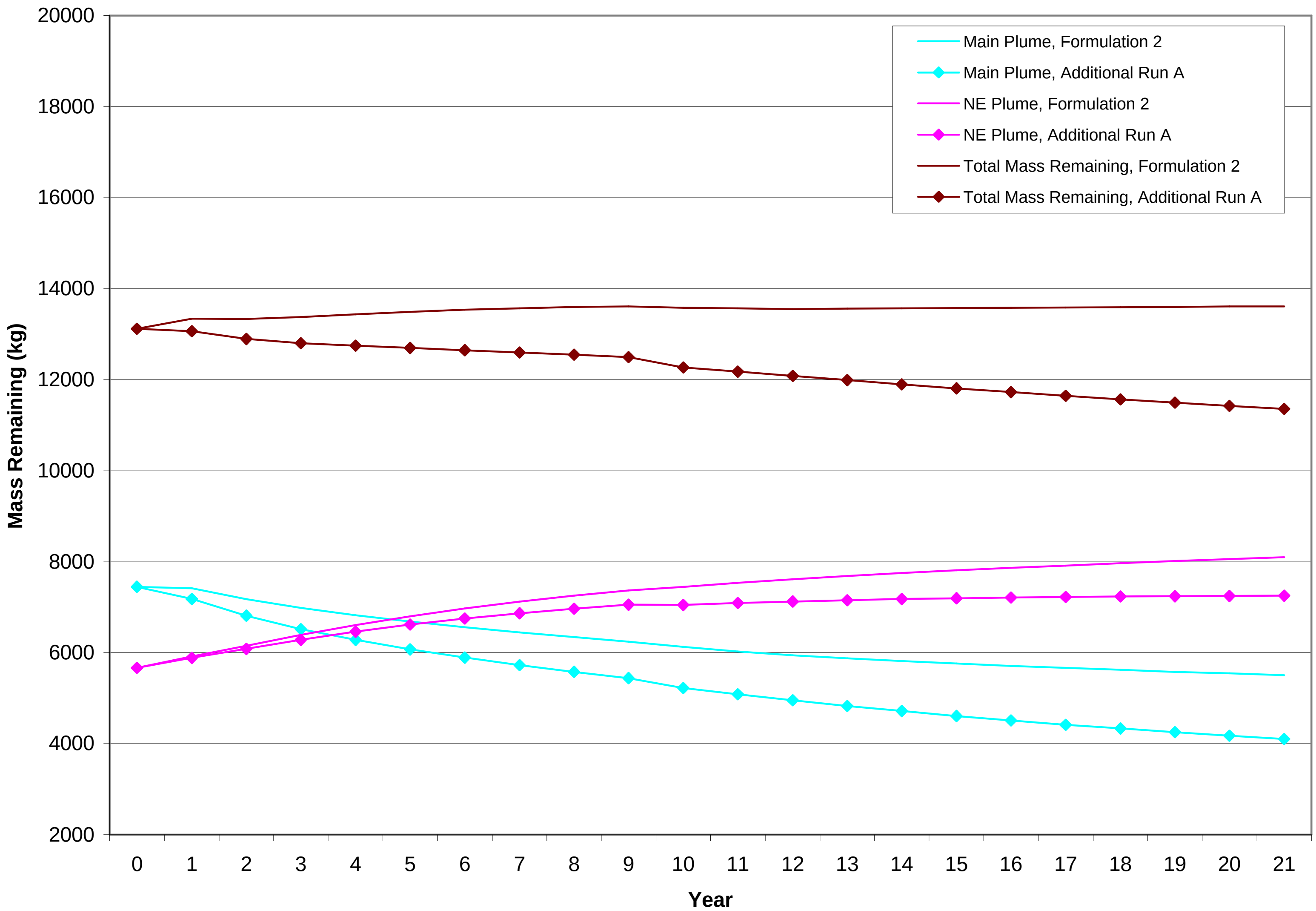


Figure 2-13 TCE Distributions After 21 Years, Model Layers 1 and 2, Additional Simulations B

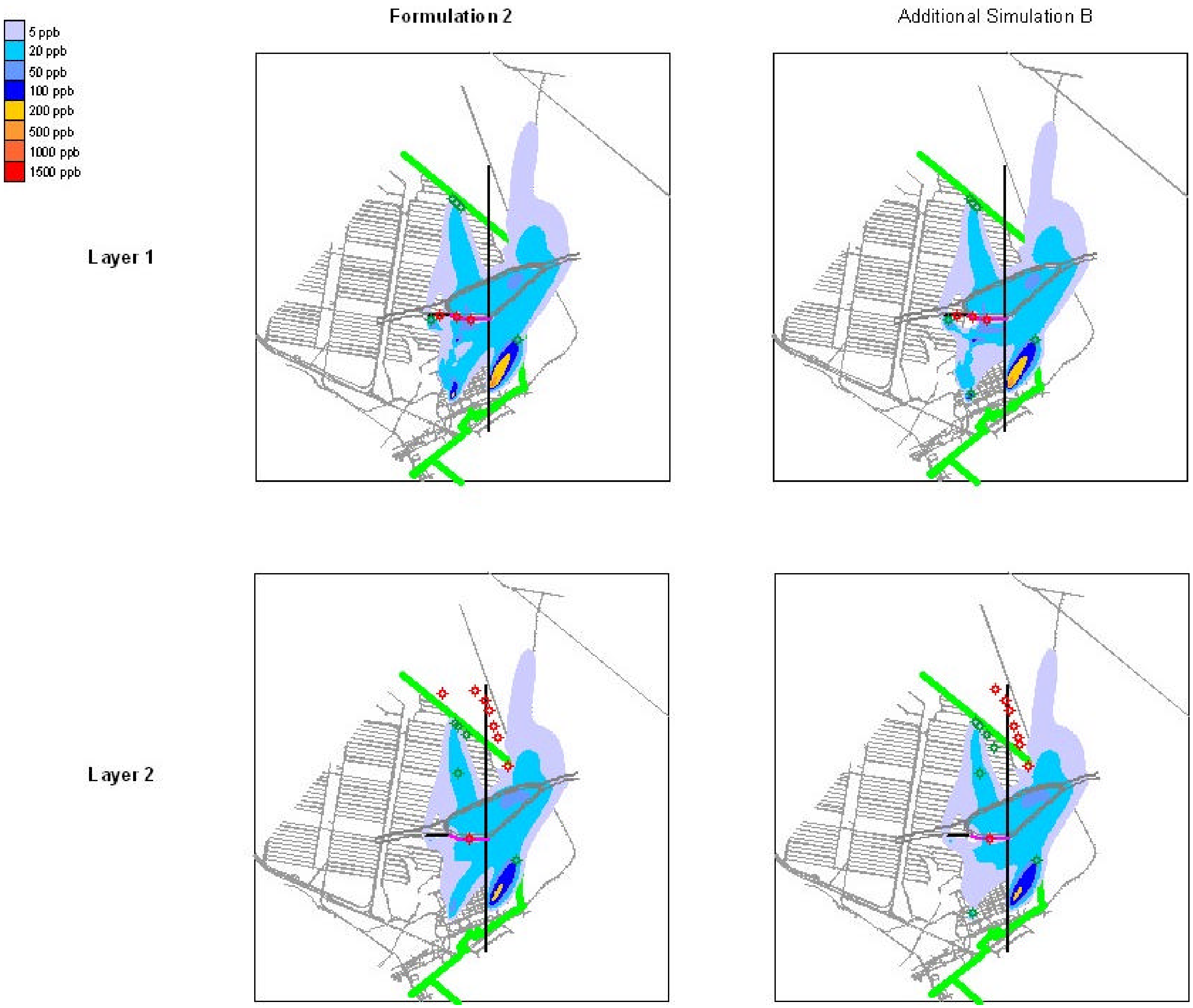


Figure 2-14   Mass Remaining After Each Year, Additional Simulations B

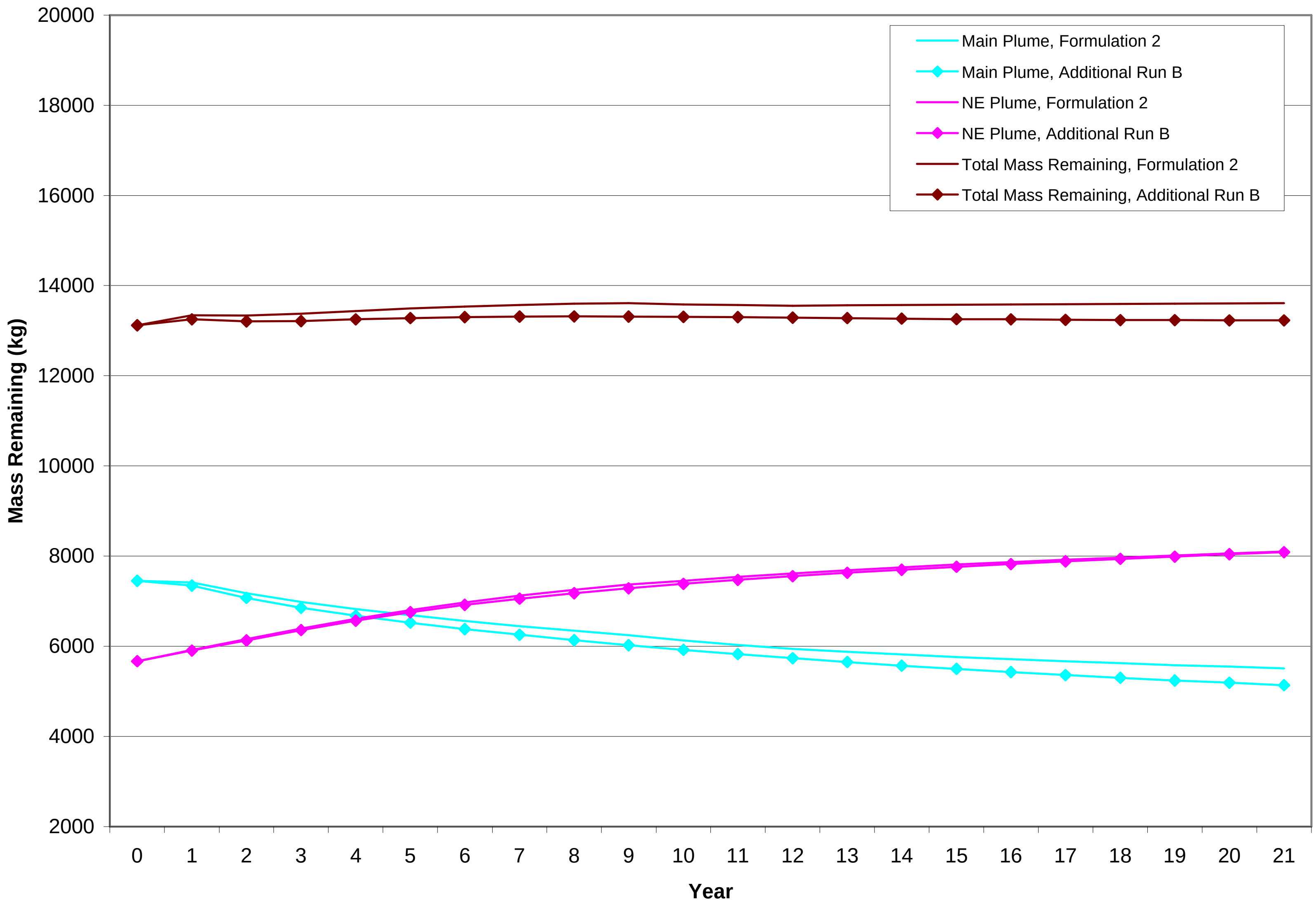


Figure 2-15 TCE Distributions After 21 Years, Model Layers 1 and 2, Additional Simulations C

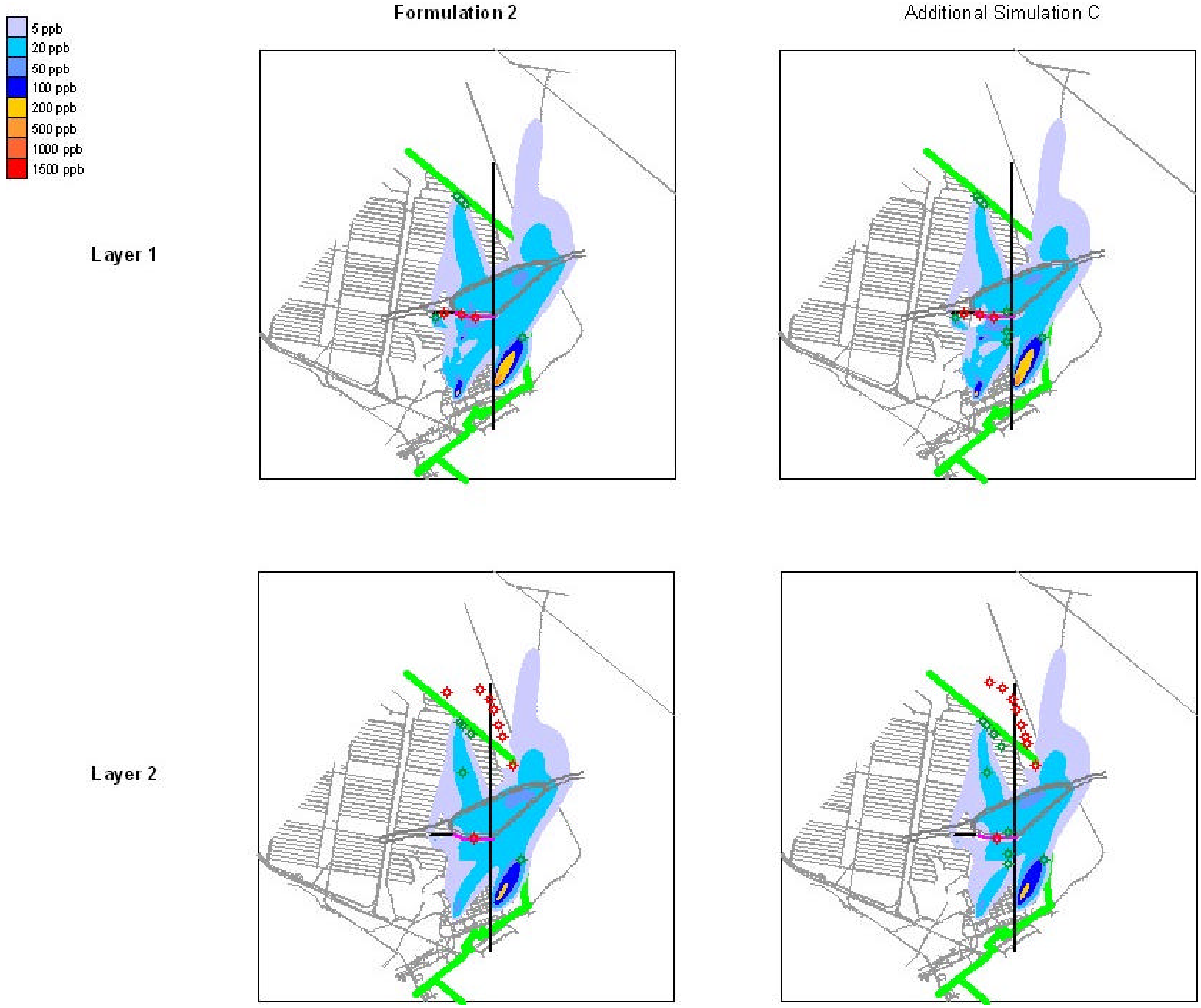
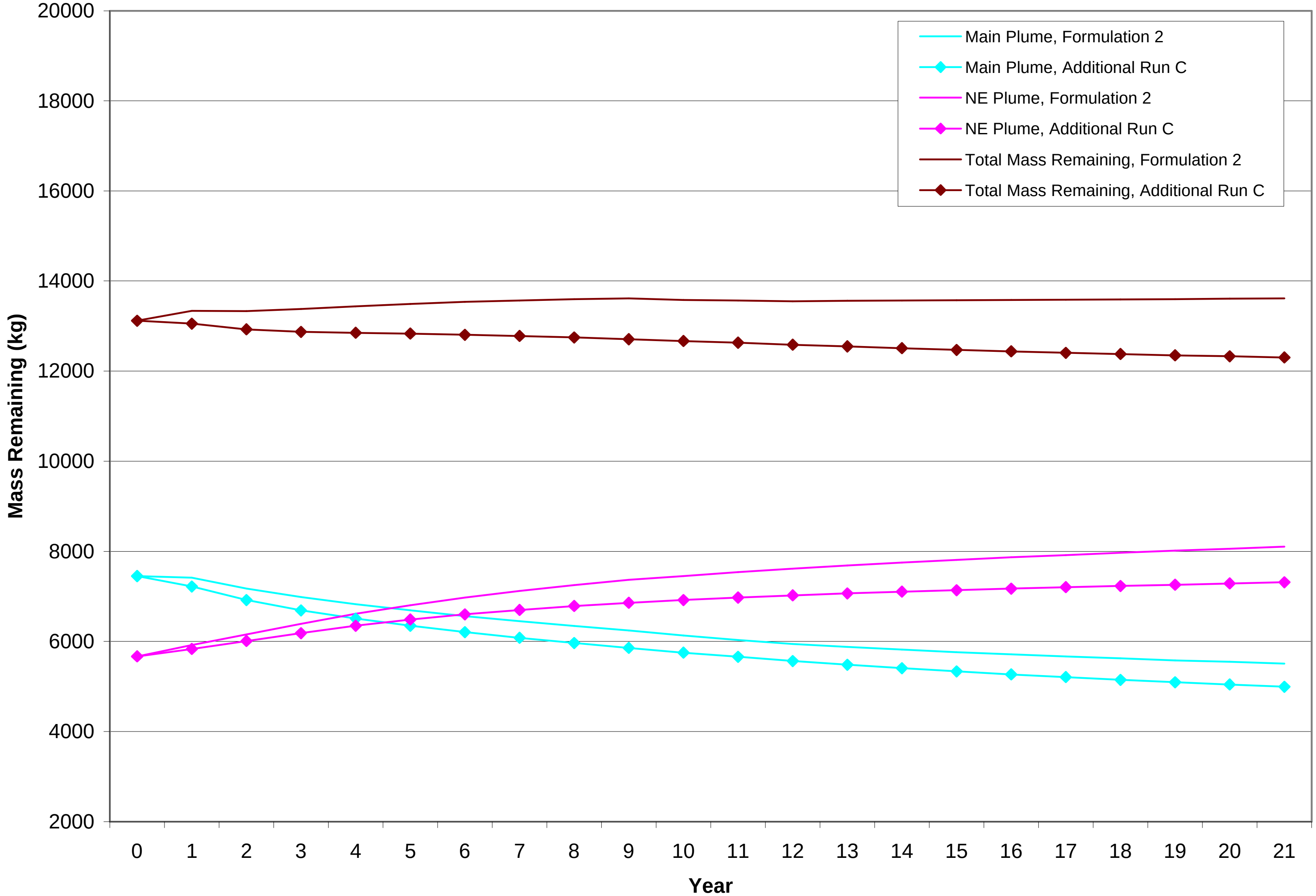


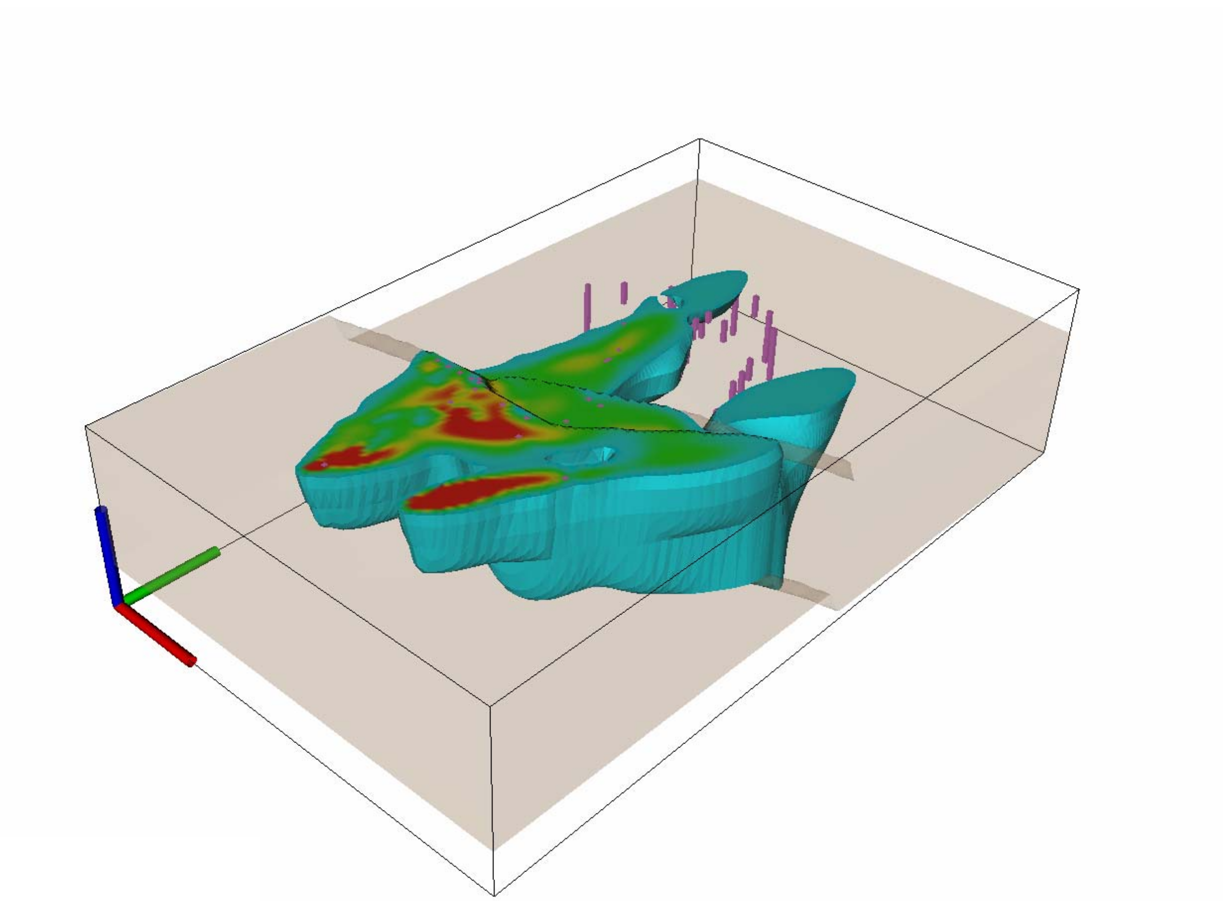
Figure 2-16   Mass Remaining After Each Year, Additional Simulations C



UA Report on Tooele

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

Chunmiao Zheng and Patrick Wang
The University of Alabama



The Hydrogeology Group
The University of Alabama

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

Chunmiao Zheng and Patrick Wang
The University of Alabama

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.

1

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.

2

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:

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

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:

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

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:

$C^{\max} \leq 5$ ppb at all POE-MP locations for $t \geq 3$ 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:

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

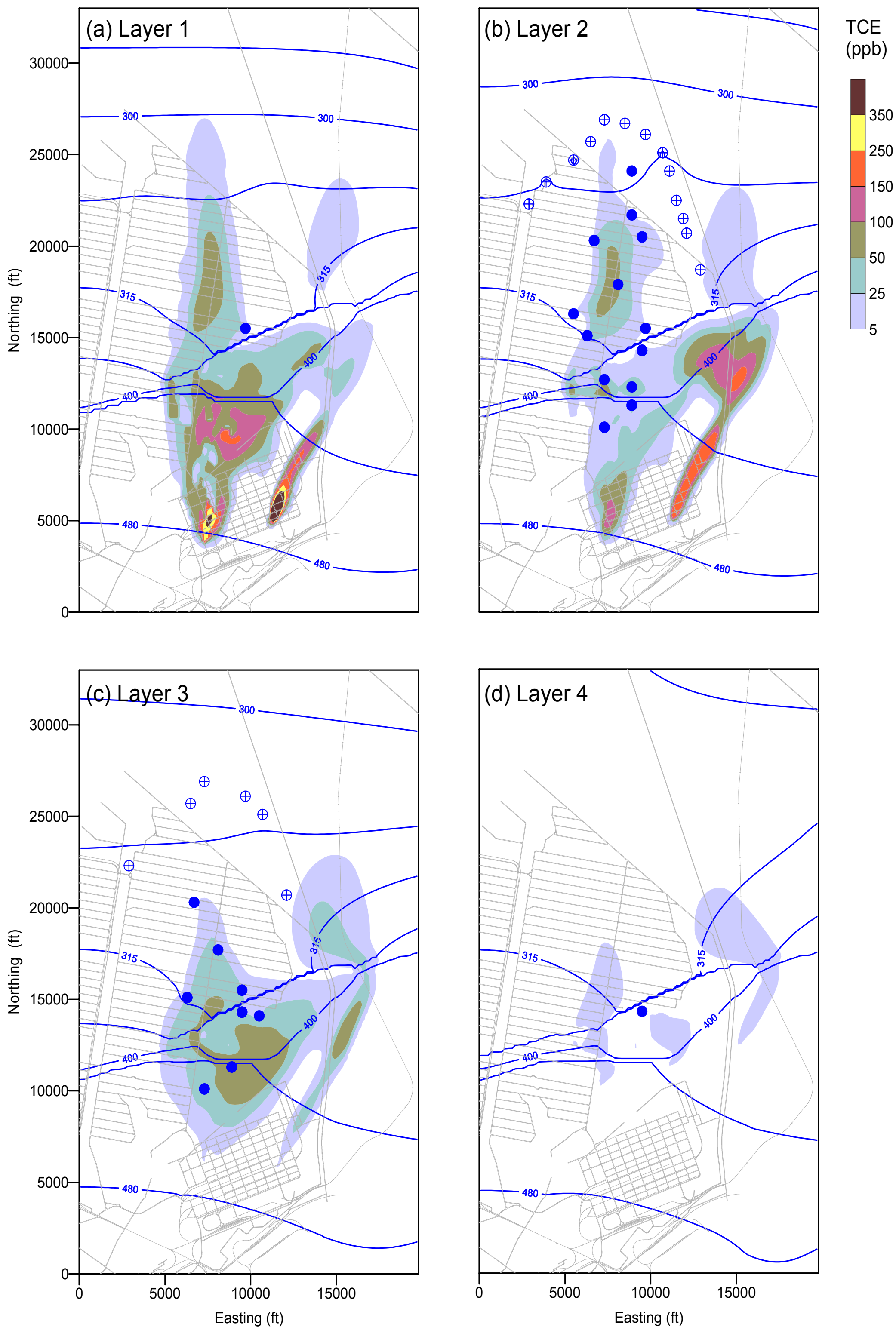


Figure 2.1. Calculated heads and TCE plumes at Tooele Army Depot, Utah for January 2003, the starting date assumed for the optimization analysis: (a) model layer 1; (b) model layer 2; (c) model layer 3; and (d) model layer 4. The existing pump-and-treat system consists of 16 extraction wells (solid dots) 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.

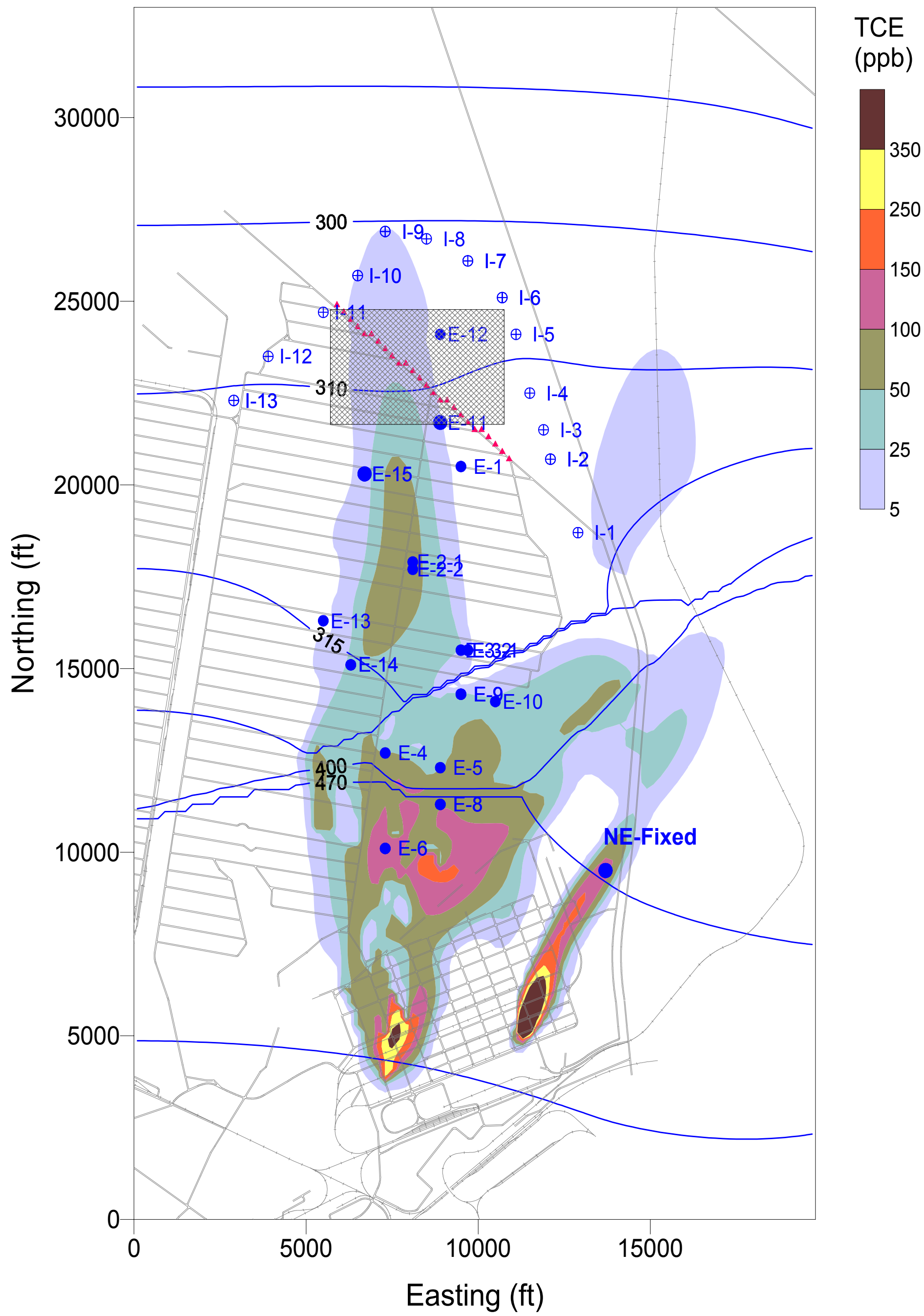


Figure 2.2. Locations of the "point of exposure" constraints for the main plume (POE-MP), shown as red triangles, where the TCE concentration must be at 5 ppb or lower by the end of year 3 and thereafter. The rectangle with cross-patterned lines indicates the 'moving well' region within which the optimal 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.

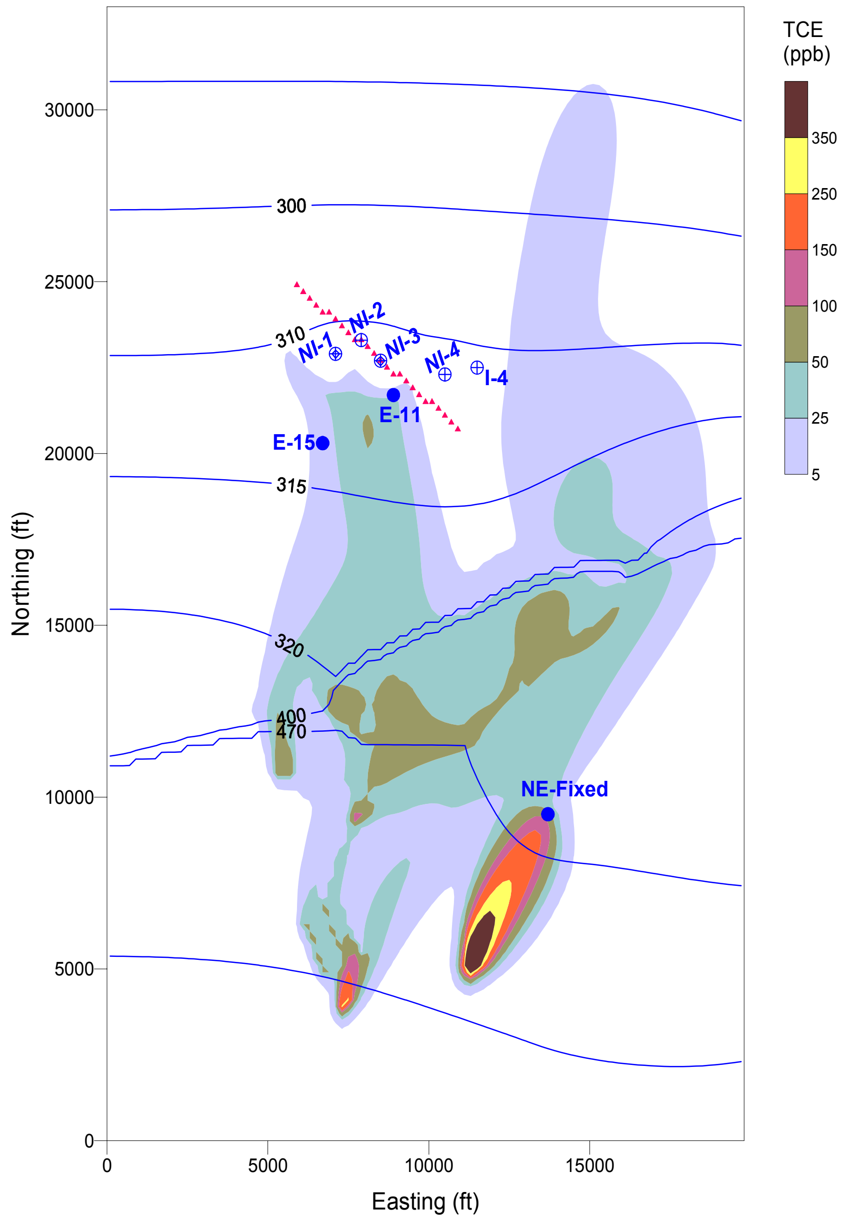
In all the runs up to this point, only steady-state solutions were sought. In other words, the well locations and flow rates were assumed to be constant throughout the entire projection duration. After the well locations were determined, a final run was carried out to develop an optimal dynamic strategy 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

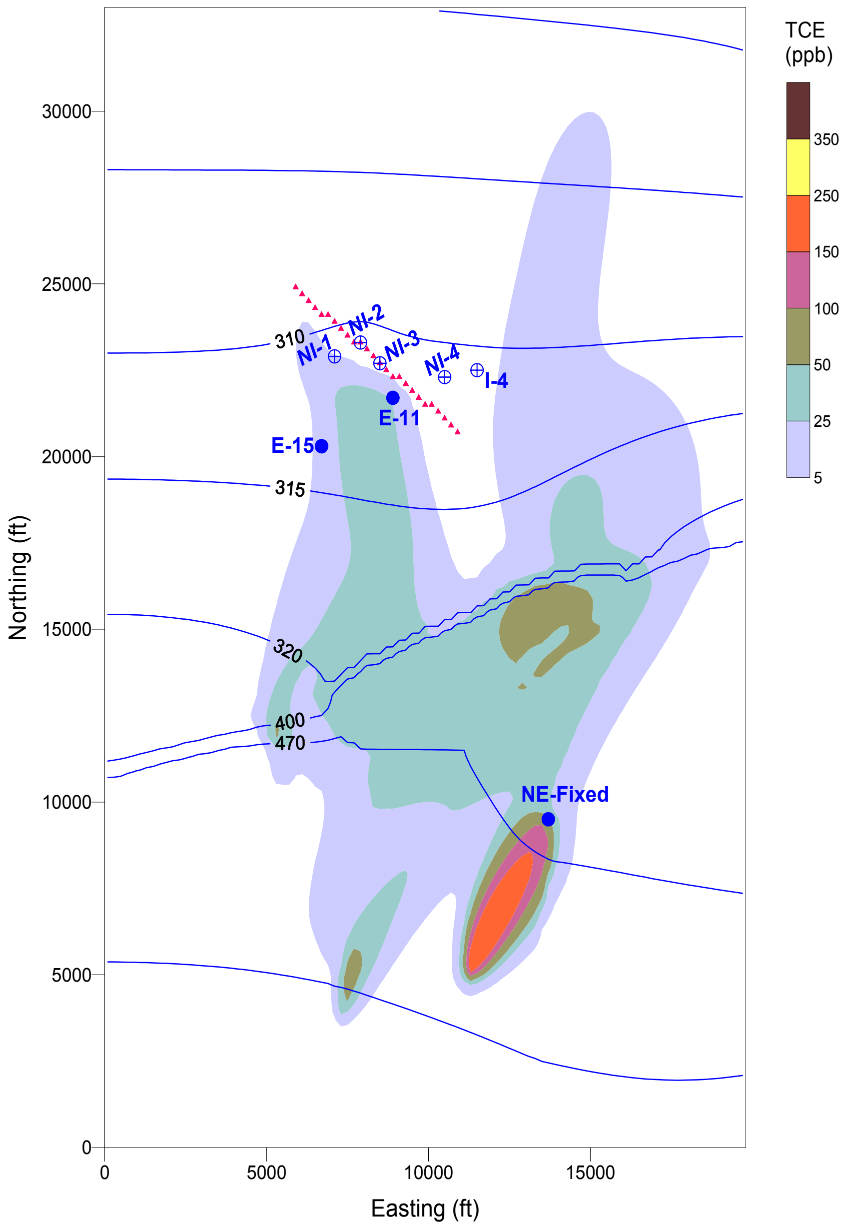
The optimal solution obtained for Formulation 1 is illustrated in Figures 2.3(a) through 2.3(c). It is noteworthy that no new pumping well is required and all existing wells are turned off except for pumping wells E-11 and E-15 and injection well I-4. One new injection (NI-1) is placed on the upgradient 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).

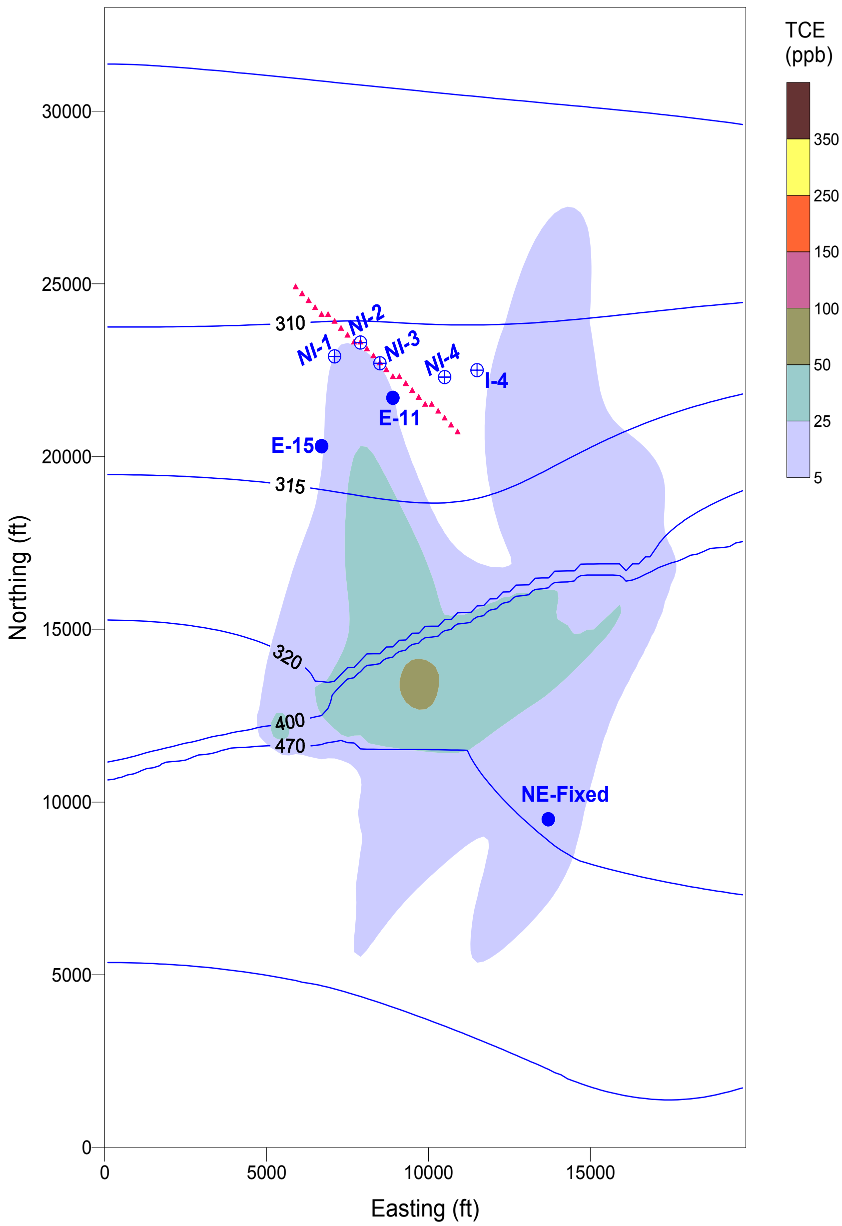
The cost objective function for the optimal strategy is $12.67 million in net present value. Of which, 56% is the fixed O&M costs which cannot be reduced as long as the pump-and-treat system is in operation. Another 32% of the total costs is related to sampling, which is dependent on the plume size. 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.

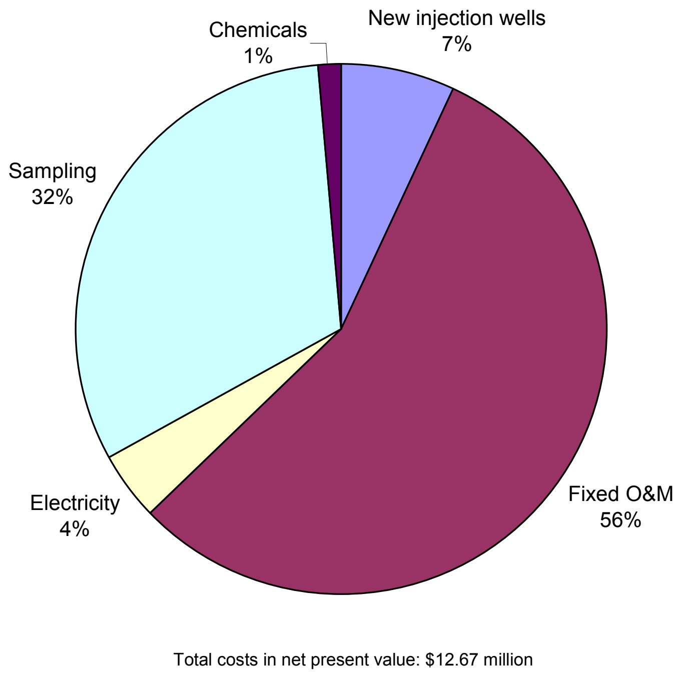


Figure 2.4. Distribution of the various cost items for the optimal solution for Formulation 1.

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’.

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). 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.

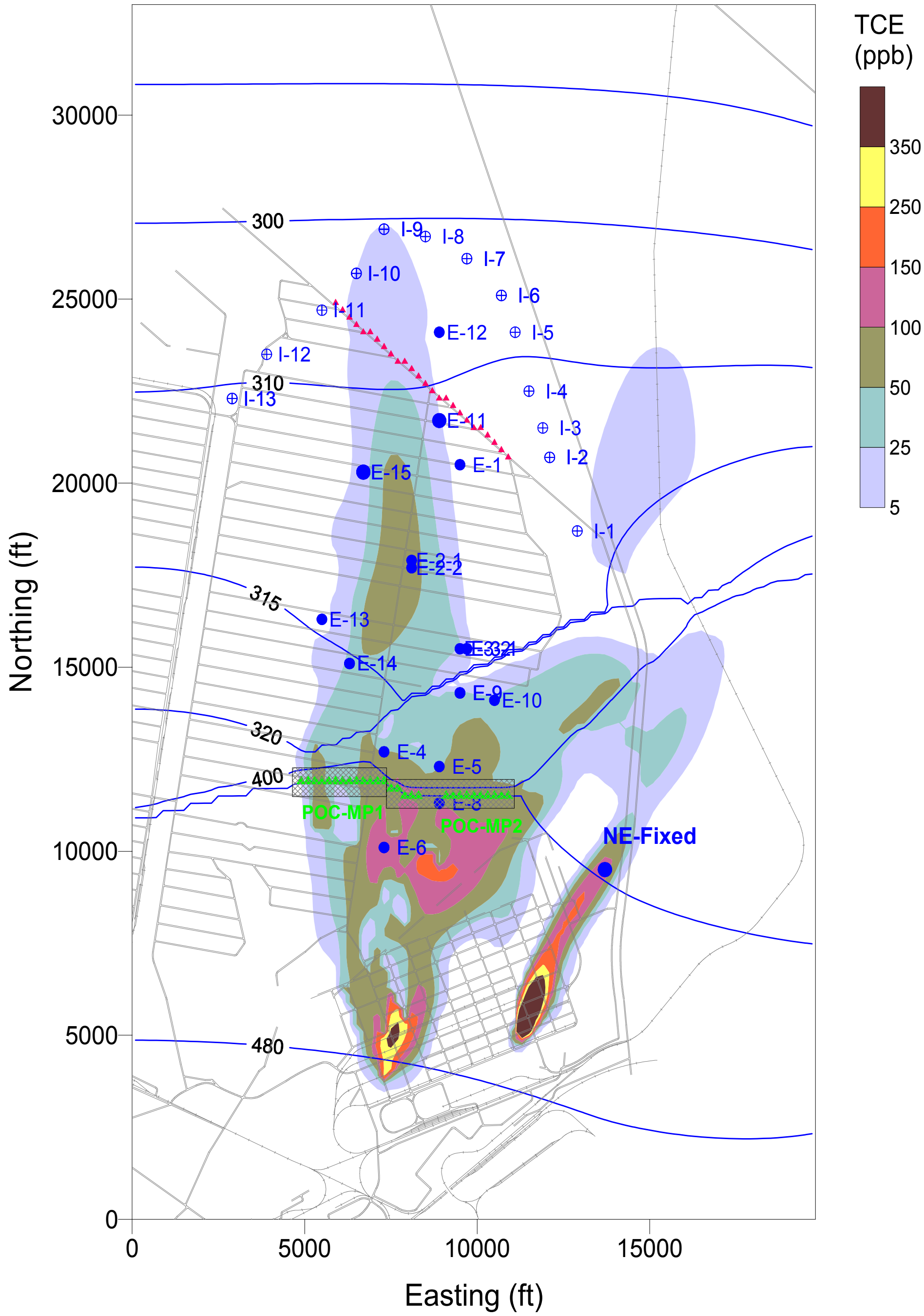


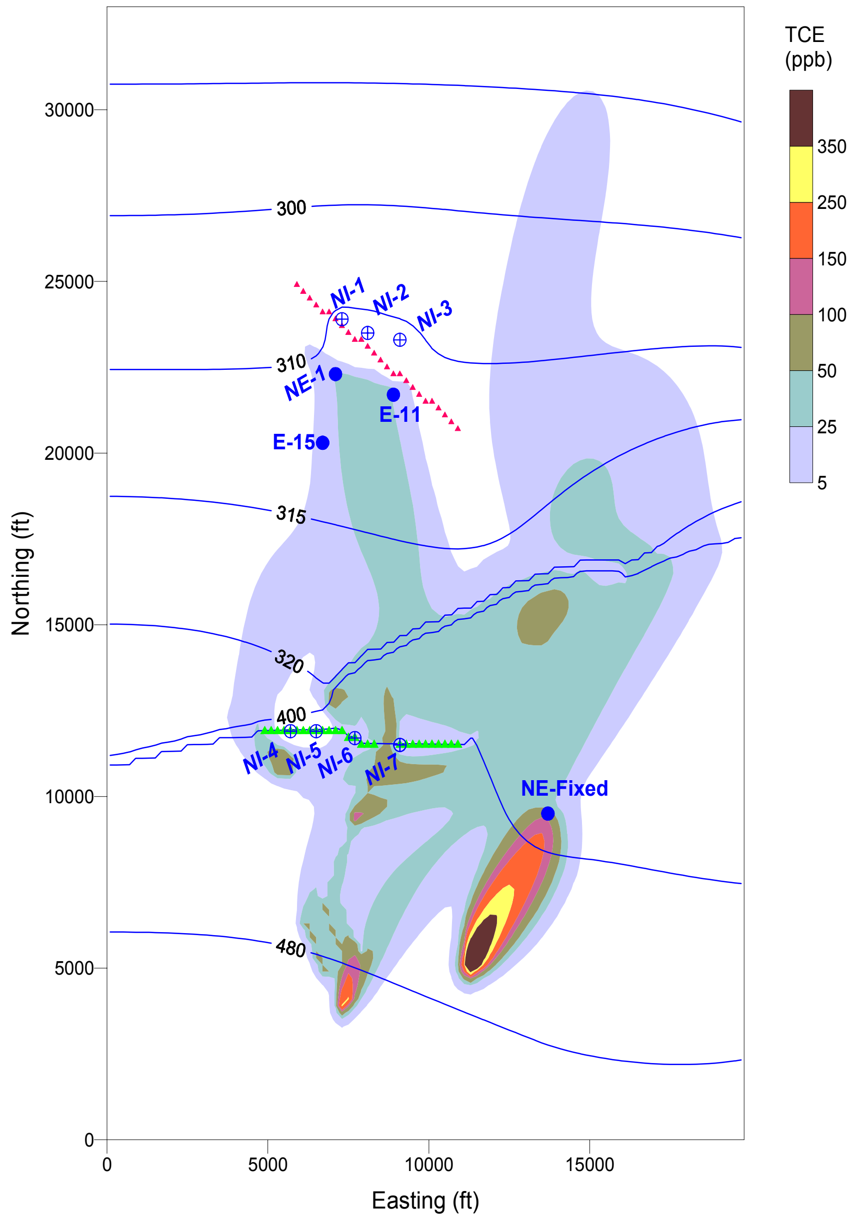
Figure 3.1. Locations of the "point of compliance" constraints for the main plume (POC-MP1 and POC-MP2) shown as green triangles. The rectangle with cross-patterned lines indicates the 'moving well' region within which the optimal locations for potential new pumping/injection wells are sought. Also shown 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.

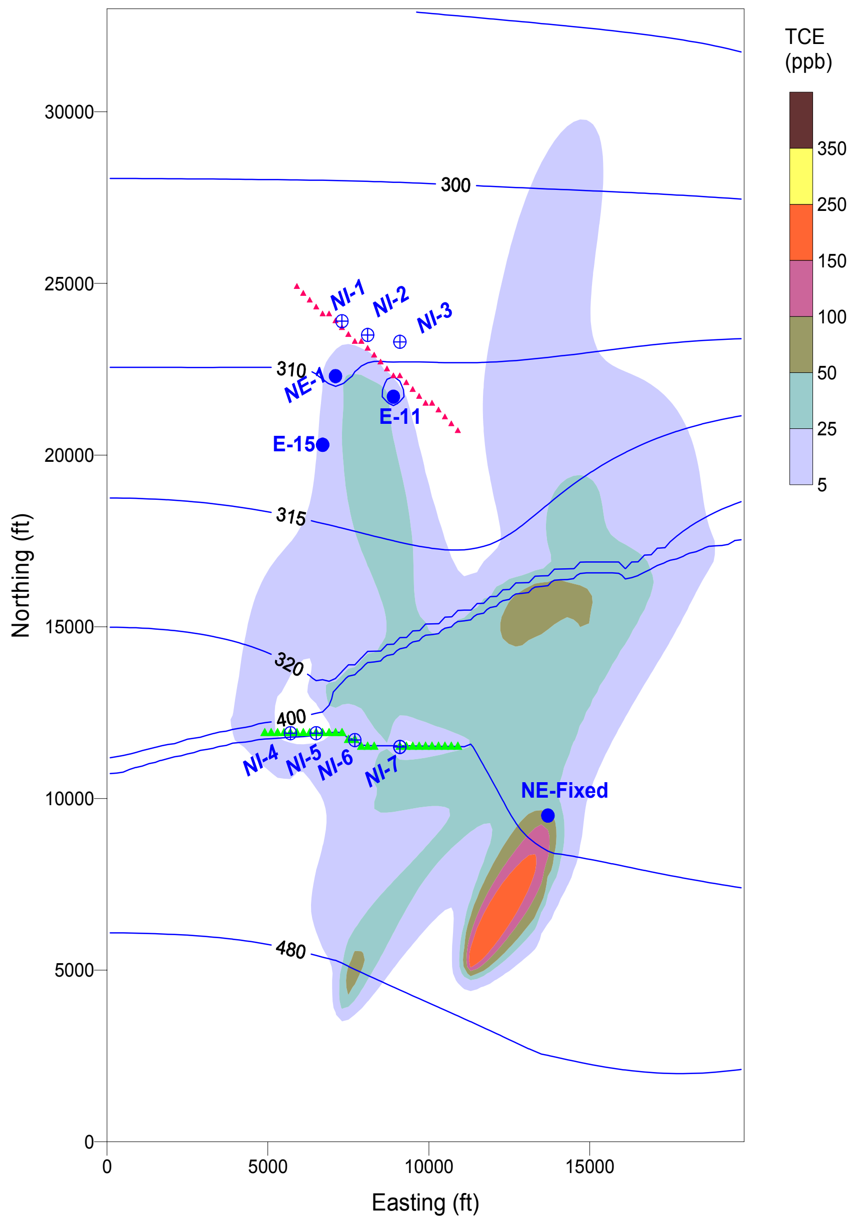
3.3 OPTIMAL SOLUTION

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.

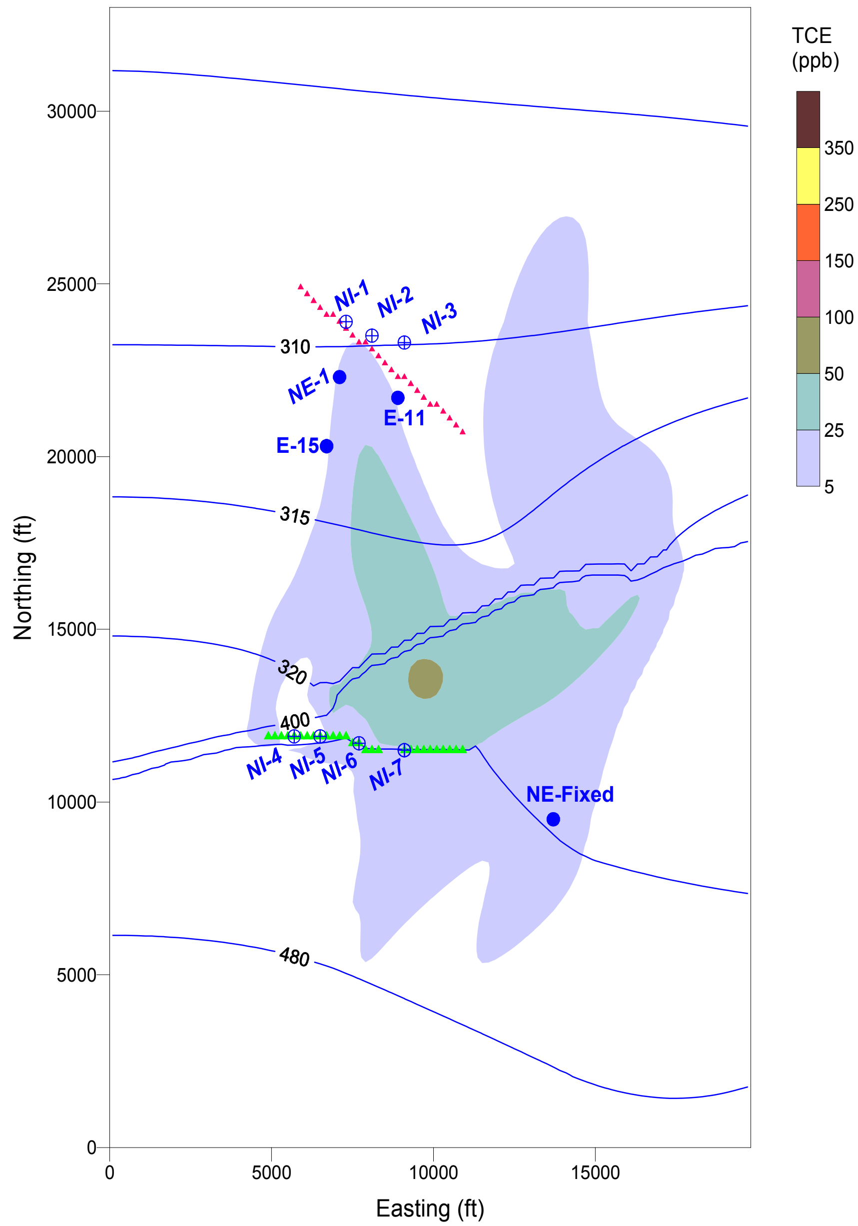
The pumping and injection rates for the optimal dynamic strategy are listed in Table 3-1, and well locations are included in the input file for the MODFLOW Well Package submitted with this report. All prescribed constraints are satisfied, including the maximum concentration limits at all POE-MP, POC-MP1, 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'.

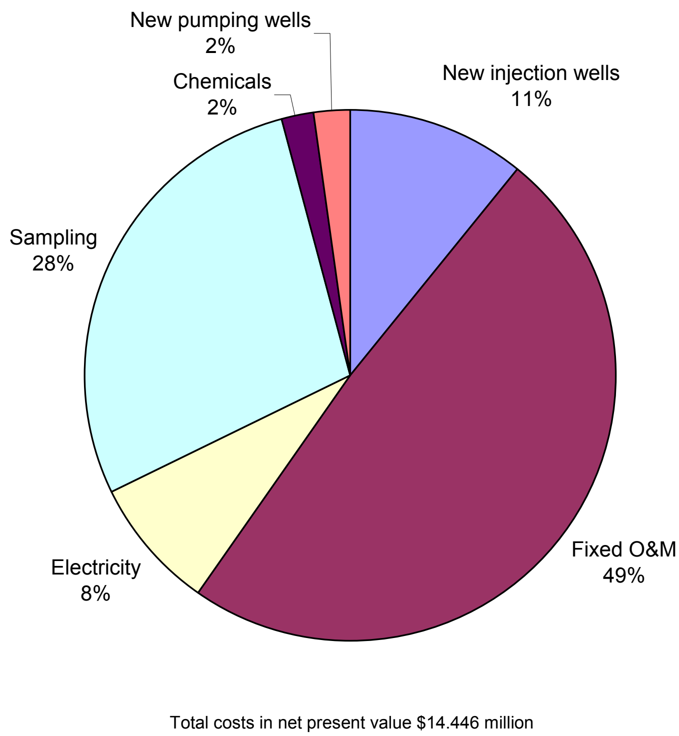


Figure 3.3. Distribution of the various cost items for the optimal solution for Formulation 2.

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.,

$C^{\max} \leq 50$ 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.

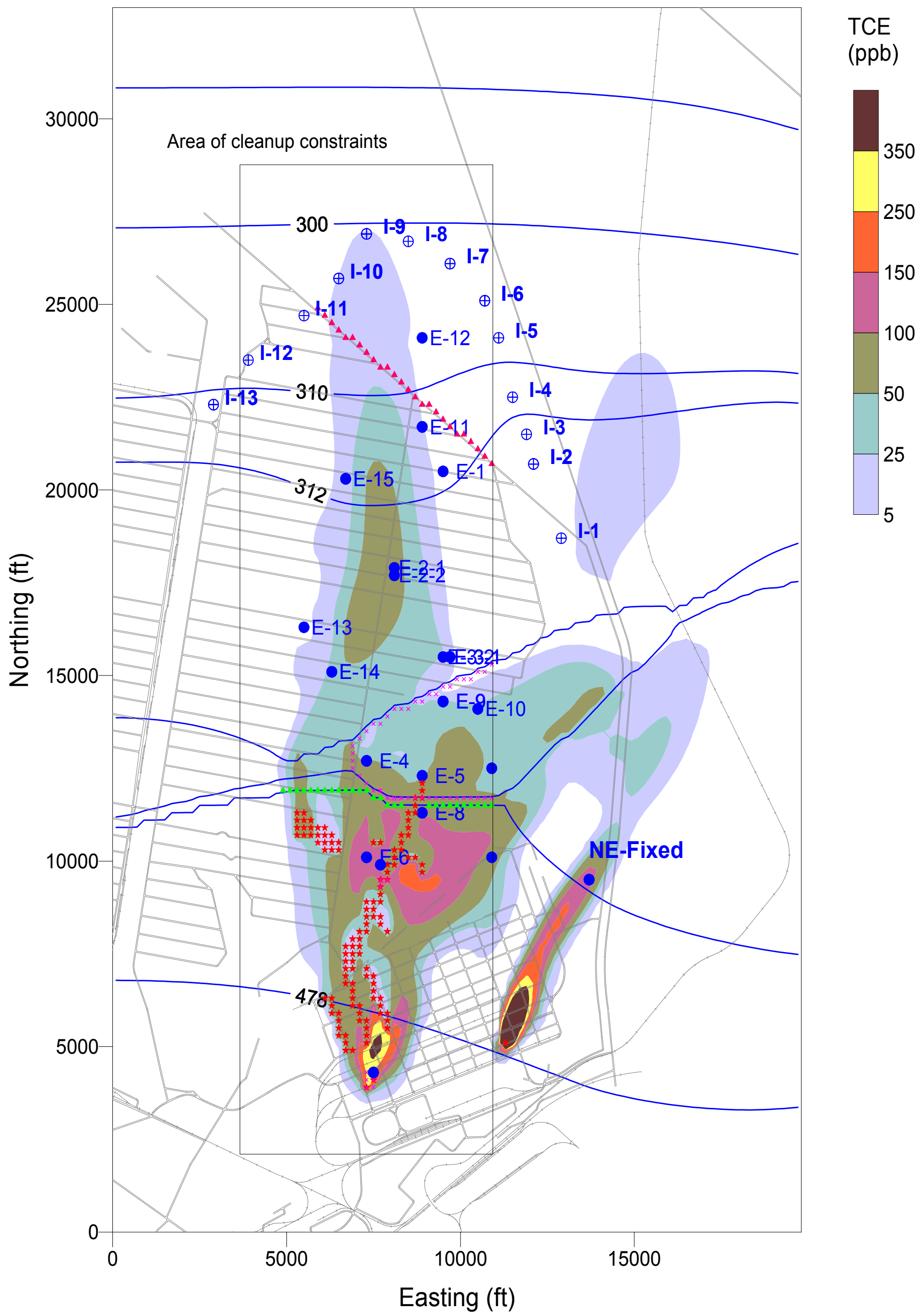


Figure 4.1. Locations of the "cleanup" constraints for the main plume shown as the area within the rectangular box. The star and cross symbols indicate the contaminant sources and other "buffer" cells, where the cleanup constraint was not applied. Also shown are the POE and POC constraints, along with 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.

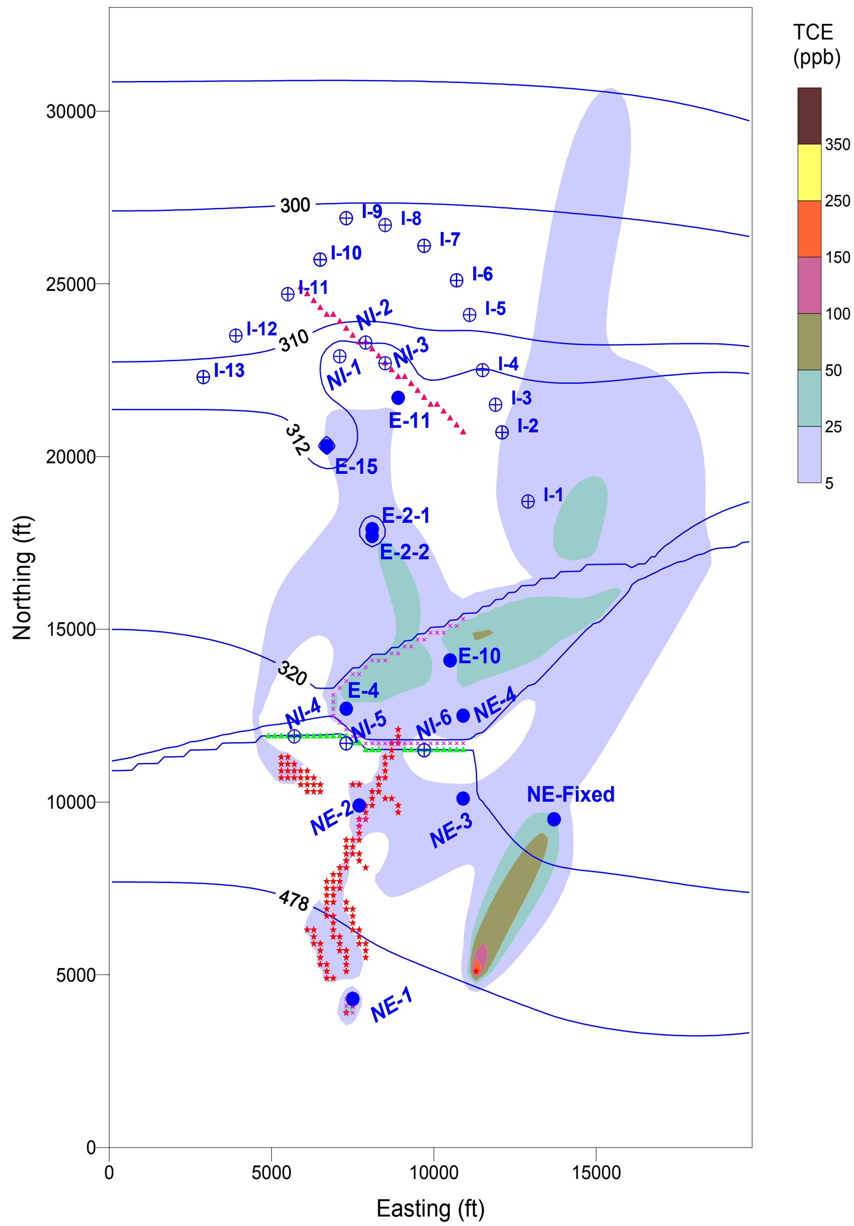


Figure 4.2. Calculated TCE plume and well layout for Formulation 3-1 in model layer 1 at the end of the project duration of 21 years. NI-1 through NI-6 are new injection wells. NE-1 through NE-4 are new pumping wells. Wells labeled with prefixes E and I are existing pumping and injection wells, respectively.

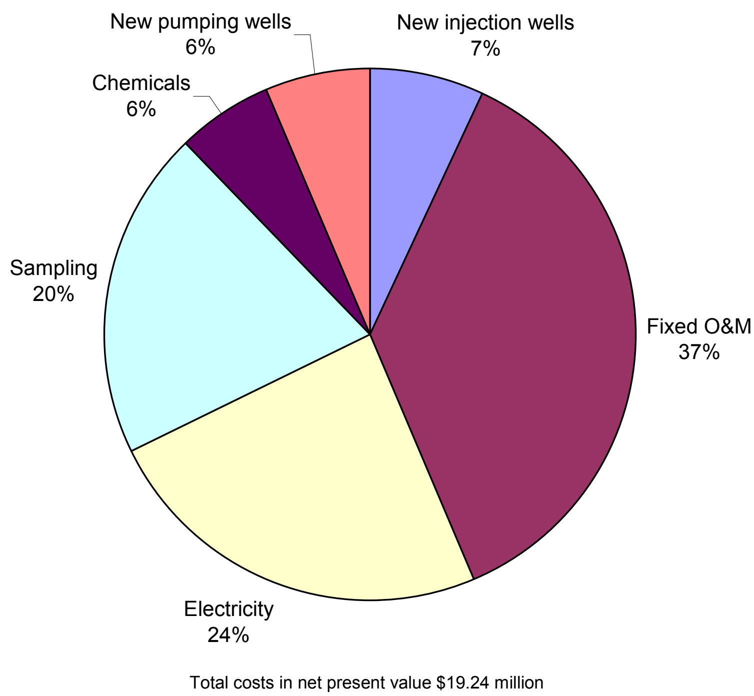


Figure 4.3. Distribution of the various cost items for the optimal solution for Formulation 3-1.

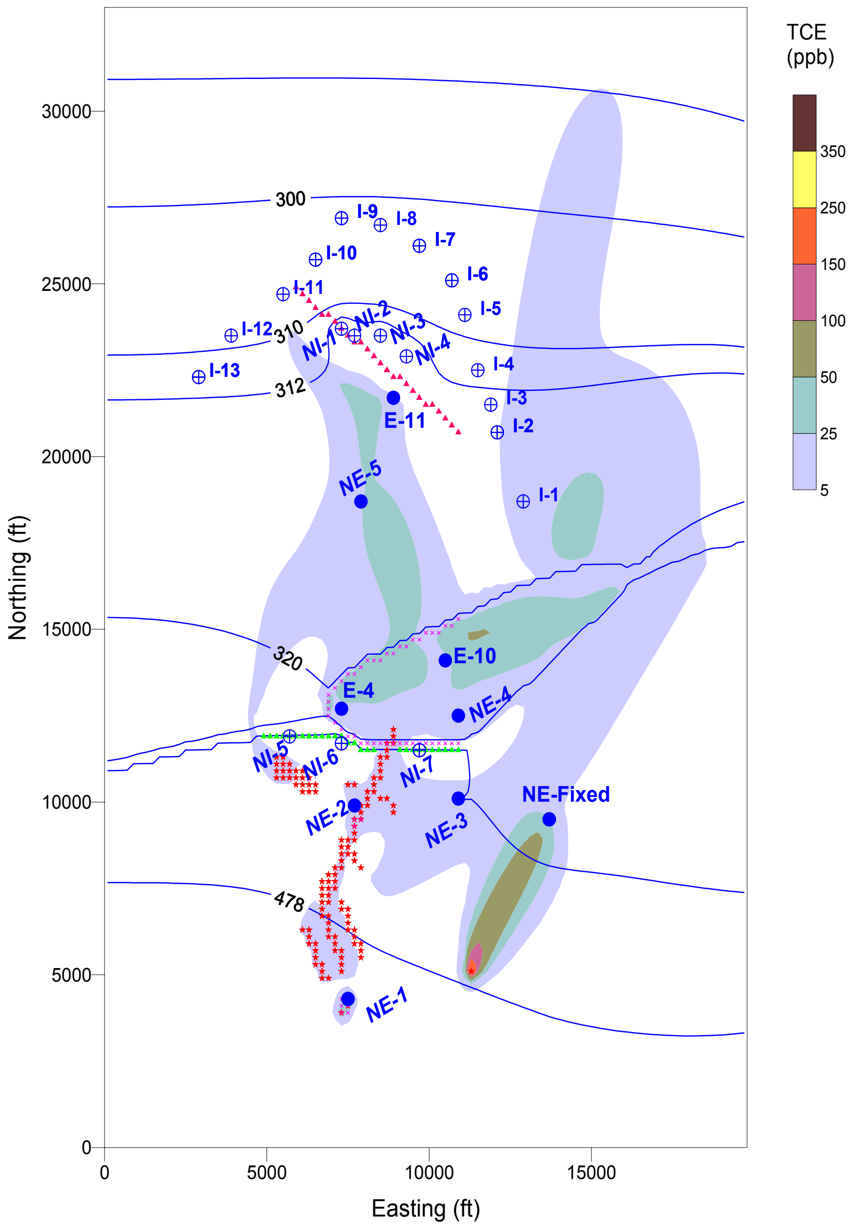


Figure 4.4. Calculated TCE plume and well layout for Formulation 3-2 in model layer 1 at the end of the project duration of 21 years. NI-1 through NI-6 are new injection wells. NE-1 through NE-4 are new pumping wells. Wells labeled with prefixes E and I are existing pumping and injection wells, respectively.

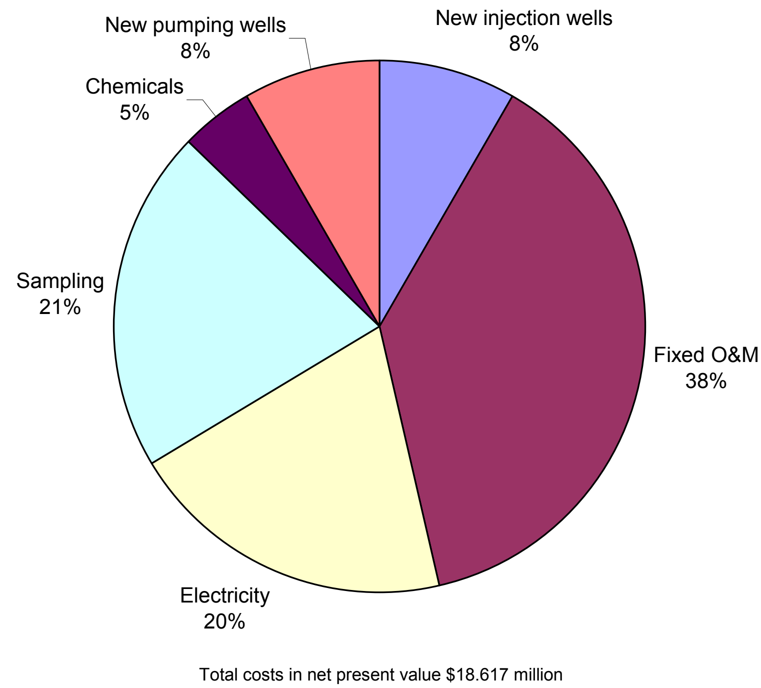


Figure 4.5. Distribution of the various cost items for the optimal solution for Formulation 3-2.

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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USU Report on Tooele

FINAL

OPTIMAL PUMPING STRATEGIES

FOR

TOOELE ARMY DEPOT MAIN TCE PLUME

Presented to

Navy Facilities Engineering Command
NAVFACENGCOMDET-SLC

Per

Contract No. N47408-00-C-7153

Prepared by

Systems Simulation/Optimization Laboratory
Dept. of Biological and Irrigation Engineering
Bldg EC-216
Utah State University
Logan, UT 84322-4105

23 Dec 2002

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Executive Summary

Utah State University (USU) was to develop pumping strategies for the main TCE plume (MP) at Tooele Army Depot (TAD). Strategies were to minimize the present value cost of satisfying posed optimization problems for a 21-year period. Three pump and treat (PAT) optimization problems were posed to USU. Formulation 1 addresses plume containment at the Point of Enforcement (POE), along the TAD boundary. Formulation 2 addresses plume containment at a Point of Compliance (POC), in addition to all Formulation 1 constraints. The POC is along an internal operable unit boundary. Formulation 3 includes all Formulation 1 and 2 constraints, a cleanup constraint, and limits on the numbers of extraction wells (EW) and injection wells (IW) that can be constructed. Formulations 1 and 2 assume contaminant source cells having temporally constant concentrations. Formulation 3 assumes temporally decreasing concentration at source cells.

Per its contract, USU here reports and distinguishes between work performed during two periods. These periods are: from project commencement through March 1, 2002; and from that first deadline to March 18, the date of USU's formal presentation and draft final report (SSOL, Mar 18, 2002). Table 1 summarizes results.

While addressing Formulation 1, USU intended to lay the groundwork for Formulation 3. Therefore, USU developed alternative Formulation 1 strategies that use different numbers of wells and their placements. In its approach to Formulation 1, USU assumed that a pumping strategy would need to extract the contaminated flux moving northward toward the POE boundary.

The first two strategies (USU1A and USU1B), require constructing only two extraction wells (EW), but require extracting from many existing wells. Because of the annual cost associated with pumping at an EW, the twenty-one year costs of USU1A and USU1B were larger than that of a strategy requiring constructing three EWs (USU1C). It seemed unlikely that we could reduce USU1A and USU1B costs enough to make them competitive with USU1C. Therefore, we only slightly optimized Strategies USU1A and USU1B before ceasing work on them.

Both new EWs required by USU1A and USU1B would have to pump near the maximum allowed by the posed optimization problem. If TAD can significantly relax that limit, possibly only one new EW would need to be constructed to address the Formulation 1 POE containment constraint.

Strategy USU1C has a present value cost of about $14.14 M and requires constructing 3 EW. The most northern of those three wells is needed because of sharp angle between the facility boundary and the flow direction, and is needed only in the first stress period.

An IW costs less than an EW. Therefore, USU developed another strategy by substituting an IW for the northernmost EW of USU1C. The resulting Strategy USU1D costs slightly less than USU1C, but is less robust and spreads contamination laterally. Therefore for Formulation 1 USU recommended strategy USU1C. USU did not try other applications of

injection for Formulation 1. An alternative solution might suffice if regulators allow TAD to delay containment until four or five years (i.e. until after the end of the current first three-year period). In such case, no EW or IW well might be needed to the north, and only two EWs (or one well pumping at a greater rate than is currently allowed by Formulation 1) might economically provide a solution.

USU began addressing Formulation 2 by considering that Strategy USU1C EW positions were appropriate to address the POE constraint, and by adding 4 IWs and no EWs to address the POC constraint. However, one week before the March 1st due date, USU realized that strategy eventually caused high TCE concentrations to bypass the POC to the west. The strategy satisfied all TAD Formulation 2 constraints, but was unacceptable to USU. Environmental regulators do not usually accept strategies that cause much clean aquifer material to become contaminated.

Thus, without vigorous optimization, on 1 Mar 2002 USU presented strategy USU2A for a Formulation 2 problem that was somewhat more restrictive than that posed by TAD. That modified Formulation 2 problem includes what USU terms a Zone 4 constraint in column 29, rows 106-140. This constraint prevents TCE concentrations of 5 ppb or greater from moving to the west of the POC into previously uncontaminated aquifer.

USU2A costs $17.110 M. USU2A involved constructing 4EW and 4IW. Of these, new injection well UI4 aids robustness in the field, and would only be constructed if needed at the beginning of year 2011 (stress period 3). UI4 is in an area having source concentration cells, competing hydraulic stresses in multiple layers, and time varying concentration constraints. UI4 could help assure that flows and resulting concentrations can be tailored to management needs even if the physical system differs from the modeled system.

In the computer model, one can decrease Formulation 2 lifetime cost by screening the adjacent Layer 1 well (UI3) in two layers, instead of one, when it is constructed. Thus strategy USU2B (developed 5-17 March) requires one fewer IW than USU2A (it does not use UI4). USU2B involves constructing 4EW and 3IW and costs $15.731 M. It also satisfies the additional Zone 4 constraint. Because it builds one less IW (near the eastern POC), it provides a little less control over flows in that area than USU2A.

Formulation 3 as posed to USU was infeasible. USU invoked its contractual option of not preparing a substitute formulation by March 1. As allowed, USU developed an alternative during March 5-17. Strategy USU3-1 costs $17.928 M and requires constructing 9 EW and 3 IW. USU3-1 is a compromise between minimizing westward TCE spread and minimizing cost. In addition to applying TAD concentration constraints it applies Zone 4 constraints for the first three stress periods only. In period 4 USU3-1 turns off one new EW to reduce cost. The consequence is that concentration almost reaches 10 ppb in the northernmost Zone 4 cell in period 4. After that the maximum Zone 4 concentration is below 4 ppb. Alternatively, to satisfy the Zone 4 constraint for all stress periods requires less than $0.060M more—merely continuing pumping in the westernmost new EW through period 4.

Introduction

We present optimal pumping strategies to address the Tooele Army Depot (TAD) TCE plume as it is projected to exist in January 2003 (Figures 1 and 2). We developed these strategies ``using the heuristic optimization capabilities of the SOMOS simulation/optimization model (SSOL and HGS, 2001). We tried to balance the desire for mathematical optimality with practicality. We verified the concentration constraint feasibility of our pumping strategies using the Geotrans postprocessor.

We submitted strategies USU1A-1D and 2A by March1, 2002. We were not obligated to submit a Formulation 3 strategy by then. Between March 5th and the March 18th draft due date, we did additional evaluation, resulting in strategies USU2B and USU3-1. (In that period USU also developed strategy USU1E using the same wells as USU1C and costing a slightly improved $14.132M).

Optimization Technique

Formulations Addressed

We present optimal pumping strategies for three optimization problems (Formulations 1-3 posed by TAD or modifications thereof). All three involve minimizing present value of the cost of operating a PAT system for 21 years. They differ in the applied constraints. For Formulations 1 and 2 contaminant source concentrations are constant in time. For Formulation 3, contaminant source concentrations decline with time.

A Formulation 1 strategy must cause concentrations in POE cells in all layers to not exceed 5 ppb by the end of year 3. Figure 3A shows the line of cells included in this POE constraint.. A Formulation 2 strategy must satisfy the POE constraint and prevent concentrations in POC cells (Layers 1 and 2) from exceeding time varying limits. Figure 3B shows the cells in rows 106, 107 and 108 included in the POC constraint.

USU added a line of concentration constraint cells (Zone 4) to assure the plume did not expand into previously uncontaminated aquifer to the west (Figure 3B, Column 24). Such expansion could otherwise result from injection along the POC.

A Formulation 3 strategy includes POE and POC constraints and requires that all cells (except for excluded cells) must be below 50 ppb by the end of year 9. Excluded cells include: all those in model columns 56 and greater; and cells having high source concentrations or extremely low conductivity.

The Optimization Process

USU developed optimal pumping strategies for Tooele Army Depot (TAD) using the SOMO3 module of SOMOS (SSOL and HGS, 2001). The SOMO3 optimization module uses heuristic optimization and artificial intelligence capabilities. SOMO3 heuristic optimization modules include genetic algorithm (GA) and simulated annealing (SA). In its spacetube or ANN-GA Moving System (AGMS) mode, it trains artificial neural networks (ANN) for state variables and uses a GA for optimization. For Tooele optimization we employed GA without artificial intelligence.

For each optimization problem formulation, our computer runs are generally partitionable into two phases:

- Exploratory simulation and optimization. We began this phase by performing exploratory flow and transport simulation. Then we tested and evaluated several candidate well locations using transport optimization.
- Optimization. We performed transport optimization for limited sets of candidate well locations.

Formulation 1 is supported by Figures 3A, and 4-7 and Appendix B. Formulation 2 is supported by Figures 3B and 8-13 and Appendix B. Formulation 3 is supported by Figures 14-17 and Appendix B. Appendix B contained postprocessor outputs for those respective strategies.

Formulation 1

After considering the optimization problem and the site boundary, USU decided its ultimately proposed strategy should extract all the contaminated water approaching the POE boundary constraint. Doing otherwise could cause the contamination to move into undesirable locations, and possibly to ultimately escape the facility. This meant that USU emphasized extraction, rather than injection, for this problem.

Preliminary optimization runs revealed that the cost objective function value (OFV) was most significantly affected by he number of EWs that pump and the cost of installing any new wells. Therefore USU's general approach was to try to use as few existing EWs and to install as few new wells as possible.

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To initially evaluate candidate well locations, USU simplified the optimization problem by addressing only the first stress period. Runs included:

- Installing 2 EWs, and pumping at those and existing EWs. (Because of the bounds on pumping at individual wells, we had to install at least 2 wells to satisfy the POE containment constraint.
- Installing 3 EWs.

USU optimized for both situations, using different combinations of candidate well locations. Table 2 lists representative GA optimization input parameters. After identifying a desirable batch of candidate well locations, USU performed sequential optimization for all stress periods. Then, USU tried to reduce cost further. For a strategy requiring constructing 3 EWs, USU replaced the northernmost EW with an IW, and optimized. However, using injection spread the contamination laterally. Although the strategy with injection was less expensive, it was not desirable, and was neither recommended nor used further.

Formulation 2

Because the Formulation 2 problem includes the Formulation 1 constraints, USU began strategy design using the wells employed for the best Formulation 1 strategy (one that required constructing 3 EWs). Thus, USU focused on determining how to best address the additional POC constraints.

After making some simulations, USU judged that it would not be physically practical to satisfy the POC constraints via extraction. Then USU made optimization runs exploring candidate IW locations upstream of the POC zones. USU concluded that satisfying the POC constraints would require installing at least 4 IWs, if installing no EWs.

To reduce computational effort, initial optimizations focused on the first three stress periods (the most crucial periods with respect to satisfying the various POC constraints). After USU obtained satisfactory candidate wells for the first three periods, it optimized for all seven periods. Those strategies required constructing 4 IWs.

One week before the deadline for submitting the strategies, USU noticed what it considered a major problem. As a result of the injection, TCE moved significantly to the west around POC-mp1 (Fig. 3B), contaminating formerly clean aquifer. Although allowed by the problem formulation, this seemed unacceptable.

USU then replaced the westernmost IW with an EW, but even this change was insufficient to keep the plume from moving into formerly clean aquifer during optimization. Thus USU added a zonal concentration constraint on concentration moving to the west. At first the zonal constraint was a line of cells diagonal with respect to flow direction (roughly running from the western end of the POC-mp1 to the southwest). However, that orientation made it more difficult to get feasible solutions for all periods).

Thus USU added a constraint on the maximum concentration allowed in a specified line of cells running roughly to the south from the western end of the POC-mp1 (Zone 4 in Fig. 3B). Figure 9 shows the revised optimization problem. At that moment there was insufficient time to optimize much, but the result was strategy USU2A.

In the two weeks between the first deadline, and the time of formal results presentation, USU optimized for the 7 stress periods, reducing cost significantly (Strategy USU2B). Table 3 displays representative GA parameters.

Formulation 3

The TAD-posed Formulation 3 problem included all the Formulation 2 constraints, plus cleanup constraints and limits on the numbers of EWs and IWs that could be constructed. Experience with Formulation 2 and exploratory evaluations led USU to believe Formulation 3 was infeasible as posed. As contractually permitted for an infeasible strategy, USU did not present a strategy by the first deadline.

Before March 18, USU developed a strategy that satisfied all TAD concentration constraints and Zone 4 constraints for all stress peiods, but used more wells than TAD allowed. To develop that strategy, USU used as candidates all Formulation 2 wells, existing wells and EWs at high-concentration locations that would otherwise not be remediated. USU did not report this $18M strategy after noticing that the source concentrations near the western edge of POC-mp1 dropped significantly by the end of period 3. This means that in the later periods, there is less need for the Zone 4 constraint.

After developing the above strategy, USU faced a dilemma. As with previous formulations, there was a conflict—increasing strategy desirability increases costs. Because the Zone 4 constraints were conceived and imposed solely by USU, USU chose to remove the Zone 4 constraints after period 3 to reduce cost from that of the above strategy. Figure 14B shows the optimization problem formulation.

In essence, USU tried to 'straddle the fence' in developing strategy USU3-1--a compromise between minimizing westward TCE spread and minimizing cost. This action is particularly appropriate because Formulation 3 source concentrations decrease in time. This means that with time, the need for a western extraction well to satisfy the Zone 4 constraints decreases. It made sense to evaluate the extent to which relaxing the Zone 4 constraint with time reduces cost.

USU only briefly optimized USU3-1. There was no time to thoroughly explore alternative candidate well locations. Table 4 shows GA input parameters. As seen later, USU3-1 cost less than $18M and resulted in only a little westward spread of TCE.

Optimization Results

Strategies USU1A and USU1B (Formulation 1)

Figure 4 shows the formal Formulation 1 cost minimization optimization problem objective function. Figure 5 shows the total optimization problem. USU presents four strategies for Formulation 1 in Table 1. The first two (USU1A and USU1B), require constructing only two EWs, but require extracting from many existing wells. Because of the annual cost associated with pumping at an EW, the twenty-one year costs of USU1A and USU1B are larger than those of strategies that require constructing an additional well but extract via fewer wells.

USU1A and USU1B cost more than USU1C and USU1D because they extract at more wells and extract more water. This also means that USU1A and USU1B remove more contaminant mass. We only slightly optimized Strategies USU1A and USU1B before ceasing work on them.

Strategies USU1A and USU1B differ in locations of the new EW and in pumping rates. USU1A costs less than USU1B (Table 1), but USU1B uses the same locations as USU1C. Therefore USU1B could be ungraded to USU1C more easily. This can be useful if TAD budget restrictions prevent constructing three EW in the first year.

Strategies USU1C, USU1D, and USU1E (Formulation 1)

Strategy USU1C requires constructing 3 EW, and clearly satisfies the POE constraint (Fig. 6). USU1C costs slightly more than USU1D, (which requires only 2 EW and 1 IW). However, Figure 7 shows that USU1D pushes some contamination laterally, potentially leading to eventual escape from hydraulic capture.

For Formulation 1 and subsequent formulations, USU chose the well locations of USU1C over those of USU1D. Figures 10-13 show results of applying the three USU1C EW wells within strategy USU2A.

After March 1st, USU very slightly improved its Formulation 1 pumping strategy. The well locations of this USU1E strategy are the same as USU1C, but the OFV improved slightly to $ 14.132 M.

Strategy USU2A (A More Restrictive Version of Formulation 2)

Strategy USU2A, developed by March 1st, includes an additional concentration constraint zone (Zone 4) in column 29, rows 106-140. This prevents water of 5 ppb or greater from moving to the left (west) of the POC, preventing clean aquifer from becoming contaminated. USU added this constraint about February 25th when noting that our preliminary Formulation 2 strategies caused contaminated water to bypass the POC. USU2A constructs 4 EW and 4 IW and costs $17.11M (Table 2). Figures 10-13 show the resulting plume.

Strategy USU2B (A More Restrictive Version of Formulation 2)

USU2B, developed from March 5-17, is the result of optimization refinement of USU2A. USU2B employs the Zone 4 constraint. USU2B constructs 4EW and 3IW and costs $15.731M (Table 1). Resulting plumes are similar to those of Figures 10-13.

Strategy USU3-1 (Formulation 3 Alternative)

USU3-1 was developed from March 5-17. Of the TAD-posed Formulation 3 constraints, USU3-1 satisfies all except the limit on EWs. It requires constructing 9 EW and 3 IW (Table 1, Figures 15-17). USU3-1 also constrains western TCE migration. It costs $17.928 M.

USU3-1 is a compromise between preventing contamination from moving to the west around the POC and reducing cost. USU3-1 applies the additional 5 ppb limit in Zone 4 for the first three stress periods. As a result, optimization can turn off the new EW near Zone 4 to reduce cost to $17.928M. The tradeoff is that maximum Zone 4 concentration almost reaches 10 ppb (in the northernmost cell) in period 4. After that the maximum Zone 4 concentration is below 4 ppb.

The cost is about $0.060M greater if applying the Zone 4 constraint for all stress periods. To prevent zone 4 concentrations from exceeding 5 ppb in period 4, extraction must continue at well UE4 during period 4. Possibly the Zone-4-period-4 constraint can alternatively be satisfied by decreasing injection at UI1 and UI2.

In reality, TAD might not need to construct all the wells that US3-1 says are needed. For example, TAD might prefer not to construct well UE9. UE9 extracts water that is moving to the Northeast. Instead of using UE9, one might let a future Northeastern plume system address that contamination. UE9 is used here to satisfy the 50 ppb constraint after year 9.

TAD might also not need to construct all of the USU3-1 wells located in source cells. If the source concentration degrades more quickly or if the 50 ppb constraint is relaxed, regulators might concur with not building wells UE8 or UE5.

Conclusions and Recommendations

USU has presented least-cost pumping strategies for three optimization problem formulations. The recommended strategies, present value, and numbers of new wells needed for each are:

Formulation 1: USU1E; $ 13.132 M ; 3 EW, 0 IW.
Formulation 2: USU2B; $ 15.731 M ; 4 EW, 3 IW.
Formulation 3: USU3-1; $ 17.928 M ; 9 EW, 3 IW.

Minimum-cost strategies might not be as robust as strategies that pump more water. Robustness is the assurance that a pumping strategy will achieve in the field what the model says its will. The economic benefit of minimizing pumping or other cost might be offset by reduced robustness.

To the extent possible, design projects should include interaction between the client and the designer (Hegazy and Peralta, 1997; Peralta and Aly, 1994, 1995, 1996; Peralta 2001a,b). Such interaction was not possible in this effort. Interaction can help determine whether modifications should be made to the Formulations to improve benefit to the client.

Not being able to communicate with the client cost USU a great deal of time on this project. USU sometimes had to decide whether to try to reduce cost versus trying to maintain strategy quality in other ways. Trying to do both took time and effort. Weighing noncommensurate goals without interaction is challenging.

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Table 1. Executive summary of USU pumping strategies for TAD.

Formulation #	1				2 modified with extra constraint #		3 with relaxed constraint and extra constraint # @
Option and Notes (These differ in initial cost, expandability, contamination removal, etc.)	**1A***	**1B***	**1C**	**1D**	**2A #**	**2B #, %**	**3-1 %**
Objective Function Value ($M)	16.058	16.216	14.137	14.136	17.110	15.731	$17. 928M
Number of New Extraction Wells Installed	2	2	3	2	4	4	9
Number of New Injection Wells Installed	0	0	0	1	4	3	3
Elapsed Years Until Cleanup	N/A				N/A		9

Notes: * 1A was designed for expansion into a Formulation III design. Therefore, optimization was not completed.

* 1B was designed for expansion into a Formulation II or III design. Therefore, optimization was not completed.

\# 2A and 2B employed an additional constraint preventing TCE from exceeding 5 ppb in any column west of the POC.

% 2B and 3-1 were developed during 5-17 March.

@ 3-1 required relaxing the posed Formulation 3 constraint on number of extraction wells that could be constructed. 3-1 employed an additional constraint restricting TCE movement to the west of the POC.

Table 2. GA input parameters for Formulation 1.

1. total number of simulations	400
2. total number of generations	9
3. generation size (gen. 1)	80
4. generation size (later generations)	40
5. penalty coefficient	100
6. crossover probability	0.85
7. mutation probability	0.05

Notes:

1. Total number of simulations performed by end of the number of generations specified in item 2.
2. Total number of generations used in a GA optimization.
3. The number of individuals in generation 1.
4. The number of individuals in all generations after generation 1.
5. Within the objective function, this is the coefficient used to weight unit violations of constraints. The resulting penalty makes the objective function less desirable proportionally with respect to the degree of constraint violation.

6. Probability that a pair of individuals will mate. Usually, one maintains a high probability (i.e. 0.7 ~ 0.9), since without mating, only mutation will change a strategy. Aly and Peralta (1999) report that a probability less than 0.7 produces inferior results.

7. Probability that each bit of a chromosome will mutate. The rate of mutation should generally be low (smaller than 0.1). Mutation is performed after crossover.

8.

Table 3. GA input parameters for Formulation 2.

total number of simulations	260
total number of generations	12
generation size (gen. 1)	40
generation size (later generations)	20
penalty coefficient	100
crossover probability	0.85
mutation probability	0.05

Table 4. GA input parameters for Formulation 3-1.

total number of simulations	100
total number of generations	5
generation size (gen. 1)	20
generation size (later generations)	20
penalty coefficient	100
crossover probability	0.85
mutation probability	0.05

Fig. 1. Initial (Projected 1 Jan 2003) Layer 1 TCE concentrations exceeding 5 ppb, and lines identifying hydraulic conductivity changes.

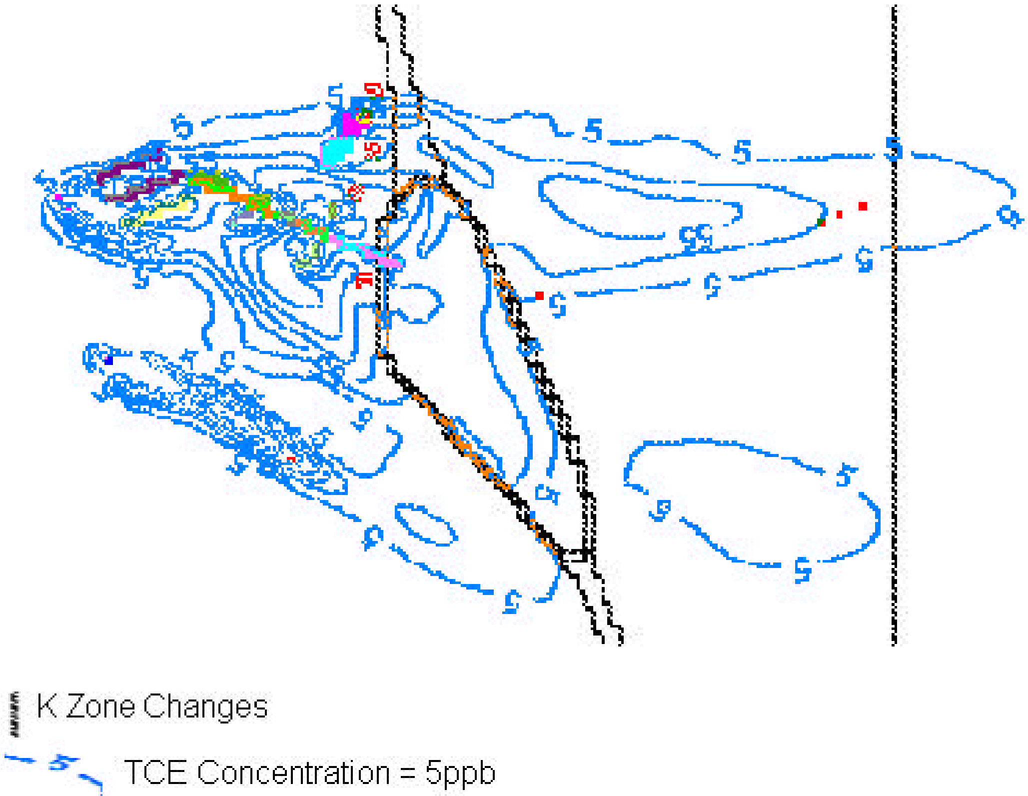

Fig. 2. Initial (Projected 1 Jan 2003) Layer 2 TCE concentrations exceeding 5 ppb, and lines identifying hydraulic conductivity changes.

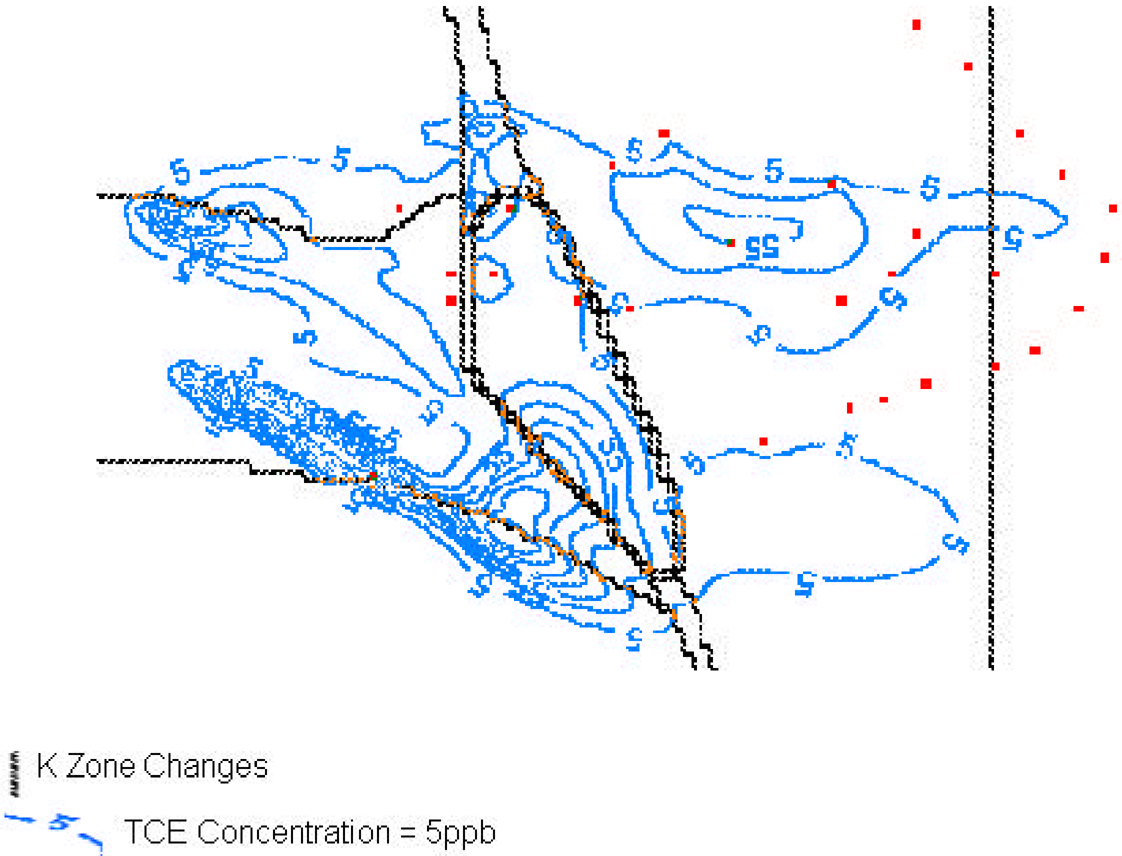

Fig. 3a. POE Constraint cells and Layer 1 TCE concentrations > 5 ppb after three years of pumping per USU2A.

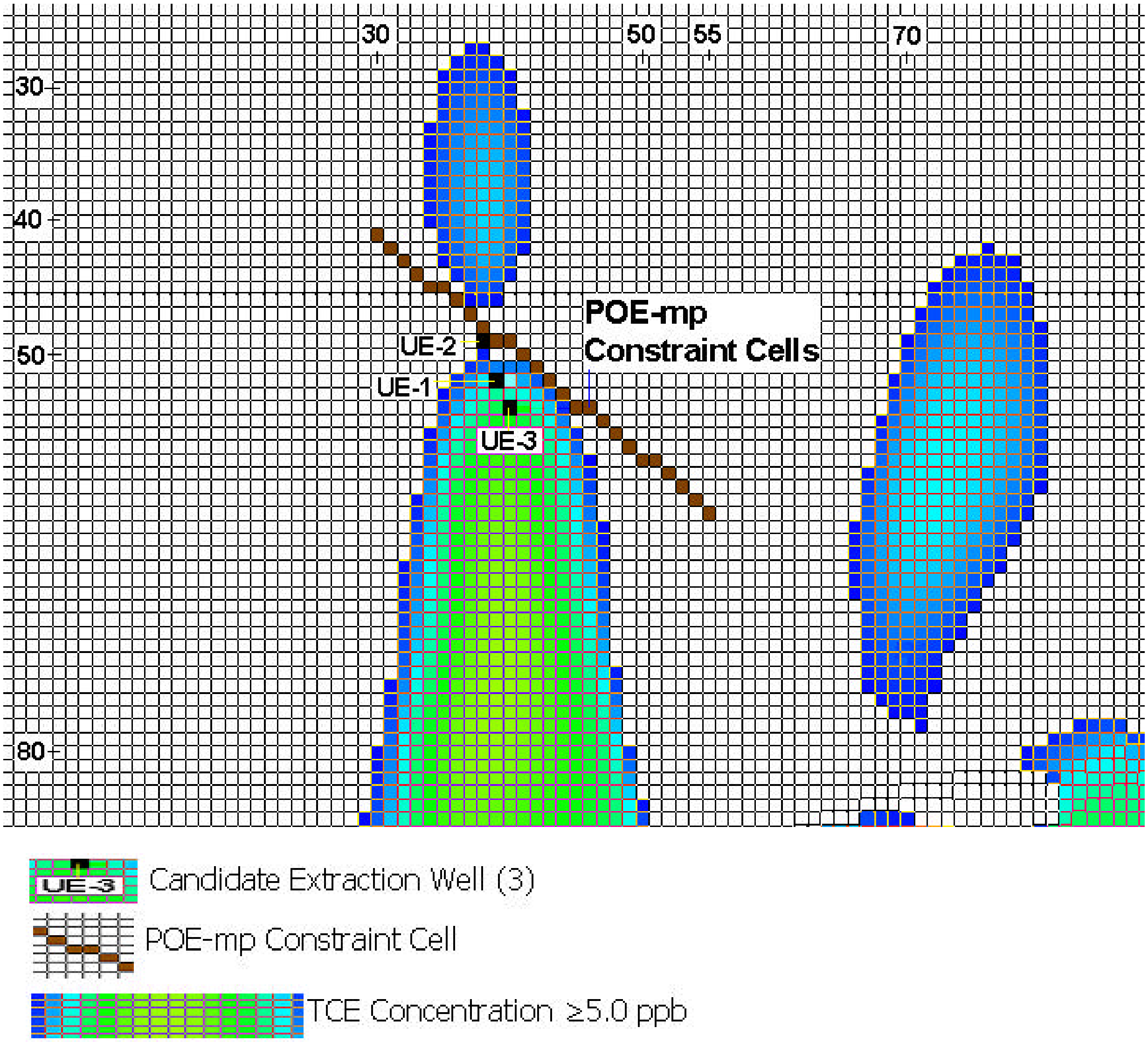

Fig. 3b. POC Constraint and Zone 4 Constraint cells and Layer 1 TCE concentrations ≥ 5 ppb after three years of pumping per USU2A.

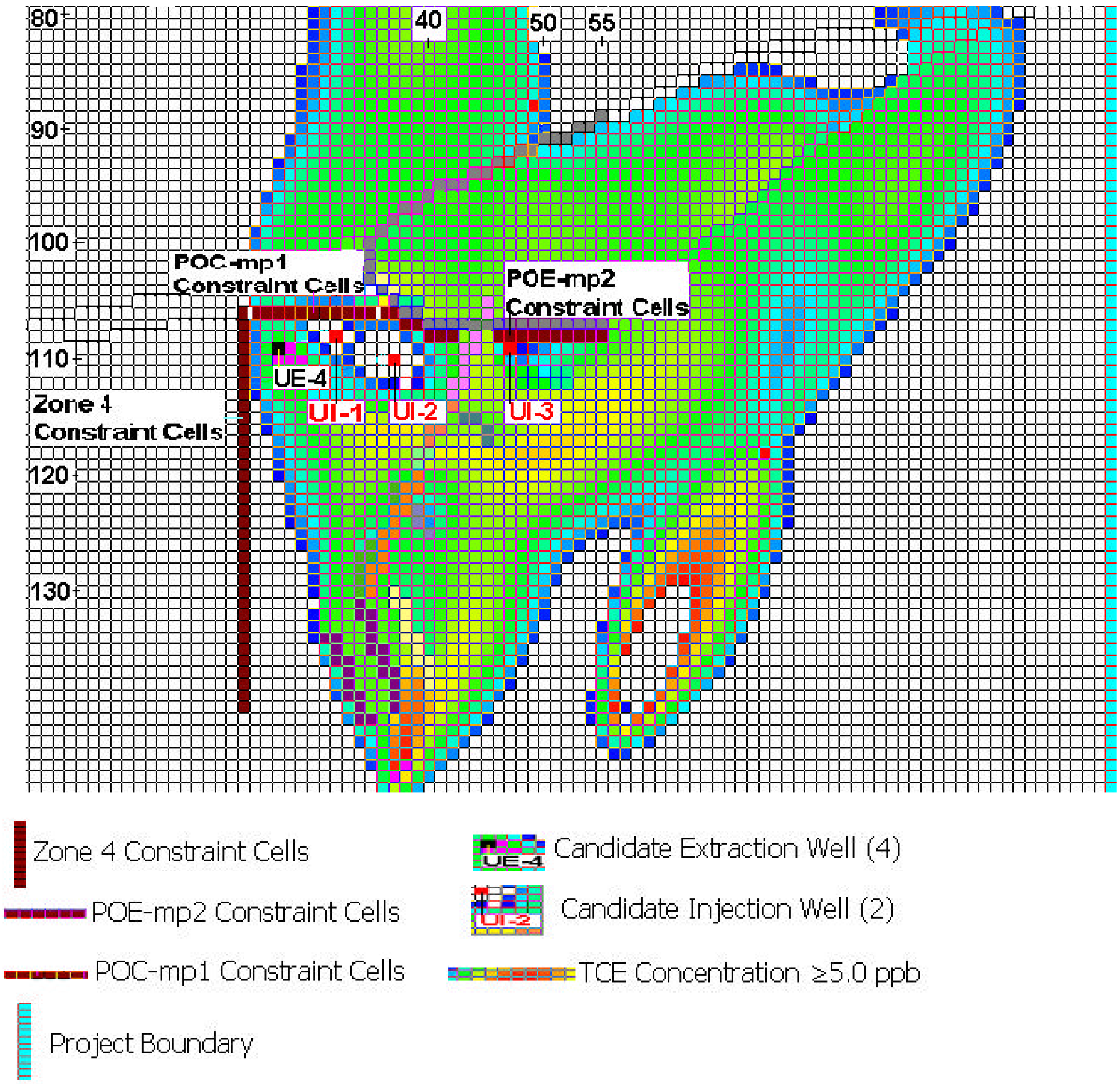

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Fig. 4. Formulation 1 objective function: minimize present value of cost.

MINIMIZE (CCE + CCI + FCO + VCE + VCS+VCC)

Where all below costs must be discounted to present value (none include proposed NE plume well at 118,69):

CCE = New well capital cost ($307K)

CCI = New recharge basin capital cost ($223K)

FCO = Fixed annual cost of O&M each year of operation ($525K)

VCE = Variable annual electrical cost ($34.5K*number of extraction wells that pump in a year)

VCC = Variable annual Chemical Cost($0.02K/gpm extraction)

VCS = Variable annual sampling cost {($208K)*plume area at beginning of a stress period/ Jan 2003 plume area}

Fig. 5. Formulation 1 optimization problem.

MINIMIZE (CCE + CCI + FCO + VCE + VCS+VCC)

Subject to:

- At year / 3 , for all POE-MP cells in all layers,TCE concentration ≤ 5 ppb
- Σ Extraction(including fixed NE plume well) ≤ (8000 gpm)*95 = 7600 gpm
- | Σ Extraction - Σ Injection | ≤ 1gpm
- Bounds on Pumping at Individual Wells
- Temporally constant TCE concentration source cells

Fig. 6. USU1C: Layer 1 TCE concentrations > 5 ppb after 3 years of pumping.

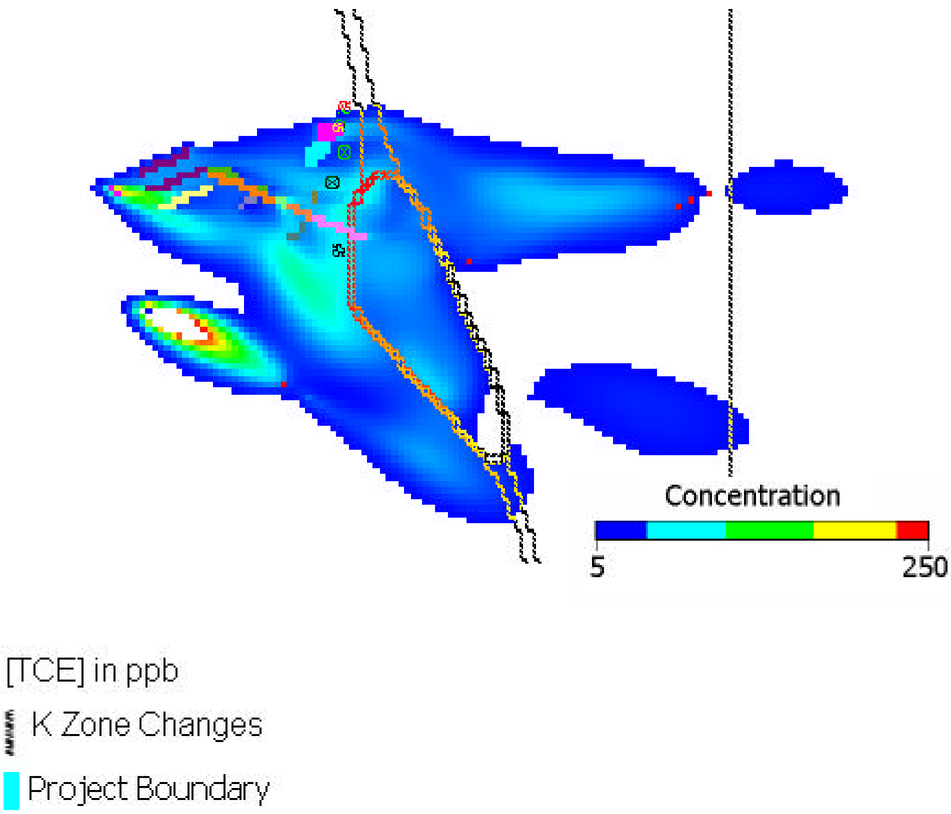

Fig. 7. USU1D: Layer 1 TCE concentrations > 5 ppb after 3 years of pumping.

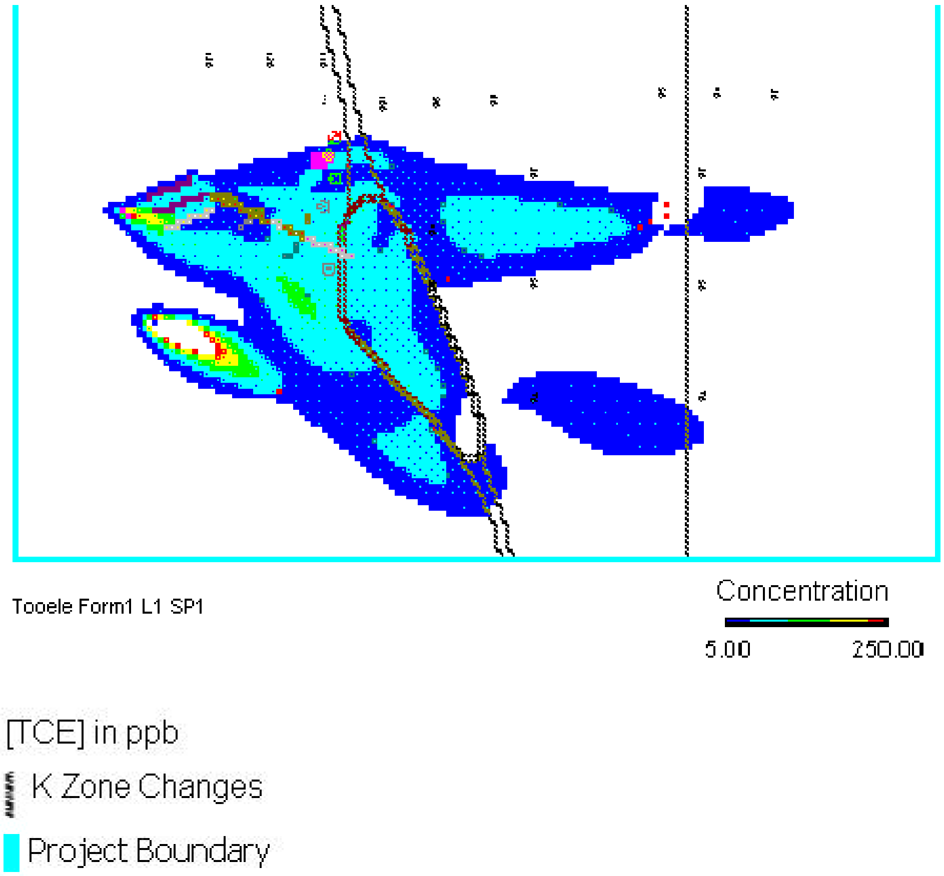

Fig. 8. Formulation 2 optimization problem.

MINIMIZE (CCE + CCI + FCO + VCE + VCS+VCC)

Subject to:

- All previous Formulation 1 constraints
- At year ≥ 3, layers 1 & 2, POC-MP1,
  TCE ≤ Max (20 ppb, ½ initial conc.)
- At year 3-8, layers 1 & 2, POC-MP2,
  TCE ≤ 50 ppb
- At year ≥ 9, layers 1 & 2, POC-MP2,
  TCE ≤ 20 ppb

Fig. 9. A more restrictive version of Formulation 2 optimization problem.

MINIMIZE (CCE + CCI + FCO + VCE + VCS+VCC)

Subject to:

- All previous Formulation 1 constraints
- At year ≥ 3, layers 1 & 2, POC-MP1,
  TCE ≤ Max (20 ppb, ½ initial conc.)
- At year 3-8, layers 1 & 2, POC-MP2,
  TCE ≤ 50 ppb
- At year ≥ 9, layers 1 & 2, POC-MP2,
  TCE ≤ 20 ppb
- At year ≥ 3, all layers, Zone 4 TCE ≤ 5 ppb

Fig. 10. USU2A: Layer 1 TCE concentrations > 5 ppb after 3 years of pumping.

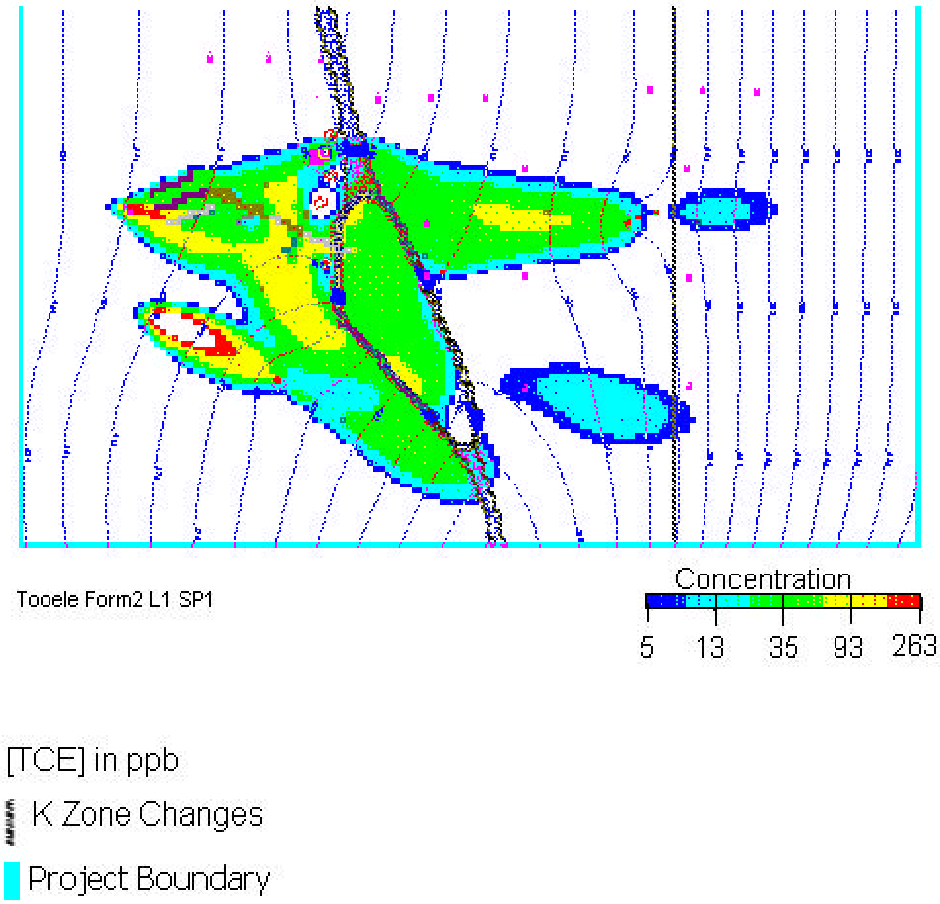

Fig. 11. USU2A: Layer 2 TCE concentrations > 5 ppb after 3 years of pumping.

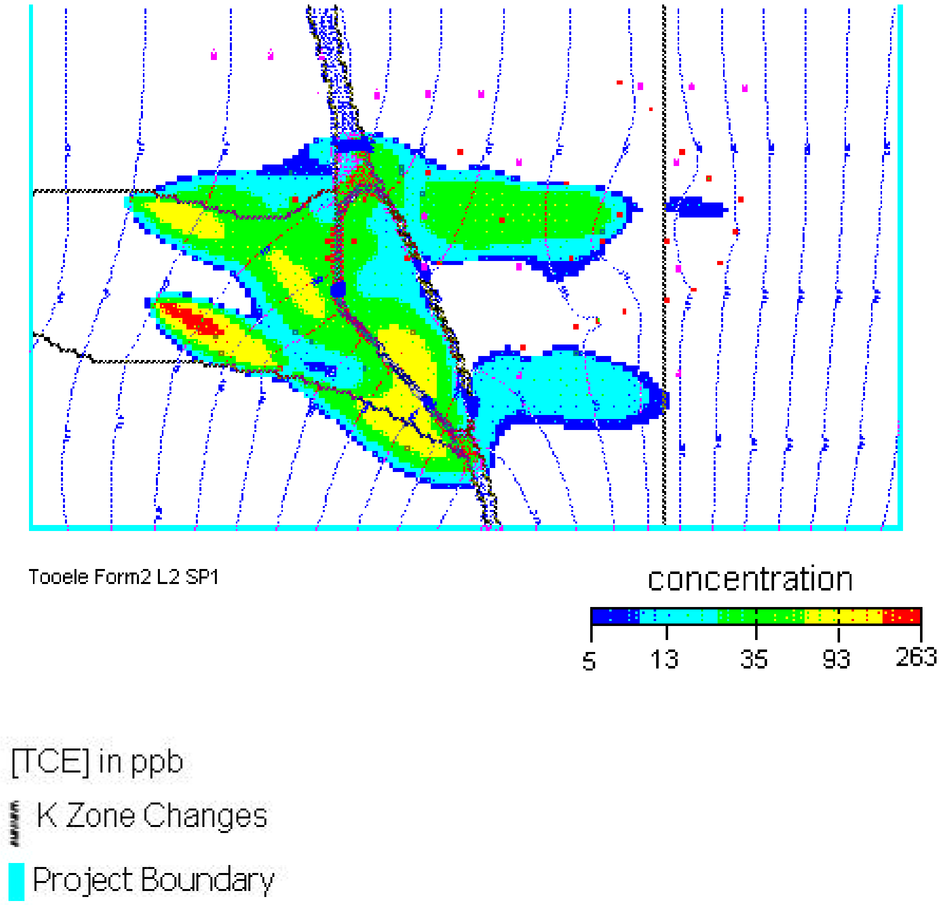

Fig. 12. USU2A: Layer 1 TCE concentrations > 5 ppb after 9 years of pumping.

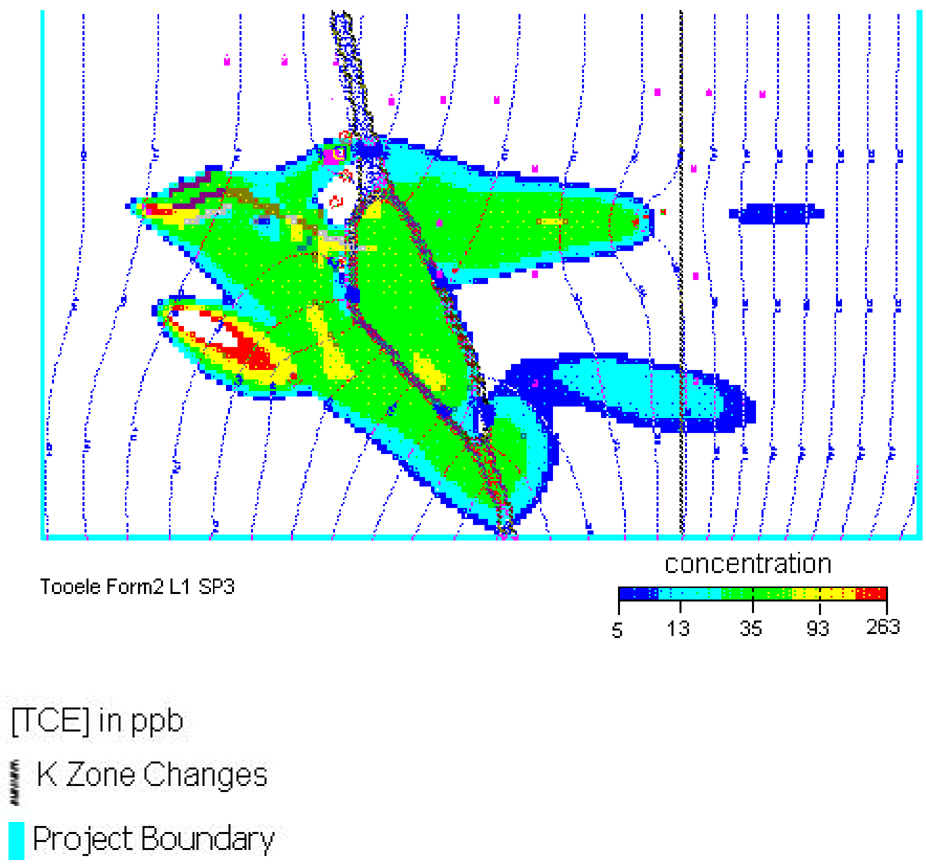

Fig. 13. USU2A: Layer 2 TCE concentrations ≥ 5 ppb after 9 years of pumping.

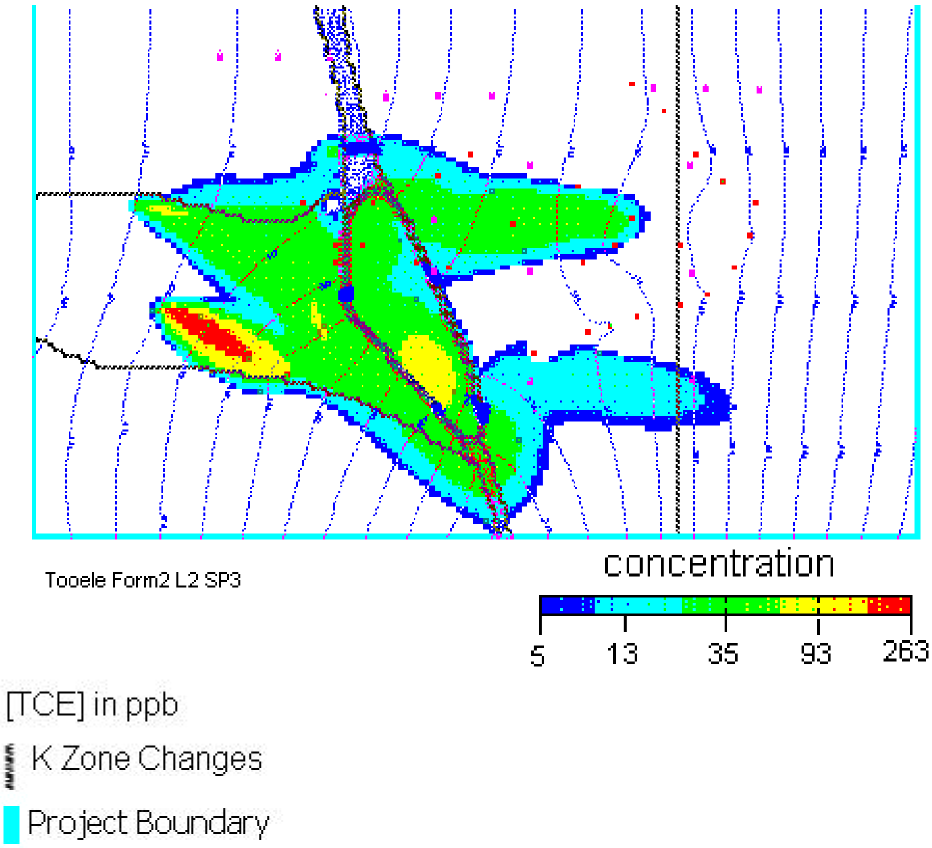

Fig. 14A. Posed infeasible Formulation 3 optimization problem.

MINIMIZE (CCE + CCI + FCO + VCE + VCS+VCC)

Subject to:

- All previous formulation 1&2 constraints and,in layer 1 and 2:
- Number of new extraction wells ≤ 4(for entire period of 21 years)
- Number of new injection wells ≤ 4 (for entire period of 21 years)
- At year ≥ 9 , cleanup zone in all layers:
  TCE ≤ 50ppb

Fig. 14B. Optimization problem for Formulation USU3-1

MINIMIZE (CCE + CCI + FCO + VCE + VCS+VCC)

Subject to:

- All Formulation 1&2 constraints
- At year $\geq$ 9 , cleanup zone in all layers:
  TCE $\leq$ 50ppb
- Temporally decreasing TCE concentration sources
- Zone 4, all layers, TCE $\leq$ 5 for periods 1-3

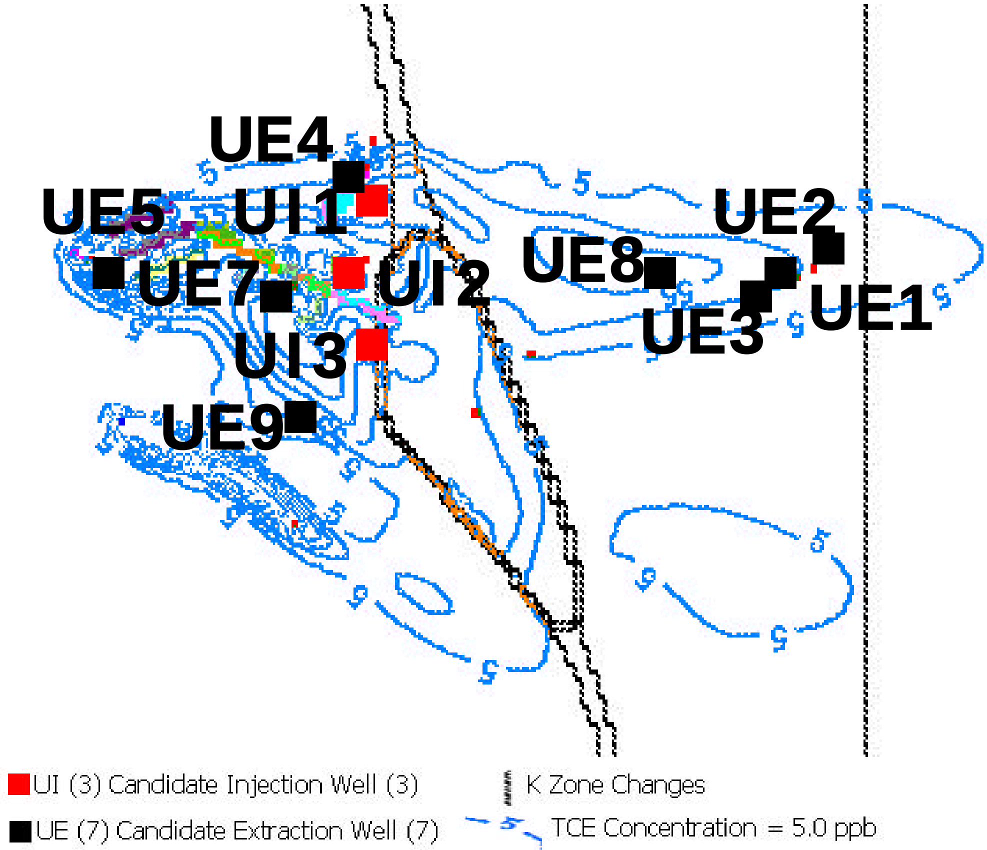

Fig15. Initial Layer 1 TCE ≥ 5 ppb concentration and Formulation 3 alternative Strategy USU3-1 new wells required.

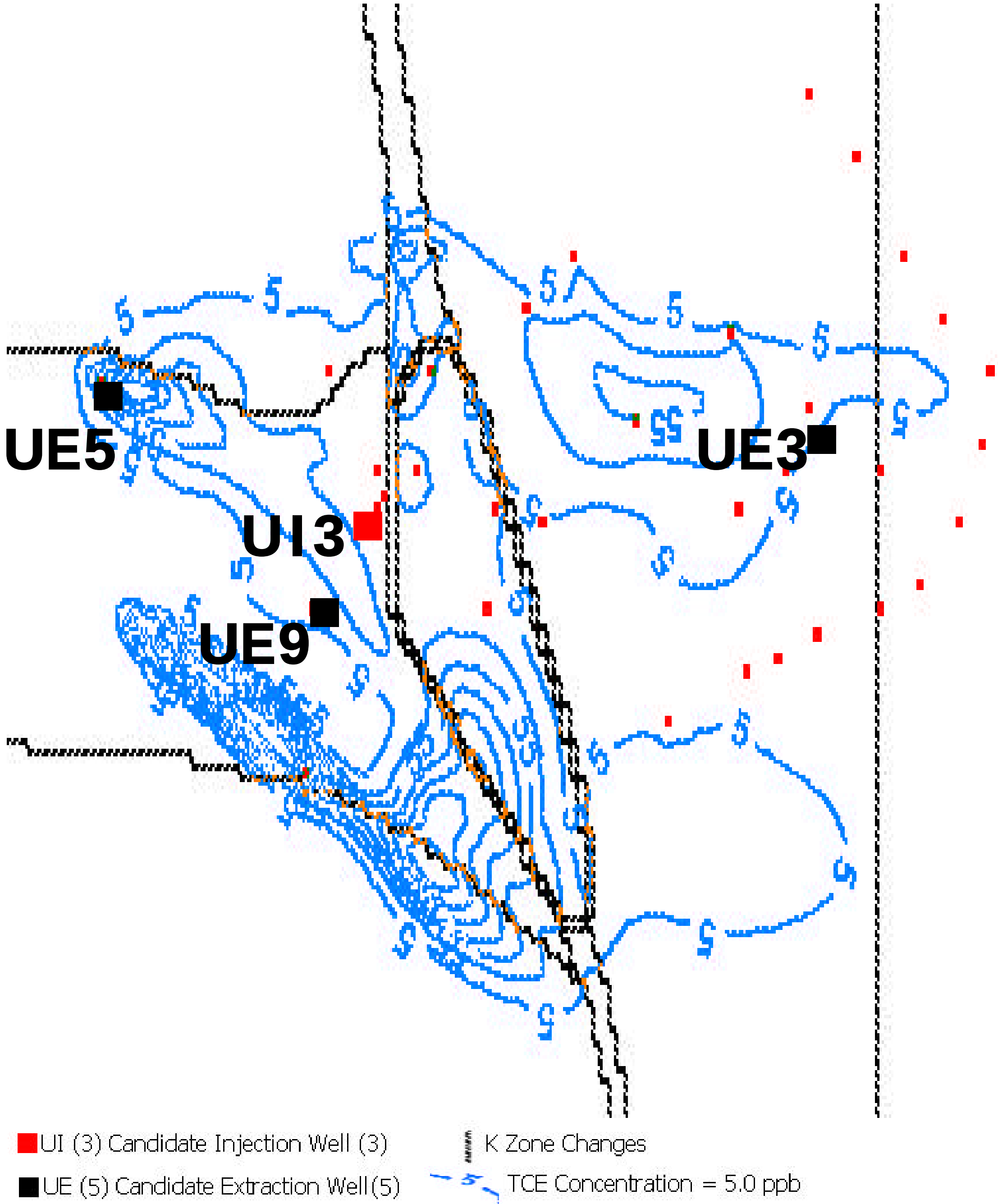

Fig16. Initial Layer 2 TCE ≥ 5 ppb concentration and Formulation 3 alternative Strategy USU3-1 new wells required.

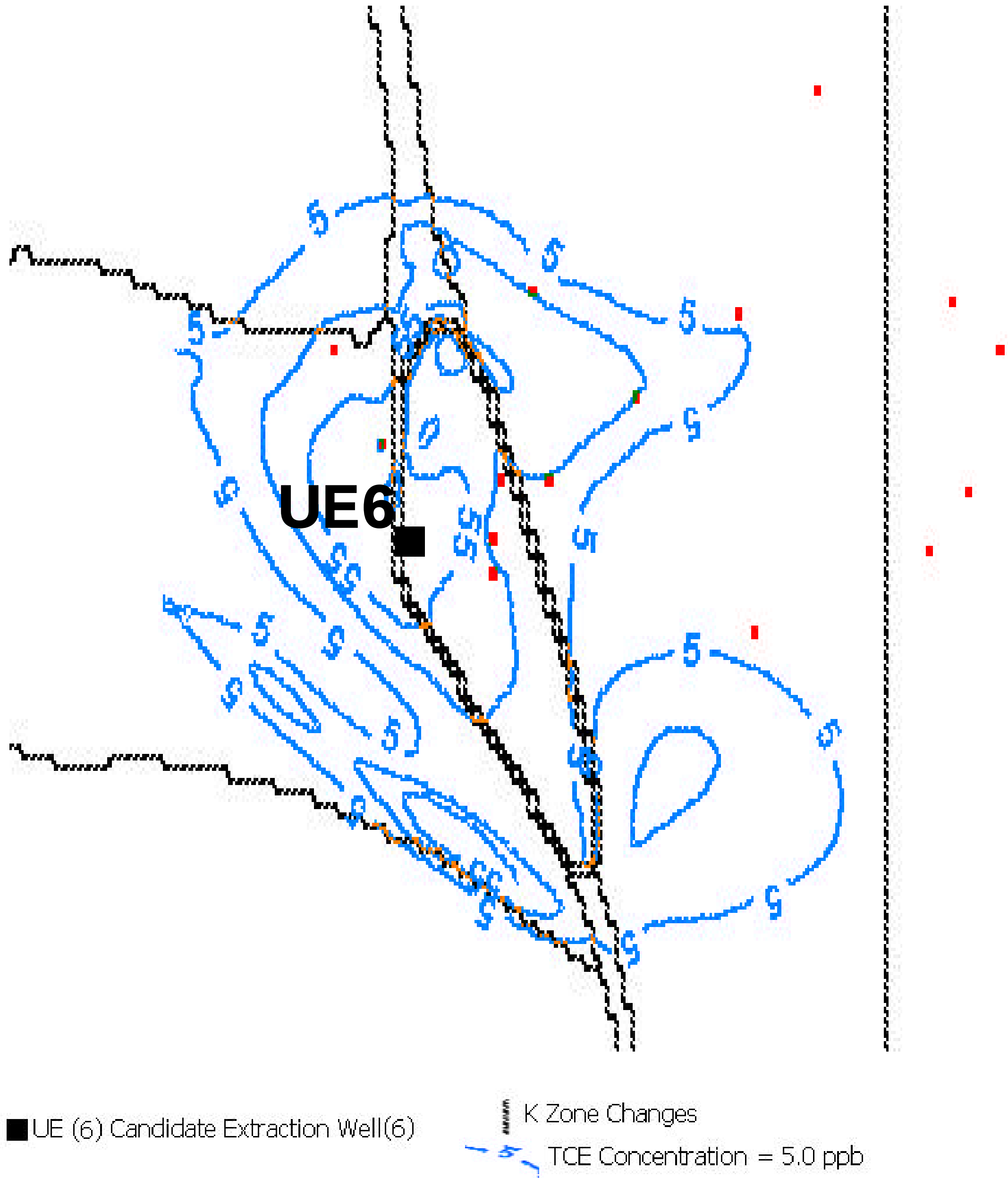

Fig17. Initial Layer 3 TCE ≥ 5 ppb concentration and Formulation 3 alternative Strategy USU3-1 new wells required.

Appendix A.

Edited Post Processor Output for Formulation 1, USU1E

Intermediate Variables Calculation

Total Number of Wells In Each Stress Period

Stress Period	Extraction Wells	Injection Wells
1	5	7
2	4	6
3	5	7
4	5	7
5	5	7
6	5	4
7	5	5

Extraction Well Rates (Combining Multi-Aquifer Wells)

Well Index	Well Rate (gpm)
Stress Period: 1	
12	608.023
30	1353.796
31	380.014
32	374.445
33	380.009
Stress Period: 2	
12	581.185
30	1353.796
31	356.263
33	380.009
Stress Period: 3	
12	602.828
16	608.023
30	1353.796
31	380.014
33	380.009
Stress Period: 4	
12	287.221
16	413.730
30	1353.796
31	380.014
33	376.695
Stress Period: 5	
12	617.519
16	282.322
30	1353.796
31	380.014
33	380.009
Stress Period: 6	
12	617.519
16	466.085
30	1353.796

31	378.367
33	326.568
Stress Period: 7	
12	617.519
16	599.373
30	1353.796
31	380.014
33	380.009

Injection Well Rates (Combining Multi-Aquifer Wells)

Well Index	Well Rate (gpm)
----------	---------------
Stress Period: 1	
19	181.061
20	65.987
21	702.073
22	129.807
23	1128.640
25	813.412
26	75.811
Stress Period: 2	
19	42.448
22	746.724
23	83.354
25	427.143
26	757.763
27	614.314
Stress Period: 3	
18	276.197
21	701.948
22	409.756
23	108.435
25	522.191
26	763.826
27	542.820
Stress Period: 4	
18	165.840
22	709.990
23	384.549
24	55.945
25	827.932
26	599.155
28	68.044
Stress Period: 5	
18	95.484
19	236.170
20	672.753
21	43.882
22	714.957
23	1082.825
27	167.596
Stress Period: 6	
22	713.544
23	1082.550
25	877.576
26	469.166

Stress Period: 7

18	350.927
22	707.549
23	1097.704
24	383.583
25	791.276

Number of New Extraction Wells in Each Stress Period

3
0
0
0
0
0
0

Number of New Injection Wells in Each Stress Period

0
0
0
0
0
0
0

Total Pumping and Injection Rates in Each Stress Period (gpm)

Pumping Rate	Injection Rate
3096.288	3096.792
2671.253	2671.747
3324.670	3325.174
2811.456	2811.456
3013.661	3013.666
3142.336	3142.835
3330.712	3331.039

Plume Area at the Beginning of Each Stress Period

Stress Period	Plume Area (ft*ft)
1	0.118720E+09
2	0.170400E+09
3	0.175320E+09
4	0.178600E+09
5	0.181200E+09
6	0.186520E+09
7	0.192160E+09

Objective Function Calculation

The Capital Costs of New Wells (thousand of dollars)
921.000

The Capital Costs of New Recharge Basins (thousand of dollars)
0.000

The Fixed Costs of O&M (thousand of dollars)
7067.663

The Variable Costs of Electricity for Operating Wells (thousand of dollars)
1772.568

The Variable Costs of Sampling (thousand of dollars)
3919.310

The Variable Costs of Chemicals (thousand of dollars)
451.611

The Objective Function Value (thousands of dollars) for Formulation # 1
14132.152

Constraints Check-Out

--- Maximum Treatment Capacity Constraint ---

The Maximum Treatment Capacity Constraint Satisfied

--- Pumping/Injection Limit Constraint ---

The Pumping/Injection Limit Constraint Not Satisfied
Stress Period Extraction Wells Injection Wells
This is caused by the format of our well package. This constraint is not violated.

--- Pumping-Injection Balance Constraint ---

The Pumping-Injection Balance Constraint Satisfied

--- POE_MP Constraint ---

The POE_MP Constraint Satisfied

Number of Constraints Not Satisfied
0

Edited Post Processor Output for Formulation 2, USU2B

Intermediate Variables Calculation

Total Number of Wells In Each Stress Period

Stress Period	Extraction Wells	Injection Wells
1	6	13
2	5	10
3	6	12
4	6	15
5	6	13
6	6	10
7	6	14

Extraction Well Rates (Combining Multi-Aquifer Wells)

Well Index	Well Rate (gpm)
Stress Period: 1	
12	539.589
30	1353.796
31	380.014
32	380.014
33	380.009
38	380.014
Stress Period: 2	
12	617.519
30	1353.796
31	380.014
33	380.009
38	380.014
Stress Period: 3	
12	607.134
16	517.874
30	1353.796
31	380.014
33	380.009
38	380.014
Stress Period: 4	
12	561.746
16	422.483
30	1353.796
31	380.014
33	380.009
38	379.599
Stress Period: 5	
12	517.531
16	588.723
30	1353.796
31	380.014
33	380.009
38	379.084
Stress Period: 6	
12	617.504

16	356.361
30	1353.796
31	380.014
33	380.009
38	332.511
Stress Period: 7	
12	607.477
16	605.649
30	1353.796
31	380.014
33	380.009
38	368.138

Injection Well Rates (Combining Multi-Aquifer Wells)

Well Index	Well Rate (gpm)
Stress Period: 1	
17	41.004
19	71.000
20	293.258
21	373.385
22	451.601
23	326.973
25	222.689
26	296.614
28	52.999
29	54.890
35	464.075
36	559.408
37	205.873
Stress Period: 2	
19	134.987
22	323.389
24	141.086
25	914.876
26	234.175
27	269.054
28	51.534
35	412.530
36	303.154
37	326.573
Stress Period: 3	
18	64.595
19	240.383
21	417.377
23	291.954
24	65.909
25	776.507
26	407.459
27	351.405
29	184.012
35	239.604
36	292.058
37	287.590
Stress Period: 4	
18	154.203

19	68.709
20	71.390
21	164.001
22	74.429
23	852.526
24	74.912
25	694.146
26	157.679
27	372.305
28	74.491
29	155.429
35	136.026
36	215.265
37	212.263
Stress Period:	5
17	158.915
18	262.649
20	158.562
22	312.858
23	836.473
24	296.422
25	300.198
26	514.206
27	117.688
28	61.311
35	201.228
36	173.201
37	205.452
Stress Period:	6
17	121.833
19	329.425
20	601.410
21	532.462
22	369.463
25	410.395
26	290.681
27	156.390
35	478.080
37	130.062
Stress Period:	7
17	70.356
18	56.459
19	422.686
20	352.247
21	67.197
22	577.216
23	613.270
24	373.682
25	181.882
26	191.155
27	269.117
35	142.327
36	206.449
37	171.045

Number of New Extraction Wells in Each Stress Period

4
0
0
0
0
0
0

Number of New Injection Wells in Each Stress Period

3
0
0
0
0
0
0

Total Pumping and Injection Rates in Each Stress Period (gpm)

Pumping Rate	Injection Rate
3413.437	3413.770
3111.353	3111.359
3618.842	3618.853
3477.647	3477.772
3599.158	3599.164
3420.196	3420.201
3695.084	3695.089

Plume Area at the Beginning of Each Stress Period

Stress Period	Plume Area (ft*ft)
1	0.118720E+09
2	0.172760E+09
3	0.177720E+09
4	0.181560E+09
5	0.184600E+09
6	0.188560E+09
7	0.193880E+09

Objective Function Calculation

The Capital Costs of New Wells (thousand of dollars)
1228.000

The Capital Costs of New Recharge Basins (thousand of dollars)
669.000

The Fixed Costs of O&M (thousand of dollars)
7067.663

The Variable Costs of Electricity for Operating Wells (thousand of dollars)
2237.015

The Variable Costs of Sampling (thousand of dollars)
3966.035

The Variable Costs of Chemicals (thousand of dollars)
563.549

The Objective Function Value (thousands of dollars) for Formulation # 2
15731.262

Constraints Check-Out

--- Maximum Treatment Capacity Constraint ---

The Maximum Treatment Capacity Constraint Satisfied

--- Pumping/Injection Limit Constraint ---

The Pumping/Injection Limit Constraint Not Satisfied

Stress Period	Extraction Wells	Injection Wells

This is caused by the format of our well package. This constraint is not violated.

--- Pumping-Injection Balance Constraint ---

The Pumping-Injection Balance Constraint Satisfied

--- POE_MP Constraint ---

The POE_MP Constraint Satisfied

--- POC_MP1 Constraint ---

The POC_MP1 Constraint Satisfied

--- POC_MP2 Constraint ---

The POC_MP2 Constraint Satisfied

Number of Constraints Not Satisfied
0

Edited Post Processor Output for Formulation 3, USU3

Intermediate Variables Calculation

Total Number of Wells In Each Stress Period

Stress Period	Extraction Wells	Injection Wells
1	10	15
2	9	14
3	11	15
4	5	9
5	5	11
6	4	10
7	4	6

Extraction Well Rates (Combining Multi-Aquifer Wells)

Well Index	Well Rate (gpm)
Stress Period: 1	
7	208.751
10	355.452
12	617.519
30	1353.796
31	379.760
32	377.967
33	380.009
38	380.014
40	380.014
43	380.014
Stress Period: 2	
12	461.669
30	1353.796
31	364.429
33	374.897
38	259.750
40	363.650
41	363.650
43	207.800
44	363.650
Stress Period: 3	
10	760.023
12	561.850
30	1353.796
31	374.170
33	380.009
38	350.740
40	377.973
41	380.009
43	378.466
44	202.002

45 380.014
Stress Period: 4
12 617.114
30 1353.796
31 380.014
33 380.009
40 281.657
Stress Period: 5
12 527.760
30 1353.796
31 380.014
33 380.009
40 216.533
Stress Period: 6
12 409.719
30 1353.796
31 380.014
33 380.009
Stress Period: 7
12 617.519
30 1353.796
31 380.014
33 379.516

Injection Well Rates (Combining Multi-Aquifer Wells)
Well Index Well Rate (gpm)
---------- ---------------
Stress Period: 1
17 54.870
18 365.686
19 315.892
20 448.121
21 217.826
22 399.137
23 901.779
24 97.115
25 391.682
26 151.294
27 196.303
29 132.550
35 383.105
36 486.938
37 271.496
Stress Period: 2
17 70.834
19 139.730
21 239.510
22 121.469
23 466.807
24 56.428
25 824.192
26 467.254
27 543.880
28 62.065
29 43.420
35 369.598

36	383.173
37	324.942
Stress Period: 3	
17	154.385
18	100.051
20	169.118
21	295.476
22	693.761
23	418.442
24	232.139
25	343.099
26	670.534
27	615.488
28	54.958
29	170.957
35	551.932
36	550.940
37	478.267
Stress Period: 4	
17	210.346
20	43.233
21	207.192
24	379.048
25	708.203
26	754.969
35	288.852
36	207.800
37	213.463
Stress Period: 5	
17	188.158
19	555.559
20	75.650
21	100.321
23	477.758
25	207.961
26	759.722
27	83.156
29	156.292
36	76.652
37	176.890
Stress Period: 6	
17	59.571
18	255.236
20	71.177
21	44.183
22	648.284
23	321.087
24	60.974
25	900.361
26	41.679
35	121.153
Stress Period: 7	
17	54.392
19	562.135
23	974.598
24	336.013

25	708.723
29	95.484

Number of New Extraction Wells in Each Stress Period

6
2
1
0
0
0
0

Number of New Injection Wells in Each Stress Period

3
0
0
0
0
0
0

Total Pumping and Injection Rates in Each Stress Period (gpm)

Pumping Rate	Injection Rate
4813.297	4813.796
4113.292	4113.303
5499.053	5499.546
3012.591	3013.105
2858.112	2858.118
2523.539	2523.705
2730.845	2731.344

Plume Area at the Beginning of Each Stress Period

Stress Period	Plume Area (ft*ft)
1	0.118720E+09
2	0.170400E+09
3	0.173800E+09
4	0.175320E+09
5	0.177800E+09
6	0.180440E+09
7	0.182720E+09

Objective Function Calculation

The Capital Costs of New Wells (thousand of dollars)
2601.485

The Capital Costs of New Recharge Basins (thousand of dollars)
669.000

The Fixed Costs of O&M (thousand of dollars)
7067.663

The Variable Costs of Electricity for Operating Wells (thousand of dollars)
3045.144

The Variable Costs of Sampling (thousand of dollars)
3859.248

The Variable Costs of Chemicals (thousand of dollars)
685.018

The Objective Function Value (thousands of dollars) for Formulation # 3
17927.557

Constraints Check-Out

--- Maximum Treatment Capacity Constraint ---

The Maximum Treatment Capacity Constraint Satisfied

--- Pumping/Injection Limit Constraint ---

The Pumping/Injection Limit Constraint Not Satisfied

Stress Period	Extraction Wells	Injection Wells

This is caused by the format of our well package. This constraint is not violated.

--- Pumping-Injection Balance Constraint ---

The Pumping-Injection Balance Constraint Satisfied

--- POE_MP Constraint ---

The POE_MP Constraint Satisfied

--- POC_MP1 Constraint ---

The POC_MP1 Constraint Satisfied

--- POC_MP2 Constraint ---

The POC_MP2 Constraint Satisfied

--- Cleanup Year Constraint ---

The Cleanup Year Constraint Satisfied

--- Maximum Number of New Wells Constraint ---

Total Number of New Wells Ever Installed
9

The Maximum Number of New Wells Constraint Not Satisfied

--- Maximum Number of New Injection Wells Constraint ---

Total Number of New Injection Wells Installed
3

The Maximum Number of New Injection Wells Constraint Satisfied

Number of Constraints Not Satisfied
1

Appendix F: Formulation Document and Final Reports, Blaine

Formulation Document

Transport Optimization Hastings Naval Ammunition Depot
Draft Mathematical Formulations
5/15/02

INTRODUCTION

Hastings Naval Ammunition Depot (NAD) consists of 48,800 acres located immediately east of Hastings, Nebraska in eastern Adams County and western Clay County. Hastings is located 25 miles south of Grand Island, Nebraska and 105 miles west of Lincoln, Nebraska.

Hastings NAD was built in the early 1940s as an active "load, assemble, and pack" ammunition facility during World War II and the Korean Conflict. The NAD was responsible for producing nearly one-half of the ordnance used by the Navy during WWII. During the World War II, the Korean Conflict, and the subsequent decommissioning process (1958-1967), waste materials were generated through discharge of wastewater to surface impoundments and natural drainage areas of the facility, and disposal of solid waste and explosives.

Beginning in the mid-1960s, large tracts of the former NAD were either sold to various individuals, businesses, and municipalities or transferred to other governmental agencies. Much of the region's economy is based on agriculture. With sale and transfer of the NAD to the U.S. Department of Agriculture (USDA) and area farmers, over 100 irrigation wells have been installed on the former NAD.

As a result of findings of groundwater contamination at the NAD in the mid-1980s, the EPA included portions of the former NAD as part of the Hastings Groundwater Contamination Site (HGCS), a regional area of groundwater contamination in south-central Nebraska. The HGCS was added to EPA's National Priorities List (NPL) in 1986.

Five operable units (OUs) have been established for restoration of the former NAD: OU4 consists of shallow soil (less than 10 feet in depth) at the Hastings East Industrial Park (HEIP); OU8 consists of vadose zone soil that separates OU4 and groundwater at the HEIP; OU14 is groundwater which typically encountered across the former NAD at a depth of approximately 95 to 115 feet; OU16 consists of three production areas of the former NAD: the Explosives Disposal Area (EDA), the Naval Yard Dump (YD), and the Bomb and Mine Complex (BMC); OU15 is comprised of those remaining former NAD areas that were not included as part of the other Operable Units.

Groundwater was first characterized during RI/FS activities from 1987 to 1990. A Supplemental RI of the Hastings East Industrial Park (HEIP) was conducted in 1990/1991 that included additional characterization of groundwater contamination. The data from the RI annual groundwater program, and the 1999 groundwater sampling event show that the VOC plumes encompass nearly six and one-half square miles beneath the former NAD. Additionally, explosives groundwater contamination extends over an area of approximately three square miles and is commingled with the VOC plume(s) in several areas.

Groundwater is encountered in the study area approximately 100 feet below ground surface. The three saturated hydrogeologic units of primary interest of this study are, in descending order:

- The unconfined aquifer (model layer 1)
- The upper confining layer (model layer 2), and
- The semi-confined aquifer (model layers 3-6)

The unconfined aquifer is comprised of sand and gravel and clayey or silty sand. It is relatively thin, with a thickness of about 10 to 15 feet. The upper confining layer is comprised of silty clay, clayey silt and clayey sand. Although this confining layer is present under most of the region, it is absent or discontinuous in a significant part of the study are. The semi-confined aquifer has a thickness of 100 to 150 feet in the study area, and consists of sand and gravel with discontinuous layers of silty clay and clayey sand. The semi-confined aquifer is the major water supply aquifer in the region, and supports municipal, industrial, and particularly, irrigation needs.

The groundwater flow directions for both the unconfined and semi-confined aquifers are predominantly to the east and southeast during non-irrigation seasons with an average hydraulic gradient of 0.001. During irrigation season, which lasts about two and half months, heavy pumping from extensive irrigation wells dramatically alters the groundwater flow direction. The present extent of the plumes indicates that groundwater contaminant migration is also influenced by the seasonal irrigation pumping.

Groundwater contamination at the former NAD is primarily due to chemical spills and/or discharge of wastewater to surface impoundments, wastewater systems, and natural drainages, mainly in production areas of the former NAD. The contaminants of concern in groundwater are VOCs and explosives.

GOUNDWATER FLOW AND TRANSPORT MODEL

Groundwater flow is simulated with the MODFLOW code. The model grid covers 134 square miles. Variable cell dimensions range from 400 ft by 400 ft in the center of the model, to 2000 ft by 2000 ft near the model edges. There are six model layers. Layer 1 is the unconfined aquifer. Layer 2 is the upper confining layer. Layers 3-6 are the semi-confined aquifer, split evenly into 4 layers with the equal thickness and properties. The groundwater flow model was calibrated to both steady-state and transient conditions, and included particle tracking to calibrate based on historical plume shape and plume length. Calibrated horizontal hydraulic conductivities range from 10 to 80 ft/day in the unconfined aquifer, and 150 to 250 ft/day in the semi-confined aquifer. Hydraulic conductivity of the upper confining bed is much lower.

Groundwater contaminant transport is simulated with MT3DMS. In the FS, the following six parameters were simulated:

- TCE (VOC)
- PCE (VOC)
- 1,1,1-TCA ("TCA") (VOC)
- 1,1-DCE ("DCE") (VOC)
- TNT (Explosive)
- RDX (Explosive)

The optimization project is restricted to simulation of two parameters. Site managers selected TCE and TNT as the parameters most important to remedial design. However, site managers also indicated a preference to not ignore the other parameters. Therefore, an approach was developed (discussed later) to incorporate the distribution of the other constituents.

SPECIAL NOTES

Stress Periods in the Model

The FS flow and transport model was set up to run one year at a time manually. The head solution and concentration solution from the end of the previous year was used as the initial condition for the following year. Each calendar year was divided into 3 stress periods in the FS model with the temporal discretization scheme as shown below:

FS Model (3 Stress Periods Per Year)

Stress Period	Length (days)	# Time Steps	Time Step Multiplier
1	76	10	1.5
2	136	10	1.5
3	152	5	1.5

The 76-day period refers to the irrigation season, which occurs in summer months.

For this project, it is important to reduce execution time for the model as much as possible. Dr. Chunmiao Zheng accomplished this by converting the model to one complete simulation containing multiple years (rather than year-by-year as different simulations), and by reducing the number of stress periods per year from 3 to 2. This could be done because stress periods 2 and 3 contained identical external stresses (e.g., pumping, recharge, and general-head boundaries). Dr. Zheng also determined the number of time steps within each stress period could be reduced without any noticeable loss of accuracy. Thus, in the revised model, the temporal discretization scheme is modified as follows:

Revised Model For This Project (2 Stress Periods Per Year)

Stress Period	Length (days)	# Time Steps	Time Step Multiplier
1	76	5	1.5
2	289	5	1.5

Since two stress periods are required for one year, there are 60 stress periods for a 30-year simulation, with the above temporal discretization scheme repeated once per year.

Initial Time For Optimization Simulations

The model used for the FS was run forward in time to September 2003, under non-remediation conditions. It is assumed that a remedy will not be in place prior to September 2003. The simulation period for the optimization simulations therefore begins in September 2003. The first stress period each year is the non-irrigation season, and the second period each year is the irrigation season.

Simulated Time Period For Optimization Runs

For formulations 1 and 2, cleanup time must be less than 30 years. Thus the maximum simulated time period is 30 years. However, in Formulations 1 and 2, the objective function and constraints are only evaluated until "cleanup" is achieved (see "Definitions" section regarding the definition of cleanup). Therefore, simulated time periods shorter than 30 years are possible, depending on the pumping solution being simulated. GeoTrans determined a solution with cleanup time of 27 years during development of the formulations, but cannot specifically conclude that optimal solutions have cleanup time of 27 years or less (because of potential tradeoffs between capital costs, annual costs, and cleanup time).

For formulation 3, the simulation period is 30 years, since the plume containment constraint (based on concentrations) is evaluated after each year for 30 years.

Discounting of Future Costs

Site managers indicate that there is some question as to whether or not it is appropriate to use discounting to convert future costs to "net present value". They sometimes use a term called "Sum of Committed Cost Analysis", which accounts for the fact that they get just the funds needed to get through the following year's (i.e., cannot invest money not spent). However, it was ultimately decided to use a discount rate consistent with OMB guidance (3.5% was selected).

Simplifications Regarding Cost Coefficients

The FS provides extremely detailed unit costs for many items, as functions of design parameters such as flow rate. There are also many variables in the FS costs, such as type of treatment (e.g., GAC versus air stripping), which were not firmly established. For the purpose of this project, the cost terms and coefficients must be simplified. Simplifications to be made include the following (based on cost coefficients provided by ACOE and their contractor):

Capital Cost Items:

1) Treatment System: $1,000/gpm
2) New Extraction Well: $400,000/well
3) Discharge Piping: $1,500/gpm
4) Infiltration Basins: not being simulated as per site managers

Variable Annual O&M Cost Items:

1) Pumping Costs (Electrical): $46/gpm/yr
2) Treatment Costs: $283/gpm/yr
3) Discharge Costs: $66/gpm/yr

Fixed Annual O&M Cost Items:

1) Fixed Monitoring Costs: $300,000/yr
2) Fixed Management Costs: $115,000/yr

The goal of the simplifications is to create optimization problems that incorporate the tradeoff of higher pumping rate and/or increased number of wells (each of which increases capital or annual costs) versus reductions in cleanup time (which can lower life-cycle costs). These costs coefficients are not a rigorous accounting of costs. It is assumed that the optimization will provide solutions that incorporate to a reasonable degree these trade-offs, and that detailed design will then be performed on the basis of pumping strategies (i.e., well locations and rates) developed by the optimization procedures.

Constituents Being Simulated

GeoTrans test runs show that the cleanup of TCE and TNT cannot ensure the cleanup of other constituents, i.e., DCE, TCA, and RDX. This is because those constituents have extents that do not completely overlap with TCE or TNT (note that site managers feel PCE will be addressed by remediating TCE, due to it's extent and relative low concentrations). Due to limitations of this project, the optimization formulations can only consider up to 2 constituents. Site managers suggested that, since the project is restricted to simulating two parameters, that perhaps it would be reasonable to use TCE as a surrogate parameter for DCE, TCA, and RDX, because the retardation factors are similar to TCE (relative to TNT):

	Retardation Factor*	**Cleanup Level (ppb)**	**Approach**
TCE	1.14	5	Simulate as TCE
DCE	1.06	7	Use TCE as surrogate
RDX	1.243	2.1	Use TCE as surrogate
TCA	1.364	200	Use TCE as surrogate
PCE	1.635	–	Do not simulate
TNT	2.885	2.8	Simulate as TNT

*for layer 1 and layers 3-6, different values are assigned for model layer 2

The approach to generate combined initial concentration is described as follows:

- Simulate DCE, TCA, and RDX independently from 6/1999 to 9/2003 to get the initial concentration distribution of each constituent for the optimization runs 9/2003;
- Normalize the concentration of each constituent in 9/2003 to a representative TCE level according to the ratio of the cleanup levels (CL), to properly account for cleanup levels of the other constituents (since the model is evaluating TCE based on the TCE cleanup level of 5 ppb):

- $Conc^S(DCE) = Conc(DCE) *CL(TCE)/CL(DCE)$
- $Conc^S(TCA) = Conc(TCA) *CL(TCE)/CL(TCA)$
- $Conc^S(RDX) = Conc(RDX) *CL(TCE)/CL(RDX)$

▪ Assign the initial concentration for the combined parameters in each cell as the maximum concentration of TCE, DCE, TCA, and RDX at that cell:

$$Conc^{Comb} = Max(TCE, DCE, TCA, RDX)$$

This last step is done to address areas where multiple constituents overlap. If constituent concentrations were added in areas of overlap, mass would be preserved, but comparing simulated concentrations to the cleanup level of TCE would be inappropriate. Using the maximum concentration, while it does not properly account for total mass of all constituents, is the appropriate method to compare simulated concentrations to the TCE cleanup level.

It should also be noted that the individual transport models have a decay term for TCE only (not DCE, TCA, or RDX). The half-life for TCE is simulated as 65 years. Given the approximations being made for this surrogate parameter approach, the fact that the other parameters are now being simulated with this half life is not a concern, since the half life is so long relative to the simulation period (30 years or less).

MODFLOW Code Modification to Improve "Dry Cell" Conditions

Starting from the hydraulic containment scenario in the FS report, GeoTrans performed some test simulations with added/modified pumping rates in high concentration areas, focusing only on model layers 3-6. GeoTrans noted that the simulation suffered from many "dry cells" in model layers 1 and 2, indicating that at some point during the flow simulation the head dropped below the bottom elevation of the layer (that cell is then set to inactive for the rest of the flow and transport simulation). GeoTrans applied a procedure developed by Dr. Zheng for MODFLOW which assigns a user-specified value of saturated thickness for cells where head is below layer bottom (i.e., the head is still below the layer bottom, but the cell remains active and transmissivity is calculated based on the minimum saturated thickness that is specified). This fixes the problem of cells going dry just because of the solution iteration process in the flow simulation, or as a result of a domino effect caused by nearby cells going dry. While this procedure allows the cells that are not truly supposed to be dry to stay active in MODFLOW, in MT3D if a cell is truly supposed to be dry (head below bottom of layer) then concentration will still be assigned a special value by MT3D as an inactive cell, which is an indicator that the solution has too much pumping. However, for the test runs GeoTrans performed, it was determined that the dry cells were being caused by the iteration process (i.e., they were not really supposed to be dry) and Dr. Zheng's procedure allowed the model to ultimately reach a more appropriate solution (i.e., without the dry cells).

Treatment of Model Layer 1

Model layer 1 is a thin, unconfined aquifer. It was noted during development of the formulations that wells placed in layer 1, in conjunction with the code modification discussed above, caused instabilities in the flow model (causing the flow model to not converge). It was empirically determined that the flow model had no convergence problems when wells in layer 1 were represented with the MODFLOW drain package rather than the MODFLOW well package. The "drains" actually represent wells with a low-level shutoff (specified as the drain elevation). Water is removed from the aquifer as long as the water level in the aquifer exceeds the drain elevation (i.e., the low-level shutoff elevation).

In the FS solutions, the vast majority of pumping at remediation wells occurs in layers 3-5. For instance, for the hydraulic containment solution in the FS, the following remediation well rates are specified:

- Layer 1: 18 gpm
- Layer 3-5: 4050 gpm

Based on discussions with site managers, it was decided that the majority of the management problem is associated with model layers 3-6. This is partly due to the ratio of pumping from layer 1 versus layers 3-6 (presented above) and also because the FS assumes individual treatment units for those shallow wells (versus centralized treatment for the deeper wells). Therefore, in the optimization formulations, drains will be fixed in model layer 1 to provide mass reduction associated with future remedial action in that layer, but the drain locations and/or parameters will not be "optimized" as part of the formulations. The items to be optimized will be well locations and rates in model layers 3-6.

Treatment of Model Layer 2

Because layer 2 is a low permeability layer, remediation wells were not included in model layer 2 in the FS. That restriction applies to the optimization project as well.

In the modeling done for the FS, the model was run for 1 year at a time. At the beginning of each year, the concentration of model layer 2 was set to the concentration of model layer 1. For the optimization project, the simulation model was modified to simulate the entire simulation period as one model run, and the concentrations in model layer 2 are not set to equal the concentrations in model layer 1 after each year. Because all simulations include mass reductions in layer 1 (discussed above), layer 2 has higher concentrations in the optimization runs than would be present if the FS approach was utilized. Thus, the approach for the optimization runs is conservative.

Discharge of Treated Water

The FS does not explicitly detail the plan for discharge of treated water. It may be discharged to surface water, or may be discharged via ponds. In the FS, recharge of treated water into the aquifer was not considered. Project managers indicate that, for the optimization project, recharge of treated water to the aquifer should not be simulated.

A unit cost for discharge ($/gpm/yr) is assigned for formulations 1 and 2. For formulation 2, it is assumed that up to 2400 gpm of extracted water can be discharged to a local utility, with no treatment or discharge costs.

Treatment of Multi-Aquifer Wells

Remediation wells may be "multi-aquifer", i.e., they screened in multiple model layers and therefore have multiple entries in the MODFLOW well package (one per model layer screened by the well). This is often done in models, and the rate specified in each model layer for a multi-aquifer well is usually calculated according to the weighted average of transmissivity in each layer.

New wells in this project are limited to layers 3-5. We will assume that a remediation well in the in the same row and column, but different layers, represent one multi-aquifer well:

- capital cost is for only one well
- maximum well rate applies to the combined well
- ratio of rates between model layers must be consistent with the transmissivity of each layer.

In this model the transmissivity for a given row/column is the same in layers 3, 4 and 5. Therefore, if the well is in multiple layers, the rate must be the same in each layer.

Site managers used specific capacity assumptions, in conjunction with the thickness of model layer 3, to determine the following well rate limits for remediation wells specified in layers 3-5:

- well screens one model layer: 350 gpm limit
- well screens two model layers: 700 gpm limit
- well screens three model layers: 1050 gpm limit

These limits are intended to provide at least 10-15 feet of saturated thickness in model layer 3 in the cell containing the well (such water elevation limits are not included as actual constraints).

Well Numbers Must Be Specified in Well Package

To help identify multi-aquifer wells, an additional column (after layer, row, column, and rate) is needed in the WEL package for each cell to indicate well number for extraction wells. Use the same number more than once to indicate a multi-aquifer well. All irrigation wells are indicated with either negative number or 0 for well number.

The FORTRAN postprocessor being provided by GeoTrans will calculate the number of new extraction wells based on well numbers assigned by users. The FORTRAN postprocessor will also check the transmissivity ratios and combined well rates for multi-aquifer wells, and output the error messages if the rates don't obey the transmissivity ratio rule or maximum well rate constraints. It will also check if the correct non-remediation pumping (number of wells and total rates) is specified.

DEFINITIONS

year – the modeling year defined by

$$year = \text{Roundup}(\textit{elapsed modeling years})$$

- September, 2003 corresponds to zero elapsed modeling years
- *year* =1 corresponds consists of 2 stress periods
- Any timestep within stress periods 3 and 4 are in *year* =2
- **Roundup**() is a function to convert a real number into an integer by rounding up (i.e., 1.0 → 1 but 1.1 → 2).

ny – the modeling year in which cleanup is achieved. That is the modeling year when

$$\text{For layers 3-6, } \left\| C_{TCE} \right\|_{\infty} \leq 5.0\ \mu g/L \quad \text{and} \quad \left\| C_{TNT} \right\|_{\infty} \leq 2.8\ \mu g/L$$

- $\left\| C_{TCE} \right\|_{\infty}$ is the infinity-norm, which returns the maximum value of two-dimensional array C_{TCE}, which is the two-dimensional concentration array in layers 3-6 for TCE. For example, if during the 17th year of the simulation "cleanup" is achieved, then costs are incurred for 17 full years.

d – indicates discounting using 3.5% discount rate to represent the conversion of capital and annual costs incurred in the future to present value (i.e., discounted) with the following discount function:

$$PV = \frac{cost}{(1 + rate)^{year-1}}$$

- PV is the present value of a *cost* incurred in *year* with a discount rate of *rate*
- No discounting is done for all costs for *year*=1 (stress periods 1 and 2)
- All costs in subsequent years are discounted at the ends of those years
- Example 1: Assuming a discount rate of 3.5% and a $1000 cost incurred at any time during *year*=1, the present value of the cost is $1000
- Example 2: Assuming a discount rate of 3.5% and a $1000 cost incurred in *year*=2, the present value of that cost is $1000/1.035=$966.18.

management period – 5-year periods (consisting of 10 simulation stress periods) during which the pumping locations/rates for remediation wells cannot be modified. Modifications may only be made during the initial time step of each management period.

FORMULATION #1

Formulation 1 – Objective Function

This function minimizes total cost up to and including *ny* (i.e., the year of cleanup). This function must be evaluated at the end of every year, rather than after every management period, to properly account for discounting of annual costs. All costs are in thousands of dollars.

MINIMIZE (CCE + CCT + FCM + FCS + VCE + VCT + VCD)

CCE: Capital Costs of new extraction wells

$$\text{CCE} = \sum_{i=1}^{ny} (400 \times NW_i)^d$$

ny is the modeling year when cleanup occurs.
NW_i is the total number of new extraction wells installed in year *i*. New wells may only be installed in years corresponding to the beginning of a 5 -yr management period.
$400K is cost of installing a new extraction well.
d indicates application of the discount function to yield Net Present Value (NPV).

CCT: Capital Cost of Treatment (applied at beginning of simulation)

$$\text{CCT} = 1.0 \times Q_{\max}$$

$Q_{\max}$ is the maximum total pumping rate at remediation wells (layers 3-6) in any management period
$1.0K is the cost per gpm of installing a treatment unit of sufficient capacity at the beginning of the simulation for all subsequent management periods

CCD: Capital Cost of Discharge Piping (applied at beginning of simulation)

$$\text{CCD} = 1.5 \times Q_{\max}$$

$Q_{\max}$ is the maximum total pumping rate at remediation wells (layers 3-6) in any management period
$1.5K is the cost per gpm of installing discharge piping of sufficient capacity at the beginning of the simulation for all subsequent management periods

FCM: Fixed Cost of Management

$$\text{FCM}=\sum_{i=1}^{ny}(115)^{d}$$

ny is the modeling year when cleanup occurs.
\$115K is the fixed annual O&M management cost.
d indicates application of the discount function to yield Net Present Value (NPV).

FCS: Fixed Costs of sampling

$$\text{FCS}=\sum_{i=1}^{ny}(300)^{d}$$

ny is the modeling year when cleanup occurs.
\$300K is the fixed annual cost of sampling and analysis
d indicates application of the discount function to yield Net Present Value (NPV).

VCE: Variable Costs of Electricity for operating wells

$$\text{VCE}=\sum_{i=1}^{ny}\left(0.046\times Q_i\right)^{d}$$

ny is the modeling year when cleanup occurs.
\$0.046K is the electrical cost per gpm
Q_i is the total pumping rate in year *i*
d indicates application of the discount function to yield Net Present Value (NPV).

VCT: Variable Cost of Treatment

$$\text{VCT}=\sum_{i=1}^{ny}\left(0.283\times Q_i\right)^{d}$$

where

ny is the modeling year when cleanup occurs.
\$0.283K is the treatment cost per gpm
Q_i is the total pumping rate in year *i*
d indicates application of the discount function to yield Net Present Value (NPV).

VCD: Variable Cost of Discharge

$$\text{VCD}=\sum_{i=1}^{ny}\left(0.066\times Q_i\right)^{d}$$

where

ny is the modeling year when cleanup occurs.
$0.066K is the discharge cost per gpm
Q_i is the total pumping rate in year *i*
d indicates application of the discount function to yield Net Present Value (NPV).

Formulation 1 – Constraints

1) Modification Occurrence Constraint: Modifications to the system may only occur at the beginning of each management period (i.e., the beginning of modeling years 1, 6, 11, 16, 21, 26).

2) Cleanup must be achieved in model layers 3-6 within the modeling period (by the end of year 30).

$$ny \leq 30$$

3) Plume containment constraint: TCE and TNT concentration levels must not exceed their respective cleanup levels in locations beyond areas specified by the Hastings (Figures 1 & 2), i.e. plume cannot spread above cleanup levels to any cell adjacent to specified areas.

   At time, *t*, and for all grid indices *i* and *j* in layers 3-6,

$$\begin{aligned}&\text{If BTCE}(i,j) = 0\\ &\quad \text{then } C_{TCE}^{ij} \leq 5.0\ \mu\text{g/L}\\ &\text{and}\\ &\text{If BTNT}(i,j) = 0\\ &\quad \text{then } C_{TNT}^{ij} \leq 2.8\ \mu\text{g/L}\end{aligned}$$

   BTCE(*i,j*): a function of model grid indices *i* and *j* that returns 1 if (*i,j*) corresponds to a location within the buffer zone for TCE and 0 if (*i,j*) corresponds to a location outside of the buffer zone for TCE

   BTNT(*i,j*): a function of model grid indices *i* and *j* that returns 1 if (*i,j*) corresponds to a location within the buffer zone for TNT and 0 if (*i,j*) corresponds to a location outside of the buffer zone for TNT

   C_{TCE}^{ij} : the concentration of TCE at grid location (*i,j*)

   C_{TNT}^{ij} : the concentration of TNT at grid location (*i,j*)

   Location of these zones is provided in matrix form with the FORTRAN post-processor

   When Evaluated: The end of each 5-year management period.

4) Limits on individual extraction well rates: Site managers used specific capacity assumptions, in conjunction with the thickness of model layer 3, to determine the following well rate limits for remediation wells specified in layers 3-5:

- well screens one model layer: 350 gpm limit
- well screens two model layers: 700 gpm limit
- well screens three model layers: 1050 gpm limit

5) Restricted area constraint: No remediation wells are allowed in specified restricted areas (Figure 3 and Table 1).

At any time, *t*, and for all grid indices *i* and *j*,

$$\text{If } NoWelZon(i,j) = 1$$
$$\text{then } \textit{No Well Allowed}$$

NoWelZon(i,j): a function of model grid indices *i* and *j* that returns 1 if (*i,j*) corresponds to a location within the restricted area and 0 if (*i,j*) corresponds to a location outside of the restricted area. Zones are provided in matrix form with the FORTRAN post-processor.

When Evaluated: The beginning of each 5-year management period

6) Remediation well location constraint: No remediation wells are allowed in cells with irrigation wells to prevent excessive dewatering in irrigation wells and/or at remediation wells.

$$\textit{Location (Remediation Wells)} \neq \textit{Location (Irrigation Wells)}$$

When Evaluated: The beginning of each 5-year management period

7) Dry cell constraint: This means that MT3D concentration array does not indicate an inactive cell due to dry conditions.

At end of simulation, and for all grid indices *i* and *j*,

$$C_{ij} = active$$

When Evaluated: The end of simulation.

8) Irrigation Well Constraint: Modeler cannot change well rates on irrigation wells in any stress period.

When Evaluated: The beginning of each simulation period.

9) Well Screen Constraint: No well is allowed screened in model layer 6

   When Evaluated: The beginning of each simulation period.

FORMULATION #2

Same as formulation 1, but assume diversion of 2400 gpm of extracted water (i.e., do not incur treatment cost or discharge cost for up to 2400 gpm of extracted water). Changes to formulation are:

CCT: Capital Cost of Treatment (applied at beginning of simulation)

If $\left(Q_{\max} \leq 2400\right)$ then

$$CCT = 0,$$

else

$$CCT = 1.0 \times \left[Q_{\max} - 2400\right]$$

where

Q_{max} is the maximum total pumping rate at remediation wells (layers 3-6) in any management period

$1.0K is the cost per gpm of installing a treatment unit of sufficient capacity at the beginning of the simulation for all subsequent management

CCD: Capital Cost of Discharge Piping (applied at beginning of simulation)

If $\left(Q_{\max} \leq 2400\right)$ then

$$CCD = 0,$$

else

$$CCD = 1.5 \times \left[Q_{\max} - 2400\right]$$

where

Q_{max} is the maximum total pumping rate at remediation wells (layers 3-6) in any management period

$1.5K is the cost per gpm of installing discharge piping of sufficient capacity at the beginning of the simulation for all subsequent management

VCT: Variable Cost of Treatment

$$\text{VCT} = \sum_{i=1}^{ny} CT_i^{\,d}$$

where

If $\left(Q_i \leq 2400\right)$ then

$$CT_i = 0,$$

else

$$CT_i = 0.283 \times \left[Q_i - 2400\right]$$

ny is the modeling year when cleanup occurs.
nwel is the total number of extraction wells.
\$0.283K is the treatment cost per gpm
Q_i is the total rate in year *i*
d indicates application of the discount function to yield Net Present Value (NPV).

VCD: Variable Cost of Discharge

$$\text{VCD} = \sum_{i=1}^{ny} CD_i^{\,d}$$

where

If $\left(Q_i \leq 2400\right)$ then

$$CD_i = 0,$$

else

$$CD_i = 0.066 \times \left[Q_i - 2400\right]$$

ny is the modeling year when cleanup occurs.
nwel is the total number of extraction wells.
\$0.066K is the discharge cost per gpm
Q_i is the total rate in year *i*
d indicates application of the discount function to yield Net Present Value (NPV).

FORMULATION #3

Formulation 3 – Objective Function

This function minimizes the maximum total remediation pumping rate in any management period over a 30-year simulation.

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

$Q_{\max}$: the maximum total pumping rate at remediation wells (layers 3-6) in any management Period over a 30 year simulation.

Formulation 3 – Constraints

Same as formulation 1, except:

- delete the second constraint (i.e., cleanup need not be achieved within 30 years in formulation 3)
- add limit of 25 on total number of new remediation wells over the entire modeling period

$$\#\ RemediationWells \leq 25$$

Figure 1. TCE Containment Zone in Layers 3-6

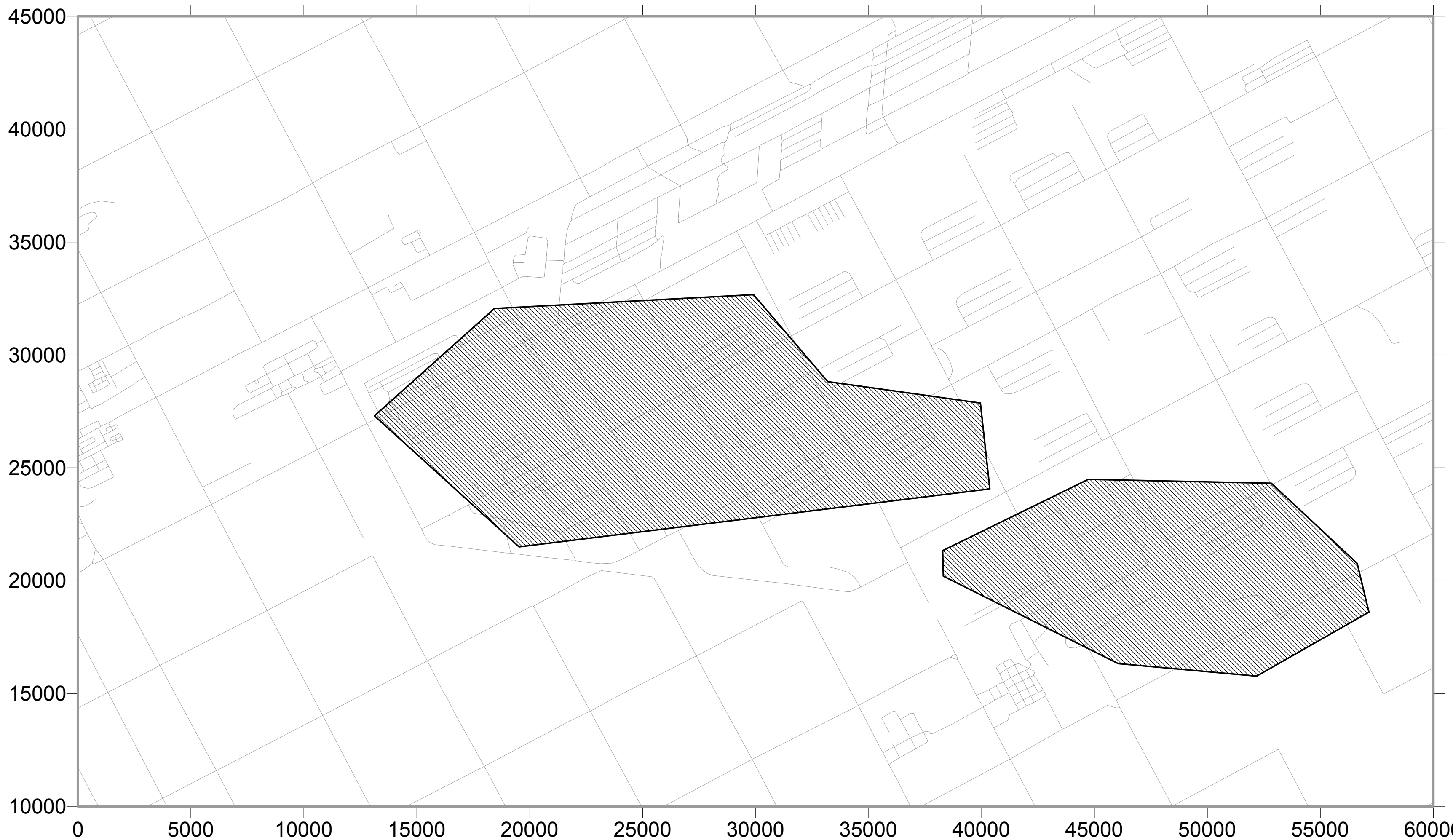

Figure 2. TNT Containment Zone in Layers 3-6

Figure 3. Restricted Areas Where No Remediation Wells Allowed

Table 1. Model Row and Column of Restricted Areas For New Wells

Row	Column
21	40
21	41
22	39
22	40
22	41
44	71
44	72
45	69
45	70
45	71
45	72
46	67
46	68
46	69
46	70
46	71
46	72
46	73
47	65
47	66
47	67
47	68
47	69
47	70
47	71
47	72
47	73
48	65
48	66
48	67
48	68
48	69
48	70
48	71
48	72
48	73
48	74
49	65
49	66
49	67
49	68
49	69
49	70

49	71
49	72
49	73
50	64
50	65
50	66
50	67
50	68
50	69
50	70
50	71
51	64
51	65
51	66
51	67
51	68
51	69

***note: in addition, new wells may not be placed in cells with existing irrigation wells

GeoTrans Report on Blaine

OPTIMIZATION RESULTS: GEOTRANS

ESTCP TRANSPORT OPTIMIZATION PROJECT
SITE #3: HASTINGS NAVAL AMMUNITION DEPOT

Prepared By:

Yan Zhang and Rob Greenwald
GeoTrans, Inc.
2 Paragon Way
Freehold, New Jersey 07728

NOTICE

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PREFACE

The goal of the ESTCP Transport Optimization project ("the project") is to evaluate the effectiveness and cost/benefit of transport optimization software for pump-and-treat (P&T) system optimization. When coupled with a site-specific solute transport model, transport optimization software implements complex mathematical algorithms to determine optimal site-specific well locations and pumping rates. This demonstration project is intended to address the following scientific questions:

1) Do the results obtained from these optimization software packages (e.g. recommended optimal P&T scenarios) differ substantially from the optimal solutions determined by traditional "trial-and-error" optimization methods?

2) Do the results obtained from these optimization software packages warrant the additional effort and costs when compared to traditional "trial-and-error" optimization methods?

The project involves the determination of optimal extraction and pumping well scenarios at three Department of Defense (DoD) P&T systems. The installations are encouraged (but not required) to implement optimization suggestions resulting from the demonstration.

For each of the three sites, three site-specific optimization problems ("formulations") will be defined. Each of three modeling groups will independently attempt to determine the optimal solution for each of the optimization formulations. Two of the modeling groups will use their own independently developed transport optimization software, and the other group (GeoTrans) will use a traditional "trial-and-error" optimization method as a control. Thus, the optimization recommendations from two separate transport optimization software programs will be compared to each other and to the recommendations from the trial-and-error control.

This report presents the "trial-and-error" results determined by GeoTrans for Site #3, which is the Hastings Naval Ammunition Depot in Hastings, Nebraska. The three formulations for this site are described in detail in a separate document.

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1.0 BRIEF SUMMARY OF FORMULATIONS

The details of the three problem formulations are provided in a separate document. A brief summary of these formulations is provided below. The initial concentrations of TCE and TNT at the beginning of the optimization simulations are presented in Figure 1 and Figure 2, respectively.

1.1 Variables To Be Optimized

The items to be optimized are well locations and rates in model layers 3-6. In the optimization formulations, drains are fixed in model layer 1 to provide mass reduction associated with future remedial action in that layer, but the drain locations and/or parameters are not to be "optimized" as part of the formulations.

1.2 Formulation 1

For Formulation 1, a cost function to be minimized was developed (in conjunction with the installation) that combines the "Up-Front Costs" with the "Total of Annual Costs" over the time it takes to reach cleanup for TCE and TNT in model layers 3-6, beginning September 2003, assuming a discount rate of 3.5%. The components of cost are:

MINIMIZE (CCE + CCT + CCD + FCM + FCS + VCE + VCT + VCD)

where

CCE: Capital cost of new extraction wells ($400/well)
CCT: Capital cost of treatment ($1/gpm)
CCD: Capital cost of discharge ($1.5/gpm)
FCM: Fixed cost of management ($115/yr)
FCS: Fixed cost of sampling ($300/yr)
VCE: Variable electrical cost of operating wells ($0.046/gpm/yr)
VCT: Variable cost of treatment ($0.283/gpm/yr)
VCD: Variable cost of discharge ($0.066/gpm/yr)

All costs above are in thousands of dollars

The solution is subject to the following constraints:

- The modeling period consists of six 5-year management periods (30 years total) beginning September 2003
- Modifications to the system may only occur at the beginning of each management period
- Cleanup, for both TCE and TNT, must be achieved in model layers 3-6 within modeling period (by the end of year 30)
- TCE and TNT concentration levels must not exceed their respective cleanup levels in locations beyond specified areas (i.e., containment must be achieved)
- Site managers used specific capacity assumptions to determine the limits on individual extraction well rates:

well screens one model layer: 350 gpm limit
well screens two model layers: 700 gpm limit
well screens three model layers: 1050 gpm limit

- Multi-aquifer wells must have equal rate in each model layer (since transmissivity is the same in model layers 3, 4, and 5)

- Some restricted areas are defined where no remediation wells are allowed

- Remediation wells are not allowed in the same model cells with irrigation wells to prevent excessive dewatering in irrigation wells and/or at remediation wells

- No inactive cell is allowed due to dry conditions when running the MT3D model

- No wells allowed in model layer 6

The specifics of the cost function and detail of the constraints are provided in the detailed problem formulation (separate document).

1.3 Formulation 2

Same as formulation 1, but assume diversion of 2400 gpm of extracted water (i.e., do not incur treatment cost or discharge cost for up to 2400 gpm of extracted water). Changes to formulation are in the terms:

CCT: Capital cost of treatment ($1/gpm)
CCD: Capital cost of discharge ($1.5/gpm)
VCT: Variable cost of treatment ($0.283/gpm/yr)
VCD: Variable cost of discharge ($0.066/gpm/yr)

In each case, gpm must be calculated by subtracting 2400 gpm from the total pumping rate at remediation wells.

1.4 Formulation 3

The objective function is to minimize the maximum total remediation pumping rate in any management period over a 30-year simulation. The constraints are the same as for Formulation 1, except:

- The constraint requiring cleanup within 30 years is eliminated

- A constraint limiting the number of new remediation wells to 25 is added

In essence, this formulation is intended to determine the minimum pumping rate at any point in time that meets all remaining constraints (after the cleanup constraint is removed), including the constraint representing plume containment.

2.0 OPTIMIZATION TECHNIQUE

GeoTrans applied "trial-and-error" optimization for each of the three formulations. The management horizon associated with each formulation consisted of six 5-year management periods (30 years total), beginning September 2003. Each trial-and-error simulation involved modifying pumping wells (locations and rates) in the MODFLOW/MT3D well package. Pumping could be modified at the beginning of each of the 5-year management periods within a specific simulation.

The simulations discussed in this report were performed by GeoTrans between May 17, 2002 to September 13, 2002. The general optimization approach utilized by GeoTrans is described below.

Step 1: Program FORTRAN Postprocessor

For each simulation, it was necessary to evaluate the objective function value, and to determine if that simulation produced an improved solution relative to previous simulations. For each simulation it was also necessary to determine if all constraints were satisfied. For "trial-and-error" optimization, it was essential that the evaluation of objective function and constraints be done efficiently. Therefore, GeoTrans coded a FORTRAN program to read specific components of model input and output, and then print out the objective function value (broken into individual components) and all constraints that were violated. GeoTrans provided this FORTRAN code to the other modeling groups, to allow those groups to check their solutions (i.e., to make sure they had not made any errors in programming associated with their methods that would invalidate their results).

Step 2: Develop "Animation" Approach

The purpose of the animations was to clearly illustrate the plume movement over time based on simulation results. The animations were developed by creating a concentration contour map for model layers at the end of each water year (August, 31) in the simulation, using SURFER, and then compiling those into a Microsoft PowerPoint file to allow the plume movement over time to be displayed as an "animation". It is time consuming updating SURFER files manually and simply using copy-and-paste command since the components of the optimization formulations apply to multiple model layers. Thus, a 3 part procedure was developed: 1) updating SURFER grid files automatically using SURFER script (31 files per layer per contaminant); 2) exporting as image files automatically using SURFER script; and 3) importing the image files into Microsoft PowerPoint files automatically using MS macro.

Step 3: Modify Pumping/Recharge, Run FORTRAN Code, and Create/Evaluate Animation

This is the classic "trial-and-error" method. After each simulation, the FORTRAN code allowed immediate determination regarding the objective function value, and whether or not the run was feasible (i.e., all constraints satisfied). Based on evaluation of the animations for TCE and TNT, modified pumping strategies were selected for one or more subsequent simulations, to better address areas of relatively high concentrations and/or areas where cleanup was not progressing fast enough, and to better address the containment of plumes.

For Formulation 3, Step 3 was modified at times to consist of particle tracking to evaluate hydraulic capture of specific scenarios, rather than MT3D simulations, due to the long execution time for MT3D.

3.0 OPTIMIZATION RESULTS

3.1 Pre-Optimization Simulations

3.1.1 FS Report Simulations

There is no existing system at Hastings. The FS report included several potential designs for extraction systems, but it is not appropriate to compare the results of the solutions determined in this optimization study to those designs. The FS designs were developed using a slightly different simulation model, and were not subject to the same goals and constraints employed in this study.

3.1.2 Initial Solution Provided By GeoTrans

GeoTrans provided each modeling group with an initial solution that was feasible for formulations 1, 2 and 3. This solution had 17 new wells, pumping a total of 6905 gpm in each of the six stress periods, with aquifer cleanup (using the definition of cleanup specified in the formulation document) achieved in 24 years. Objective function values for this initial solution were:

<u>Pre-Optimization Objective Values</u>

Formulation 1: $76,292K
Formulation 2: $56,370K
Formulation 3: 6905 gpm

3.2 Formulation 1: Minimize Total Cost

3.2.1 Optimal Solution, Formulation 1

For Formulation 1, a total of 22 major runs were performed, consisting of a total of 57 simulations (i.e., some major runs included a series of sub-runs). The best solution was found in major simulation 21 (total simulation 55), and has the following details:

Results, Formulation 1

	Optimal Solution
Objective Function (Total)	$50,335K
Cleanup Time	30 years
Number of New Extraction Wells	8

	Optimal Solution
Objective Function (Components)	
CCE: Capital cost of new extraction wells	$3,200K
CCT: Capital cost of treatment	$3,995K
CCD: Capital cost of discharge	$5,992.5K
FCM: Fixed cost of management	$2,189.114K
FCS: Fixed cost of sampling	$5,710.732K
VCE: Variable electrical cost of operating wells	$3,406.067K
VCT: Variable cost of treatment	$20,954.719K
VCD: Variable cost of discharge	$4,886.966K

A total of 8 new extraction wells are included in the optimal solution:

- 2 wells are installed in layer 3 only
- 2 wells in layers 3 and 4
- 4 wells in layers 3, 4, and 5

Extraction rates, by management period, are listed below:

Optimal Rates, Formulation 1

Well	Location (Row,Col)	Layer	Period 1 (gpm)	Period 2 (gpm)	Period 3 (gpm)	Period 4 (gpm)	Period 5 (gpm)	Period 6 (gpm)
W2	(29,57)	3,4,5	600	600	600	600	600	600
W4	(32,62)	3,4,5	945	945	945	945	945	945
W7	(47,116)	3,4,5	420	420	420	420	420	0
W20	(36,78)	3,4,5	630	630	630	630	630	630
W32	(27,32)	3,4	580	580	580	580	580	580
W43	(52,120)	3	270	250	220	220	350	350
W47	(37,39)	3,4	400	400	400	400	400	0
W49	(57,109)	3	150	150	200	200	0	0
		Total Extraction	**3995**	**3975**	**3995**	**3995**	**3925**	**3105**

Locations of extraction wells, and concentrations over time, are illustrated on the following figures:

Figure 3: TCE, Layer 3
Figure 4: TCE, Layer 4
Figure 5: TCE, Layer 5
Figure 6: TNT, Layer 3
Figure 7: TNT, Layer 4

A chart illustrating objective function value versus simulation number is provided in Figure 8.

3.2.2 General Approach to Determining the Optimal Solution, Formulation 1

<u>Major Simulations 1-3</u>

Start with the feasible solution GeoTrans sent on 5/20/02. Turn off some wells and lower the pumping rates of some wells. Lowest cost is $71,020K, 6500 gpm, 24 yrs for TCE and 21 yrs for TNT. At this point we switched to Formulation 3, and later returned to Formulation 1.

<u>Major Simulations 4-11</u>

Based on 3000 gpm solution from Formulation 3, try to increase pumping to satisfy the cleanup constraint. We found out that there is a small area in layer 1 with TCE where K value is very small, and it is hard to clean that area fast. No feasible solutions found until run 11, which had cost of $51,627K, 4045 gpm, 30 yrs for TCE and 25 yrs for TNT…many of the infeasible solutions barely exceeded the cleanup level for TCE and/or TNT, such as TCE between 5 and 10 ppb.

At this point, we decided to focus on cost saving from reducing the pumping rate rather than reducing the cleanup time, based on cost coefficients in objective function.

<u>Major Simulations 12-15</u>

Attempted to reduce pumping by removing lower screen intervals for some wells, and in process we also varied locations of some of those wells, no feasible solutions found.

<u>Major Simulation 16-18</u>

Starting from Run 11, attempted to speed up cleanup in the “hard to clean” area by modifying well rates and locations, but we just caused further problems satisfying TCE and/or TNT cleanup limits by creating stagnation areas and/or pulling contaminants away from wells where they were previously captured

<u>Major Simulations 19-22 (***optimal solution was Major Simulation 21, Total Simulation 55)</u>

Starting from Run 11, tinker with well rates and locations, especially reducing some well rates in later periods, to achieve slightly better objective function value. Best feasible solution is Run 21 with cost of $50,335K, 3995 gpm, 30 yrs for TCE and 25 yrs for TNT.

3.3 Formulation 2: Minimize Cost with Diversion of 2400gpm

Formulation 2 is the same as Formulation 1, except that some terms in the objective function are modified such that 2400 gpm of total pumping rate is diverted such that treatment and discharge is not required. While determining the optimal solution for Formulation 1, we determined via logic (but no additional simulations) that the optimal solution for Formulation 2 should be the same as optimal solution to Formulation 1. Therefore, the optimal solution presented in Section 3.3.1 is the same as that presented for Formulation 1, except for different objective function value. The logic used to make this conclusion is presented in Section 3.3.2.

3.3.1 Optimal Solution, Formulation 2.

As discussed earlier, no additional simulations were made for Formulation 2. The optimal solution is as follows:

Results, Formulation 2

	Optimal Solution
Objective Function (Total)	$28,391K
Cleanup Time	30 years
Number of New Extraction Wells	8
Objective Function (Components) CCE: Capital cost of new extraction wells CCT: Capital cost of treatment CCD: Capital cost of discharge FCM: Fixed cost of management FCS: Fixed cost of sampling VCE: Variable electrical cost of operating wells VCT: Variable cost of treatment VCD: Variable cost of discharge	 $3,200K $1,595K $2,392.5K $2,189.114K $5,710.732K $3,406.067K $8,025.620K $1,871.699K

Extraction rates for eight extraction wells are the same as optimal solution in Formulation 1 (see Section 3.2.1). Concentrations of TCE and TNT versus time are also the same as for Formulation 1 (Figures 3 to 7).

3.3.2 General Approach to Determining the Optimal Solution, Formulation 2

The objective function for both Formulation 1 and Formulation 2 is to minimize total cost, where:

$$\text{total cost} = \text{capital cost} + \text{annual cost*time}$$

There is an obvious tradeoff between annual cost and cleanup time. For instance, increasing pumping rate can increase capital and annual costs but decrease cleanup time.

During the solution of Formulation 1, we noticed that our best solution for Formulation 1 minimizes pumping, not cleanup time (which is at it's upper bound of 30 yrs). Inspection of the objective function cost coefficients (via spreadsheet analysis) confirmed that reducing cleanup time by 1 yr provides less benefit than reducing pumping by 100 gpm.

We then came to the following conclusion: If minimizing pumping rate is better than reducing cleanup time for Formulation 1, it should be even more so for Formulation 2. This is because annual costs are lower in Formulation 2, and reducing cleanup time (which is multiplied by annual costs) is therefore even less beneficial for reducing total cost in Formulation 2 than in Formulation 1. Since we already reduced total pumping as much as possible to optimize Formulation 1, that solution should also be optimal for Formulation 2.

This logic assumes that it is difficult to reduce cleanup time without adding substantially more pumping (higher capital and annual costs) and/or many additional wells (higher capital costs), which we believe to be the case based on our simulations performed for the other two formulations.

3.4 Formulation 3: Minimize Cost, Cleanup Constraint, Reduced Source Term

The objective function is to minimize the maximum total remediation pumping rate in any management period over a 30-year simulation. The constraints are the same as for Formulation 1, except:

- The constraint requiring cleanup within 30 years is eliminated

- A constraint limiting the number of new remediation wells to 25 is added

In essence, this formulation is intended to determine the minimum pumping rate at any point in time that meets all remaining constraints (after the cleanup constraint is removed), including the constraint representing plume containment.

3.4.1 Optimal Solution, Formulation 3

For Formulation 3, a total of 25 major runs were performed, consisting of a total of 57 simulations (i.e., some major runs included a series of sub-runs), including 9 simulations with only particle tracking. The best solution was found in major simulation 25 (total simulation 57), and has the following details:

Results, Formulation 3

	Optimal Solution
Objective Function: Total Pumping Rate (gpm)	2879
Cleanup Time	Not Cleaned Within 30 Years
Number of New Extraction Wells	7
Cost (Components)	
CCE: Capital cost of new extraction wells	$2,800K
CCT: Capital cost of treatment	$2,879K
CCD: Capital cost of discharge	$4,318.5K
FCM: Fixed cost of management	$2,189.114K
FCS: Fixed cost of sampling	$5,710.732K
VCE: Variable electrical cost of operating wells	$2,520.984K
VCT: Variable cost of treatment	$15,509.529K
VCD: Variable cost of discharge	$3,617.063
Total Cost:	***$39,544.922K***

Note that total cost is approximately $11M less than the optimal solution for Formulation 1. A total of 7 new extraction wells are included in the optimal solution:

- 2 wells in layers 3 and 4
- 5 wells in layers 3, 4, and 5

Extraction rates, by management period, are listed below:

Optimal Rates, Formulation 3

Well	Location (Row,Col)	Layer	Period 1 (gpm)	Period 2 (gpm)	Period 3 (gpm)	Period 4 (gpm)	Period 5 (gpm)	Period 6 (gpm)
W2	(29,57)	3,4,5	426	426	426	426	426	426
W7	(47,116)	3,4,5	396	396	396	396	396	396
W10	(37,39)	3,4,5	402	402	402	402	402	402
W20	(36,78)	3,4,5	615	615	615	615	615	615
W28	(33,66)	3,4,5	600	600	600	600	600	600
W30	(52,120)	3,4	280	280	280	280	280	280
W31	(57,109)	3,4	160	160	160	160	160	160
		Total Extraction	**2879**	**2879**	**2879**	**2879**	**2879**	**2879**

Locations of extraction wells, and concentrations over time, are illustrated on the following figures:

Figure 9: TCE, Layer 3
Figure 10: TCE, Layer 4
Figure 11: TCE, Layer 5
Figure 12: TNT, Layer 3
Figure 13: TNT, Layer 4

A chart illustrating objective function value versus simulation number is provided in Figure 14.

3.4.2 General Approach to Determining the Optimal Solution, Formulation 3

Major Simulation 1

Remove many wells from feasible solution GeoTrans sent on 5/20/02, and try to do simulations for early stress periods only to save time, but found that pumping strategies that work for early time cannot guarantee containment in the later periods. Best feasible solution is 4000 gpm.

Major Simulation 2

Turn off some wells and modify individual well rates. The best feasible solution is 3850gpm.

Major Simulation 3

Some wells not turned on until later stress periods, to lower pumping in early periods, but no feasible solution found.

Major Simulations 4-17

Perform steady-state particle tracking runs to quickly determine solution for hydraulic containment, which used averaged irrigation pumping and steady remediation pumping (runs 4-7, 9-10, 12, 14, 16). Performed 30-yr transient MT3D runs (runs 8, 11, 13, 15, & 17) based on particle tracking runs. Many were infeasible, and the best feasible solution is 3000gpm.

Major Simulations 18-25 (***Optimal Solution was Major Simulation 25, Total Simulation 57***)

Based on Run 17, try to slightly lower the pumping rates without changing well locations, best feasible solution is 2879 gpm (runs 18-25)

4.0 ADDITIONAL SIMULATIONS

GeoTrans still had budget remaining after the solution of all three formulations, and did not feel that significantly improved solutions to those already found could be determined for the three formulations with additional trial-and-error. Two sets of additional simulations were attempted.

<u>Additional Simulations "A"</u>

The simulations were similar to Formulation 1, but one small area of TCE was allowed to remain above the cleanup level. A total of 27 simulations were performed. A fixed well location and rate was assigned in that one area, and the FORTRAN postprocessor was modified to disregard the cleanup constraint in that area. The goal was to try to clean up remaining area faster than Formulation 1 results, at an equal or lower cost. The best cleanup time was 23 years (TNT=23, TCE=22) but cost was more than $13M higher than the Formulation 1 solution. We were not successful in finding a faster cleanup time that reduced the objective function relative to Formulation 1, even with the relaxed cleanup criteria in that one area.

<u>Additional Simulations "B"</u>

The goal of these simulations was to modify drains in layer 1 to see if that might lead to substantially better solutions for Formulation 1. A total of four simulations were performed. Modifications were made to drain locations and conductances. We did not succeed in finding a solution where a modified drain setup led to faster cleanup for a given pumping strategy. It must be noted, however, that we did not try very many combinations of modified drains and pumping strategies.

5.0 COMPUTATIONAL PERFORMANCE

Preliminary Items

Development of the three formulations, and development of the FORTRAN postprocessing code, were considered separate tasks from the actual solution of the problems, and are not described herein (since each of the other optimization groups started after the formulations and FORTRAN postprocessor were provided to them). However, those costs (approximately $12K) should be accounted for when evaluating the cost of the overall optimization process.

Solution of the Three Formulations

GeoTrans worked within a pre-specified budget of approximately $35,000 for developing optimal solutions for each of the three formulations. Development of the SURFER/PowerPoint animation technique accounted for approximately $1,000 of this $35,000, and the remaining $34,000 went towards solving the problems.

Each flow and transport simulation required approximately 100-120 minutes (i.e., just under 2 hours) on a Pentium IV, 1.8 GHZ computer. Running the FORTRAN code required less than one minute. Creating the SURFER grid files, contour maps, and subsequent animations for 2 to 4 model layers, for two different contaminants, required approximately 1 hour (average) per simulation. The remaining time was spent reviewing the results, deciding what modifications to make to pumping/recharge, and modifying the well package for the subsequent run.

GeoTrans ultimately made 145 total simulations (i.e., some major runs included a series of sub-runs), as follows:

formulation 1:	22 major simulations, 57 total simulations
formulation 2:	no additional simulations
formulation 3:	25 major simulations, 57 total simulations, including 9 simulations with only particle tracking
additional:	31 total simulations

Based on a cost of approximately $35,000 allocated towards solving the problems, this represents a cost of approximately $241 per simulation. That represents approximately 2.5 hours for project level staff (Yan Zhang) and approximately 0.5 hours for senior level staff (Rob Greenwald) for each simulation, associated with setting up, running, and postprocessing the simulation, and determining what to implement for the subsequent simulation.

GeoTrans would likely not have performed as many trial-and-error simulations if work was not being performed within the context of this project.

6.0 SENSITIVITY ANALYSIS (IF PERFORMED)

Sensitivity analysis, as it relates to optimization, refers to the extent to which the optimal solution changes with respect to specific changes in the optimization formulation. GeoTrans did not attempt to solve any formulations other than the three that were specified. Therefore, sensitivity analysis was not performed. The "trial-and-error" methodology is poorly suited for performing that type of sensitivity analysis, because the solution method is not automated.

7.0 SUMMARY, SITE-SPECIFIC ITEMS, AND LESSONS LEARNED

Formulations Fixed at the Beginning of the Simulation Period

For this project, the three formulations had to be "locked in" prior to the simulation period. This is not typical for optimization projects. In most cases it would be beneficial to start with one formulation, and based on those results develop different formulations, based on interaction with the Installation on an ongoing basis.

Costs of Optimal Solutions Versus FS Designs

Comparisons between the optimal solution for each formulation versus the FS Designs must be made with caution. The model used in our project differs from the model used in the FS, and the FS designs were not developed based on the objective functions and constraints used in our project.

Preferred Management Strategy

The optimal solution for Formulation 3 has a cost that is approximately $11M less than the optimal solution for Formulation 1. Although the Formulation 3 solution does not achieve cleanup within 30 years, it comes relatively close (TNT is cleanup up, and all TCE is less than 20 ppb after 30 years). If the installation believes that level of remaining concentration might be acceptable, then the solution to Formulation 3 might be more attractive. However, the solution to Formulation 1 does reduce concentrations to cleanup levels in 30 years, and if that is most important, then that solution is more attractive (albeit at a much higher cost).

Particle Tracking Versus MT3D Simulations

For some runs, we utilized steady-state particle tracking analysis to prepare a subsequent MT3D run. The goal was to quickly find solutions that would achieve containment using the faster particle tracking analysis, and then run MT3D for only those strategies. However, in many cases where particle tracking indicated containment, the MT3D constraint for containment still failed. This was probably due to a finite number of initial particle locations horizontally and vertically defined for the particle tracking, and/or, or due to transient nature of the MT3D simulations (due to seasonal pumping) versus the steady-state nature of the particle tracking.

Lessons Learned

The following factors, when combined, made the trial-and-error optimization formulations for Hastings much more complicated to solve than for Umatilla or Tooele:

- 3 model layers with wells, 4 layers with constraints (Umatilla had only 1 layer)
- 2 constituents to worry about (Tooele only had 1 constituent)
- Unable to realistically shorten the simulation period (possible for Umatilla)
- Large potential area to add wells (less so for Umatilla)
- Long simulation time relative to the other 2 sites

Many of these complications would also be expected to make the application of transport optimization algorithms more difficult.

Figure 1. Initial concentrations for TCE at beginning of optimization simulations.

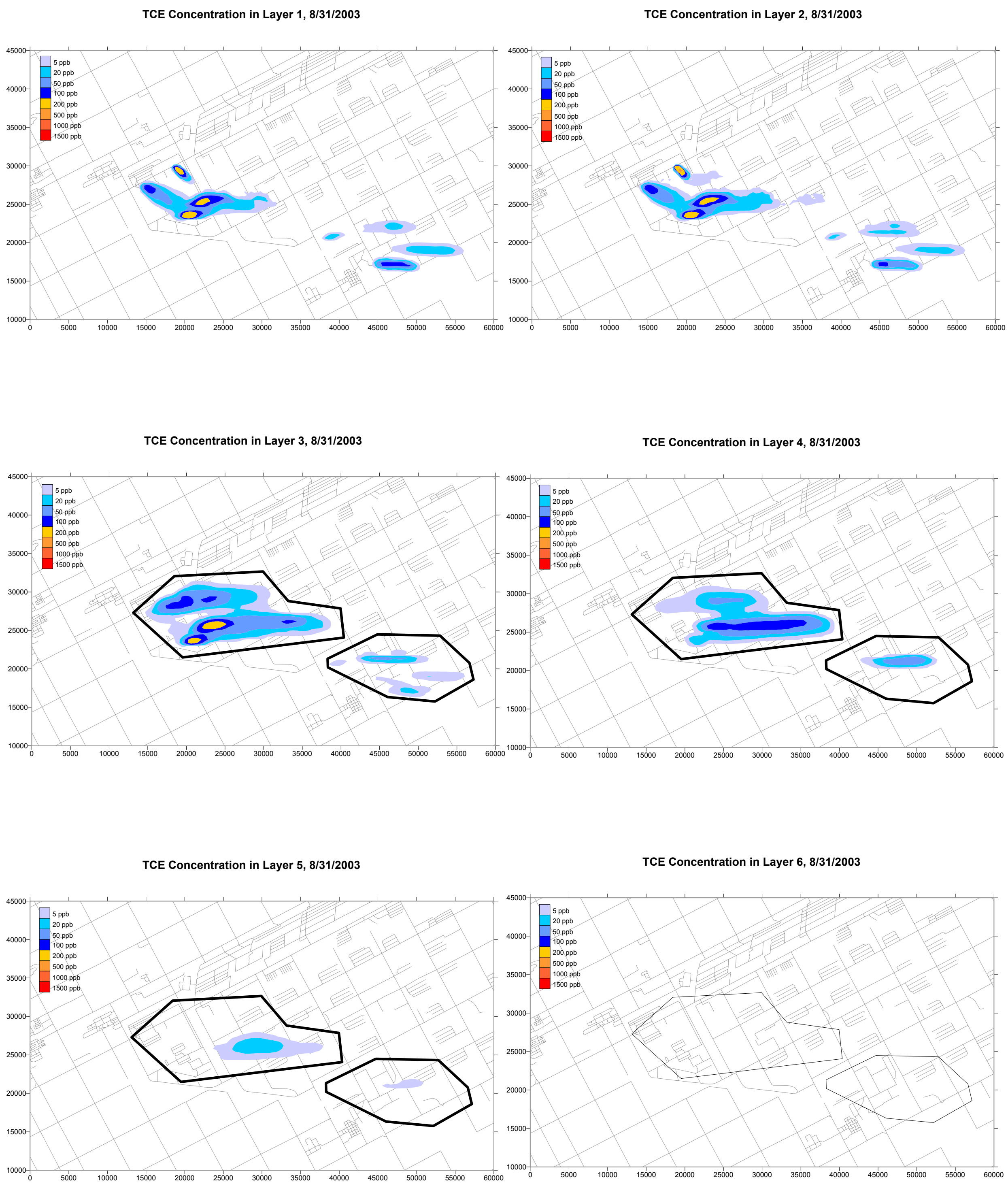


Figure 2. Initial concentrations for TNT at beginning of optimization simulations.

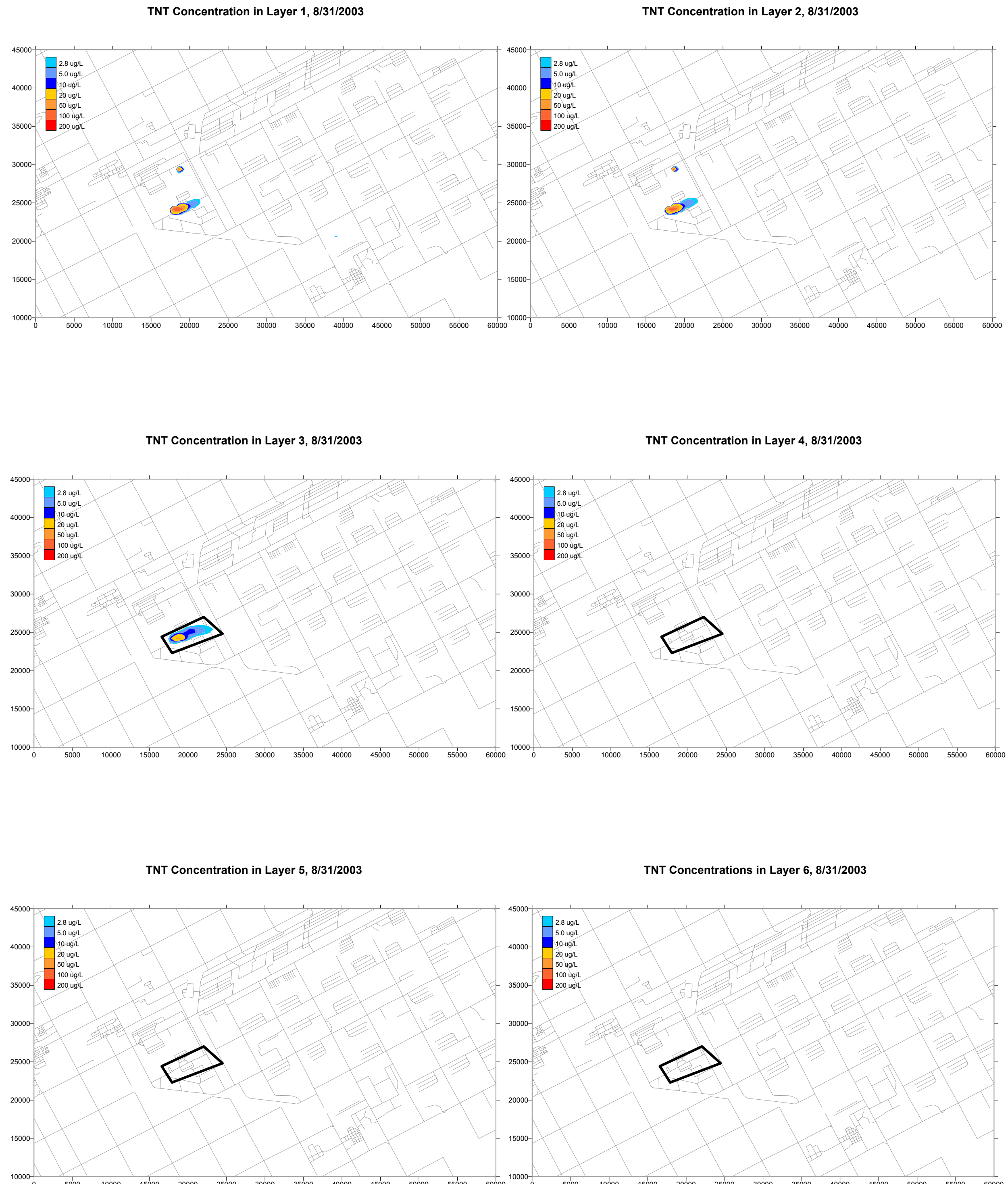


Figure 3. TCE concentrations, layer 3, Formulation 1 optimal solution

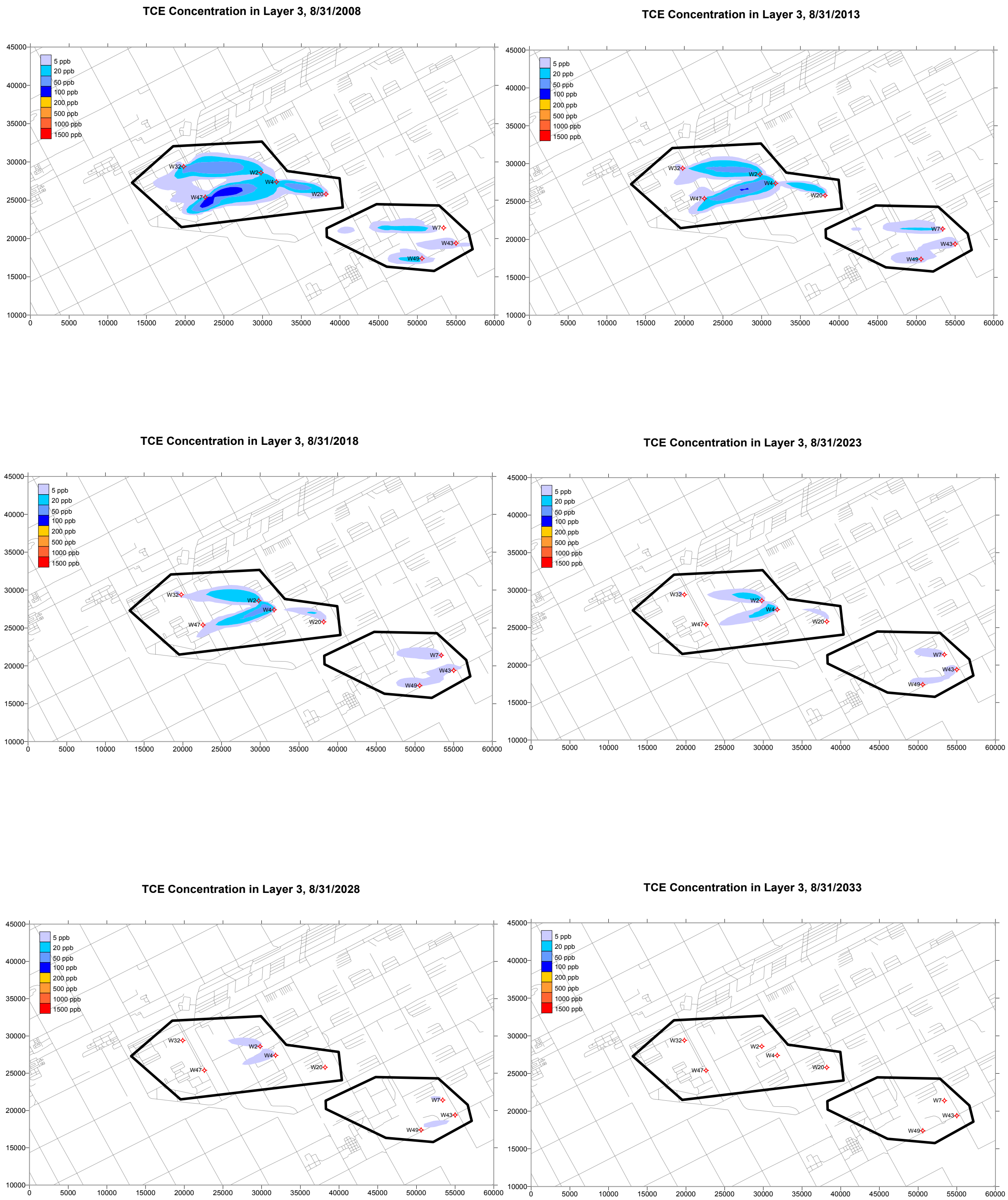


Figure 4. TCE concentrations, layer 4, Formulation 1 optimal solution

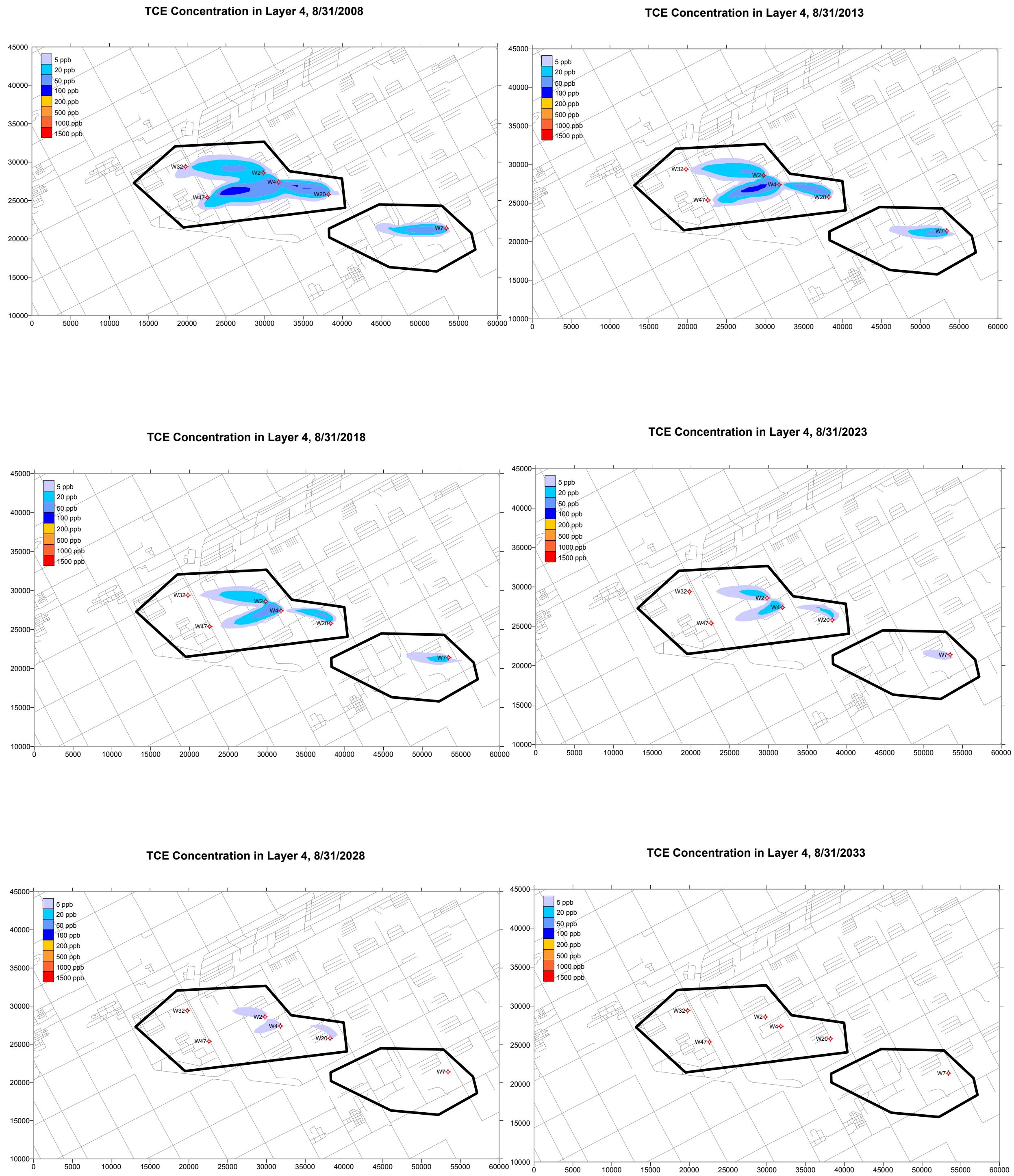


Figure 5. TCE concentrations, layer 5, Formulation 1 optimal solution

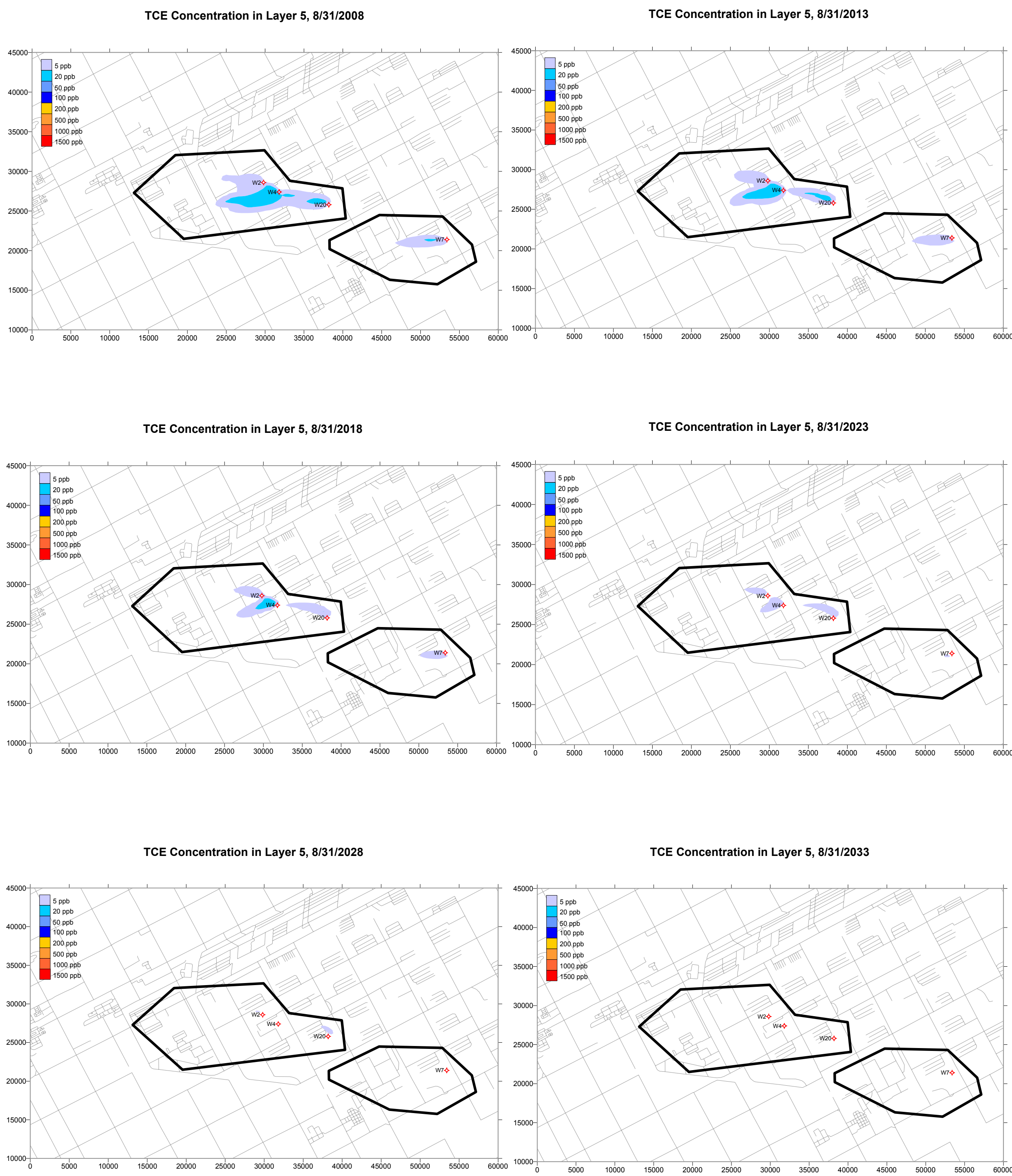


Figure 6. TNT concentrations, layer 3, Formulation 1 optimal solution

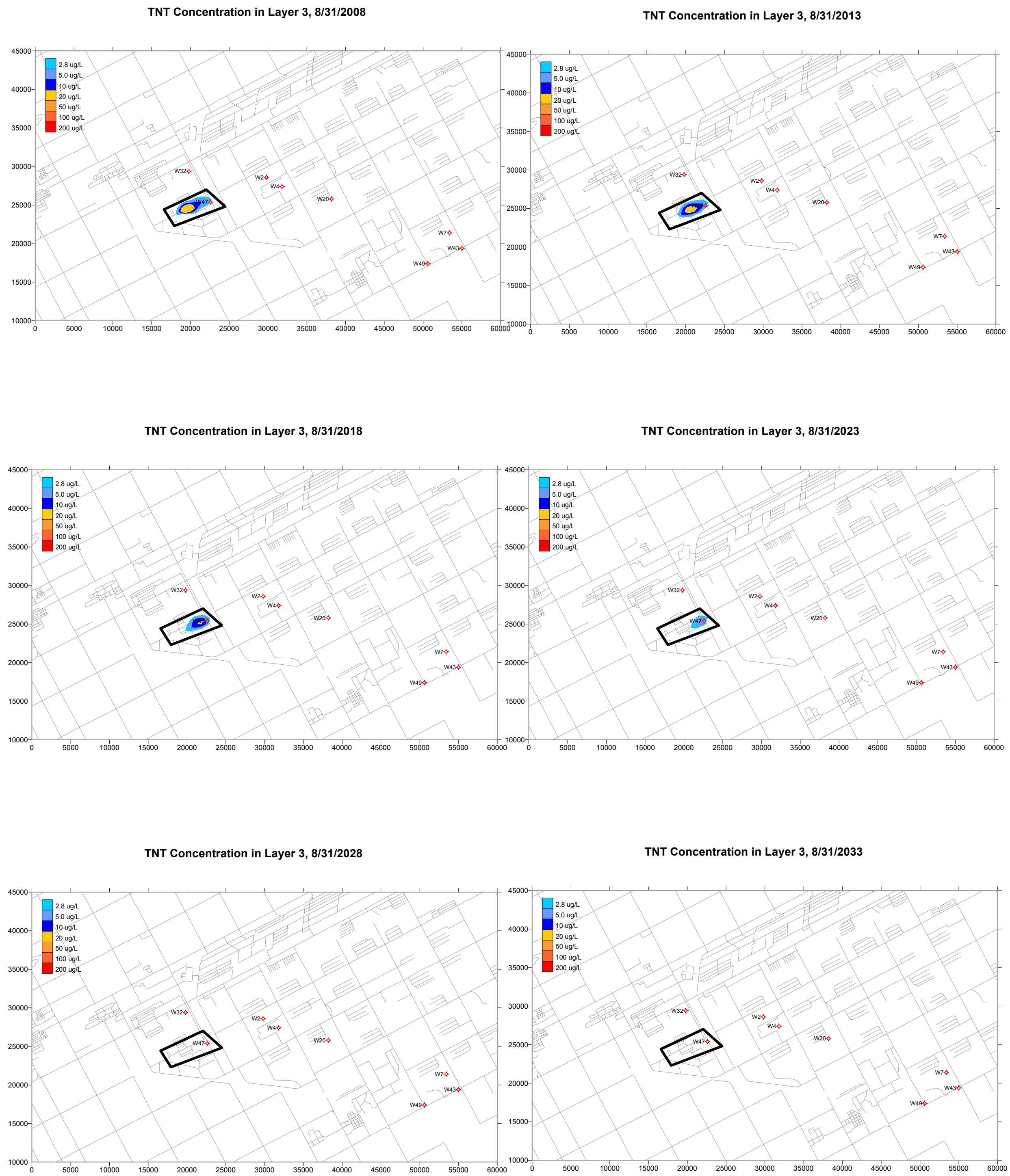


Figure 7. TNT concentrations, layer 4, Formulation 1 optimal solution

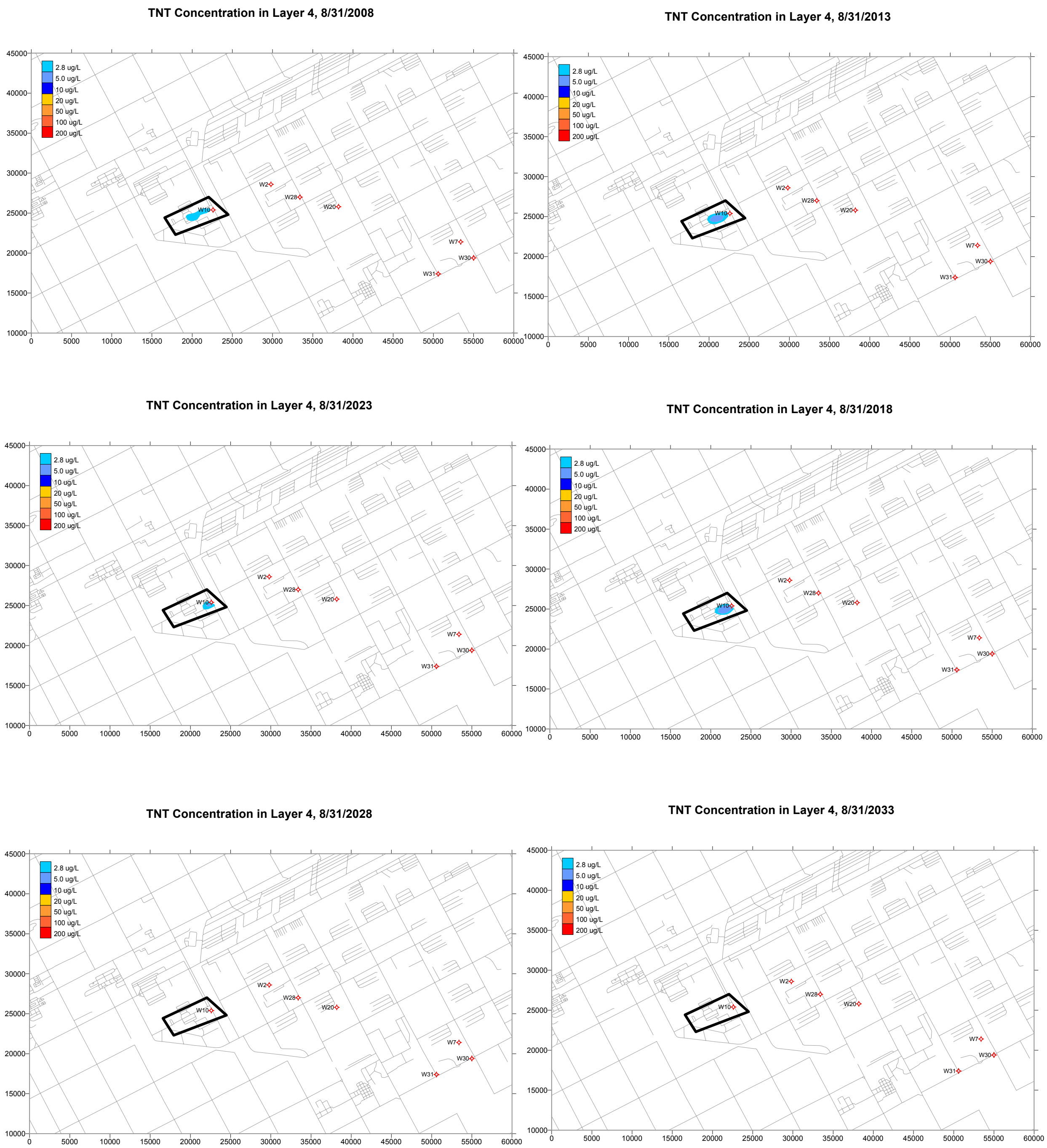


Figure 8. Objective function value by major run, Formulation 1

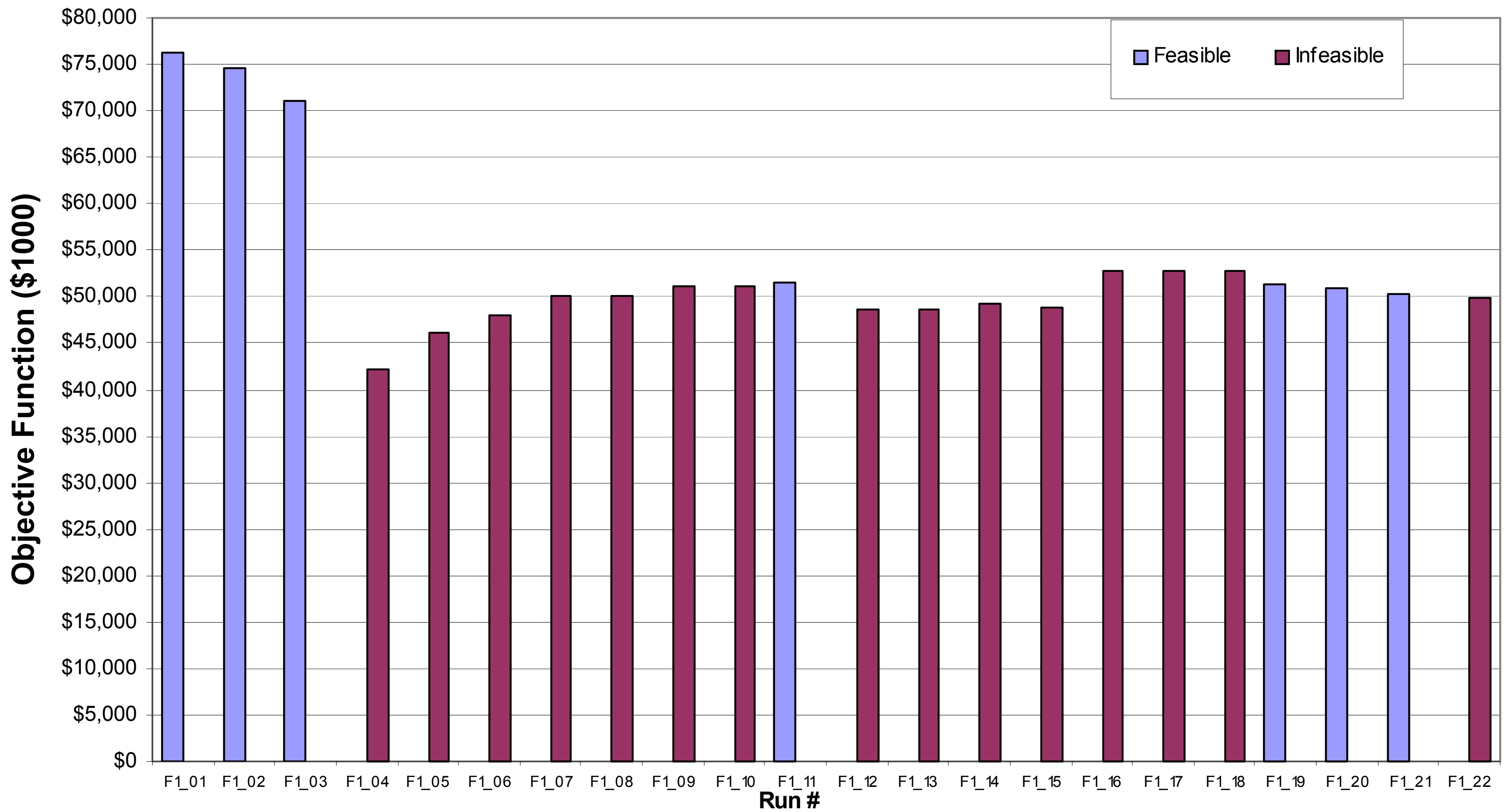
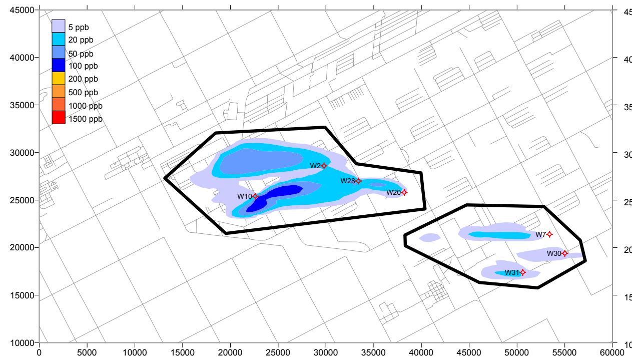
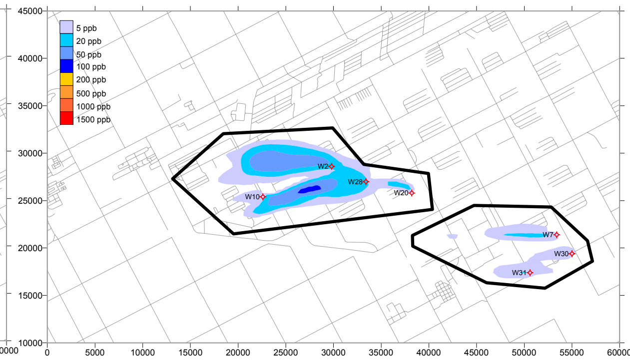


Figure 9. TCE concentrations, layer 3, Formulation 3 optimal solution

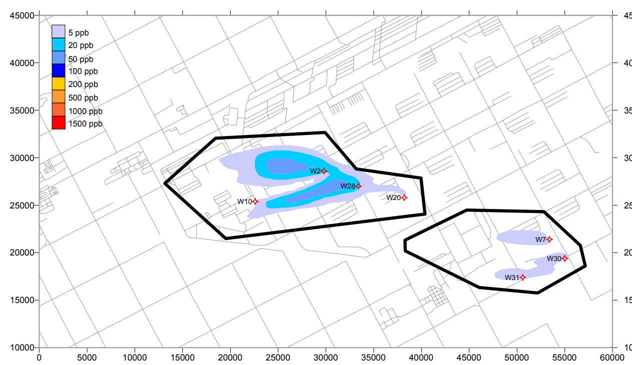
TCE Concentration in Layer 3, 8/31/2008



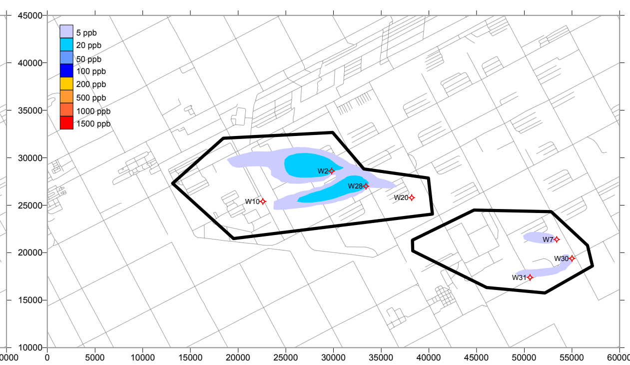
TCE Concentration in Layer 3, 8/31/2013



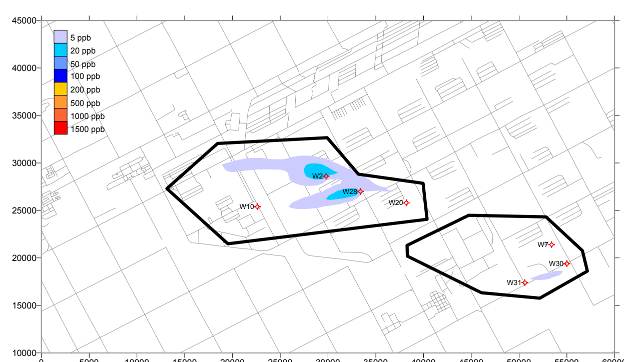
TCE Concentration in Layer 3, 8/31/2018



TCE Concentration in Layer 3, 8/31/2023



TCE Concentration in Layer 3, 8/31/2028



TCE Concentration in Layer 3, 8/31/2033

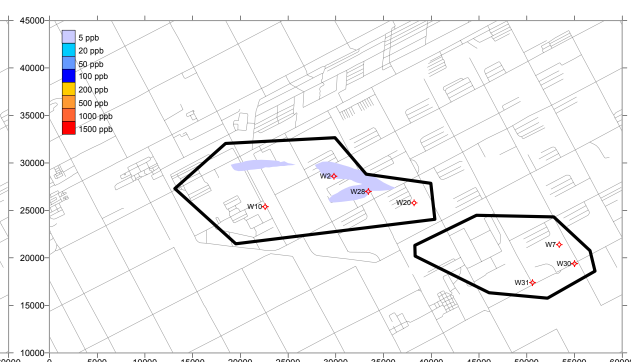


Figure 10. TCE concentrations, layer 4, Formulation 3 optimal solution

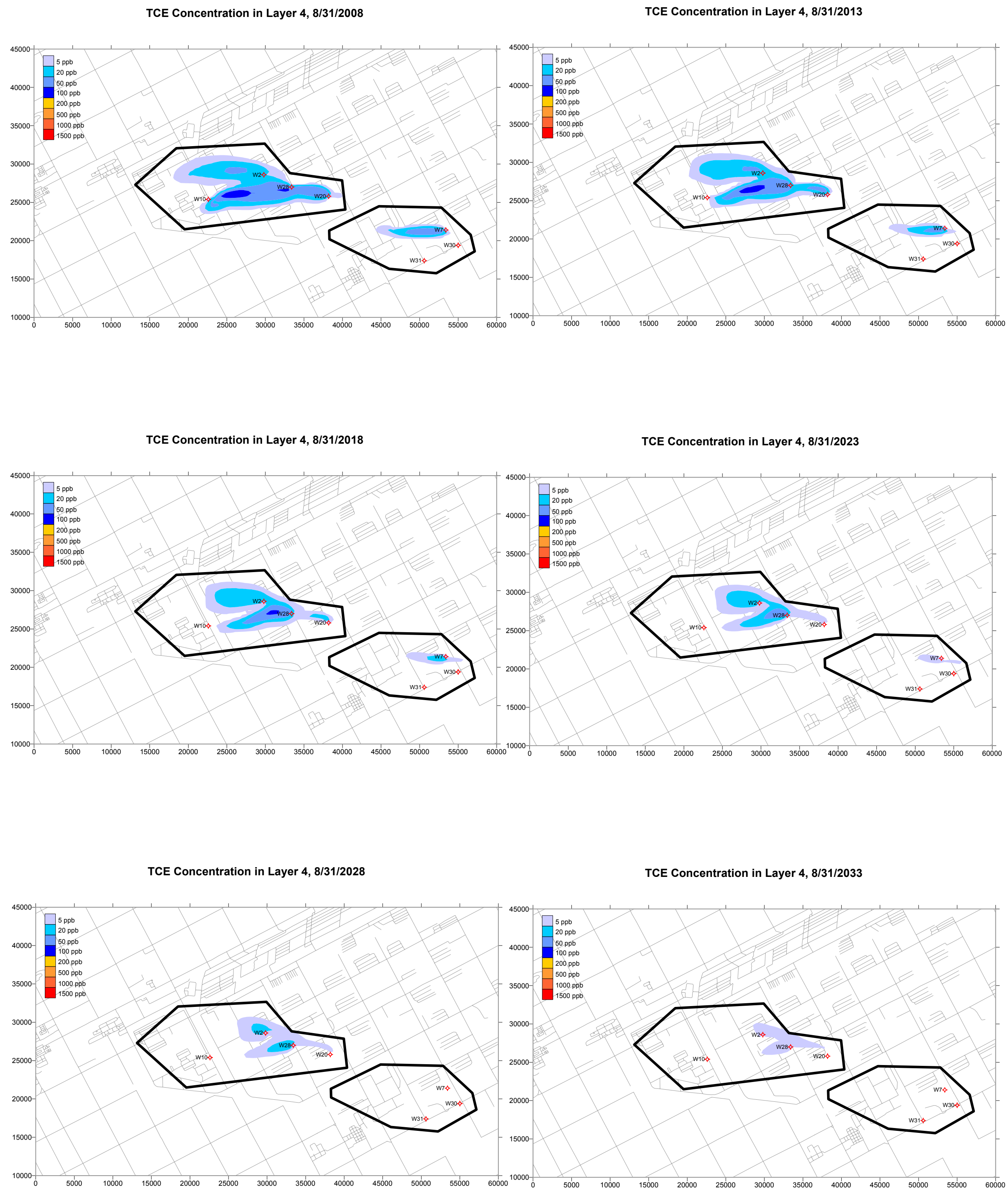


Figure 11. TCE concentrations, layer 5, Formulation 3 optimal solution

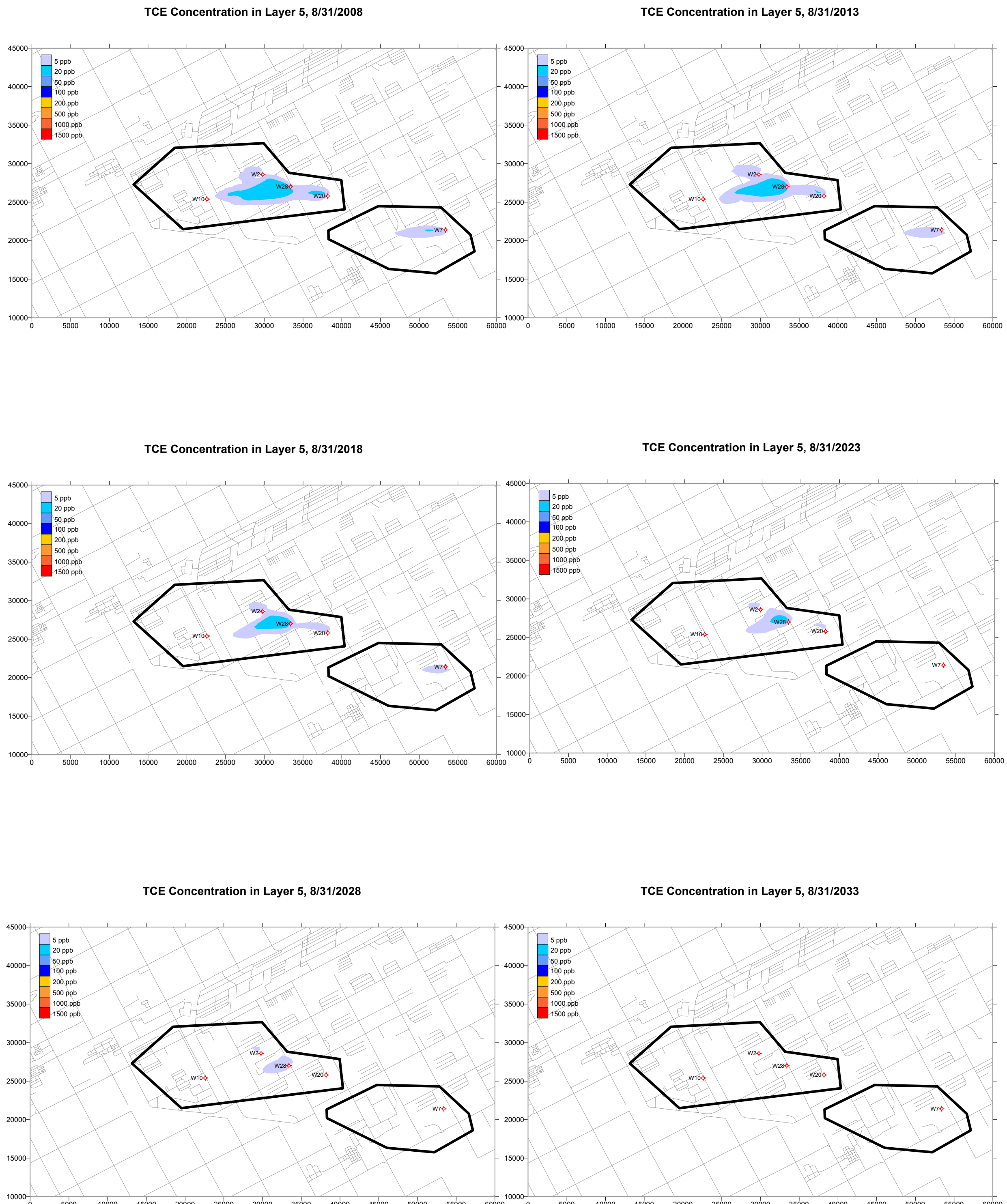


Figure 12. TNT concentrations, layer 3, Formulation 3 optimal solution

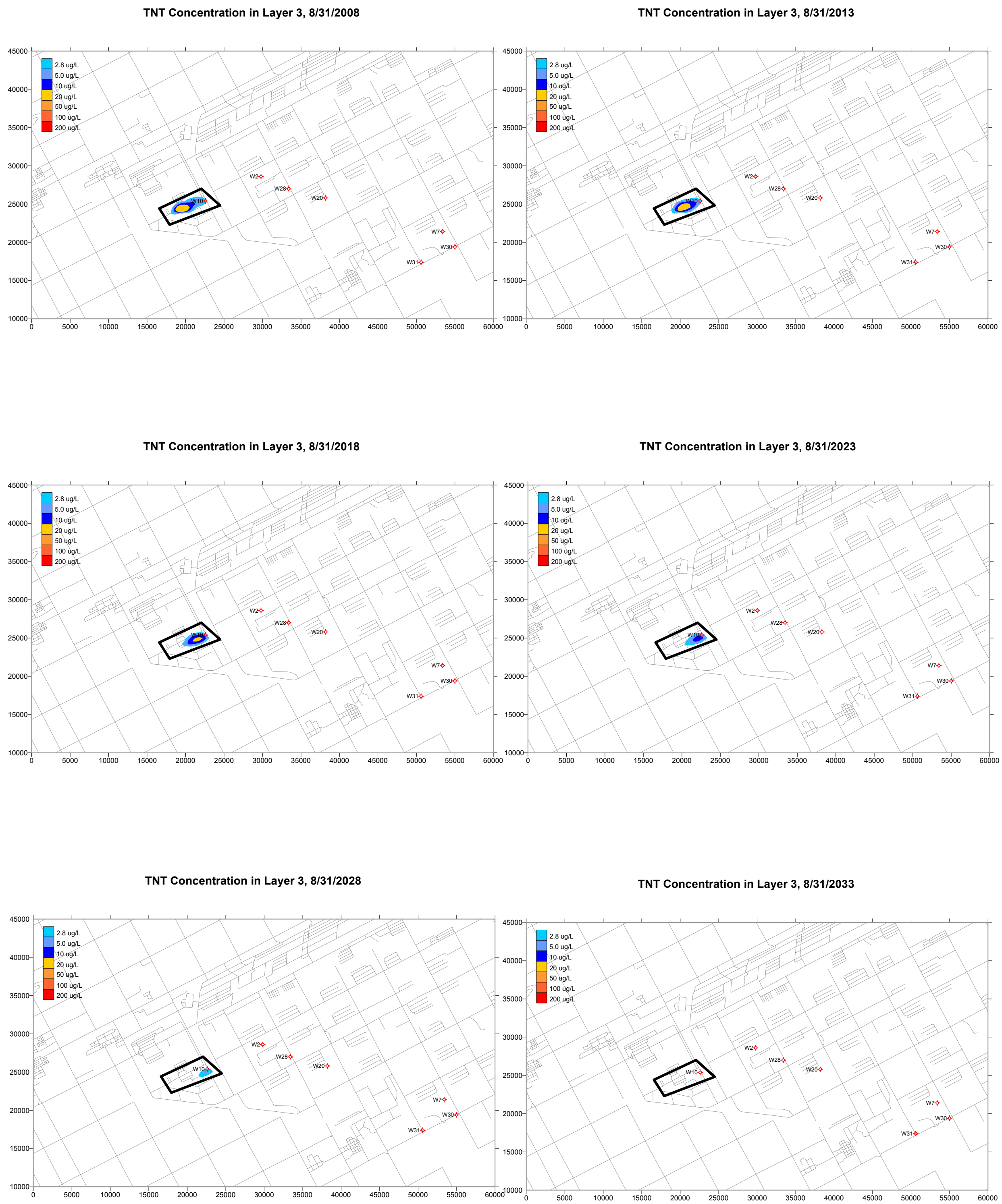


Figure 13. TNT concentrations, layer 4, Formulation 3 optimal solution

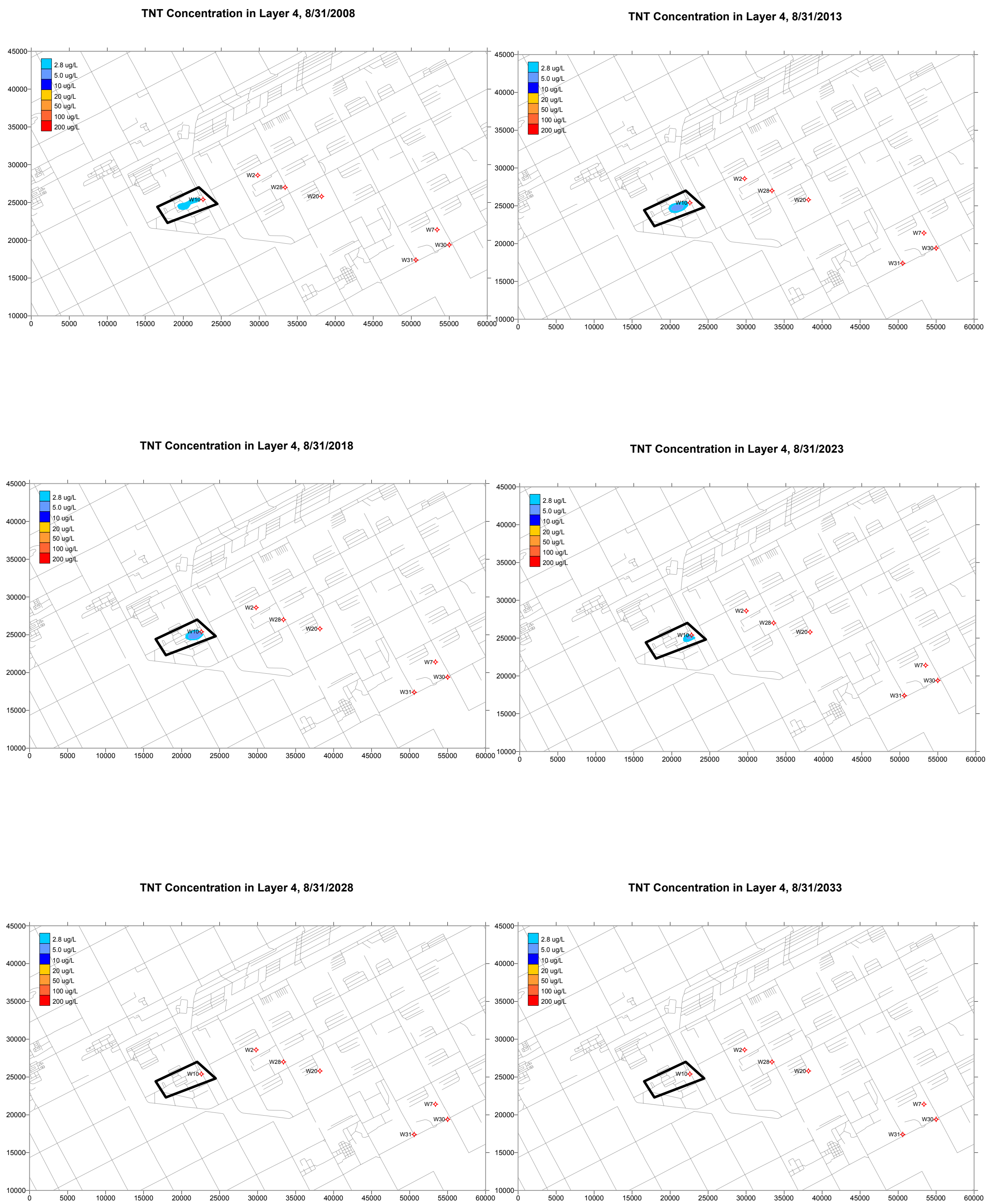
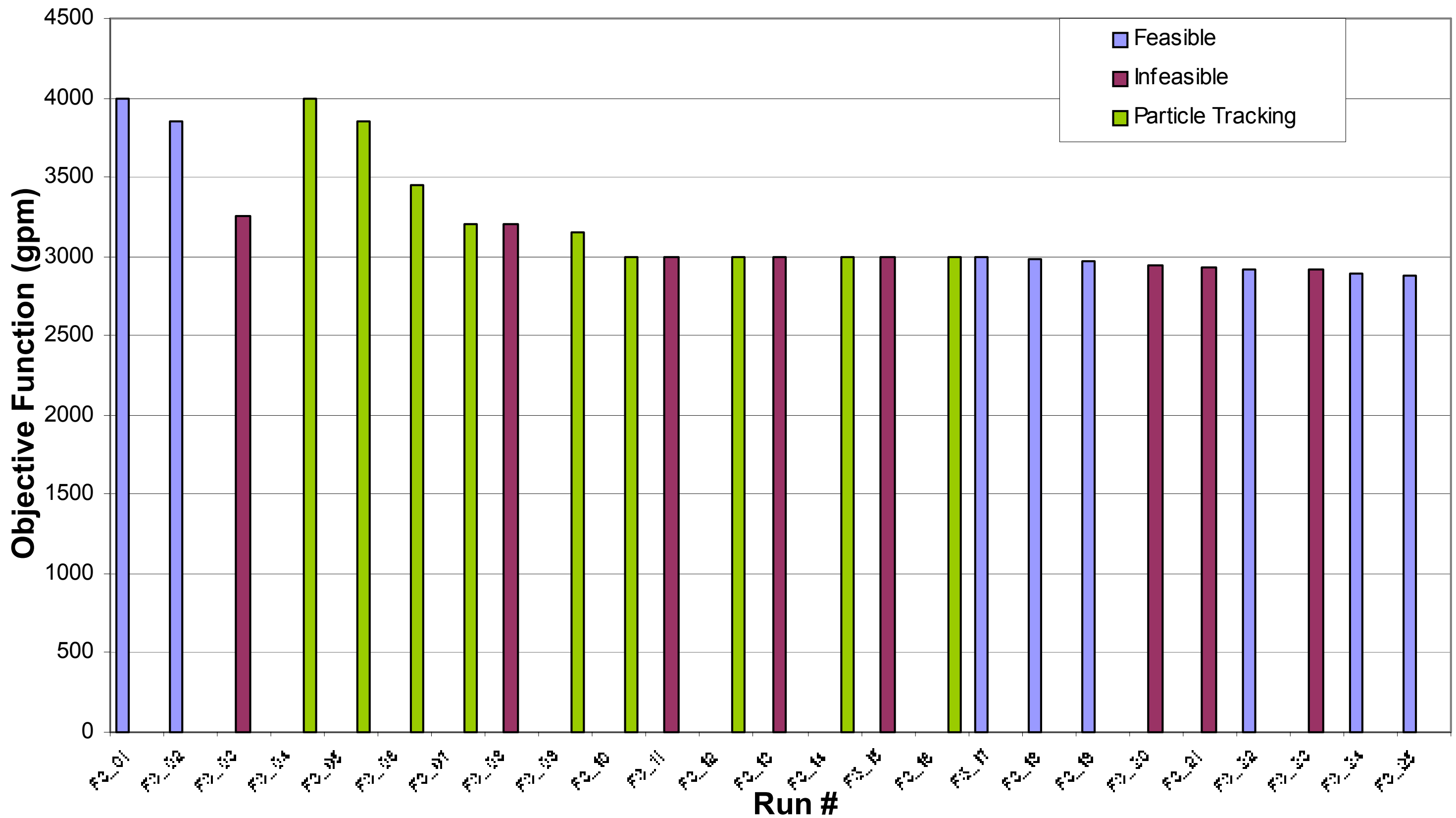


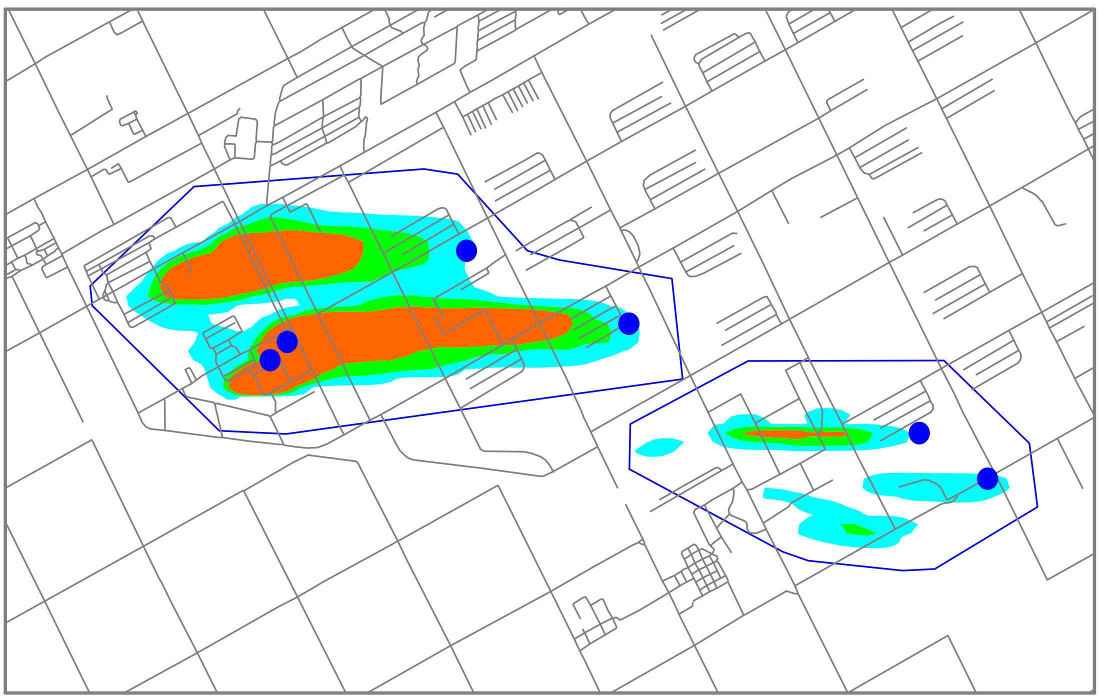
Figure 14. Objective function value by major run, Formulation 3



UA Report on Blaine

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

Chunmiao Zheng and Patrick Wang
The University of Alabama



The Hydrogeology Group
The University of Alabama

Technical Report
September 2002
Revised 2/2003

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

Chunmiao Zheng and Patrick Wang
University of Alabama

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 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 a 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:

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

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:

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

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:

<u>For Tabu Search (TS)</u>

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 (K	I	J)	P1 2003-2008	P2 2013	P3 2018	P4 2023	P5 2028	P6 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**

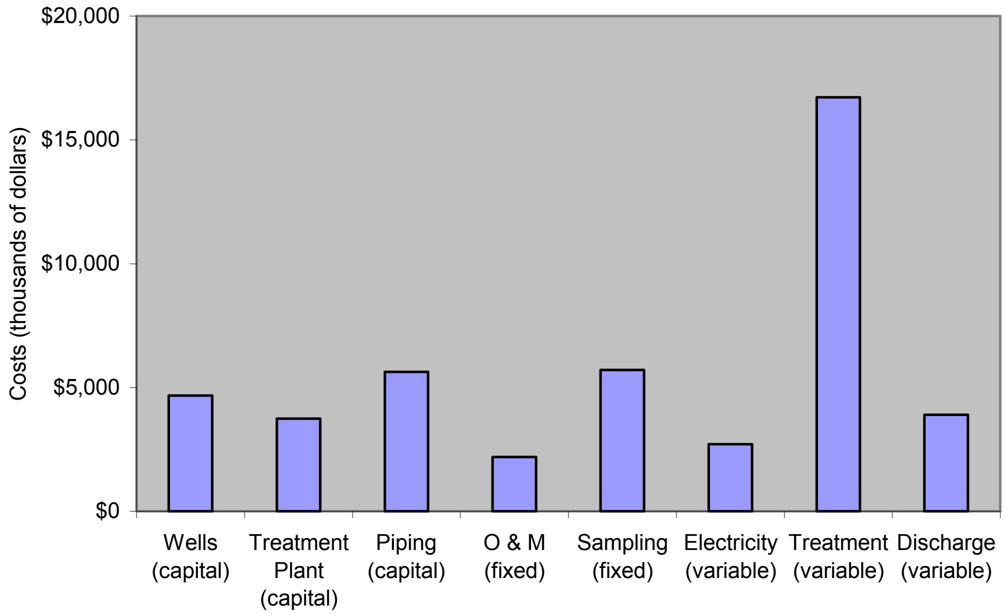


Figure 2.1. Breakdown of cost terms for the pumping strategy developed for Formulation 1.

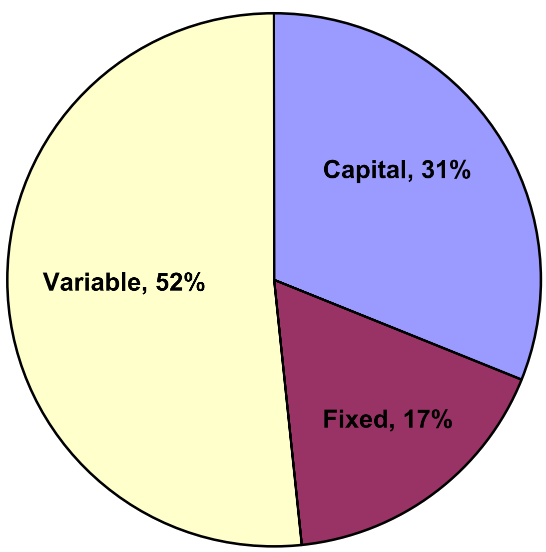
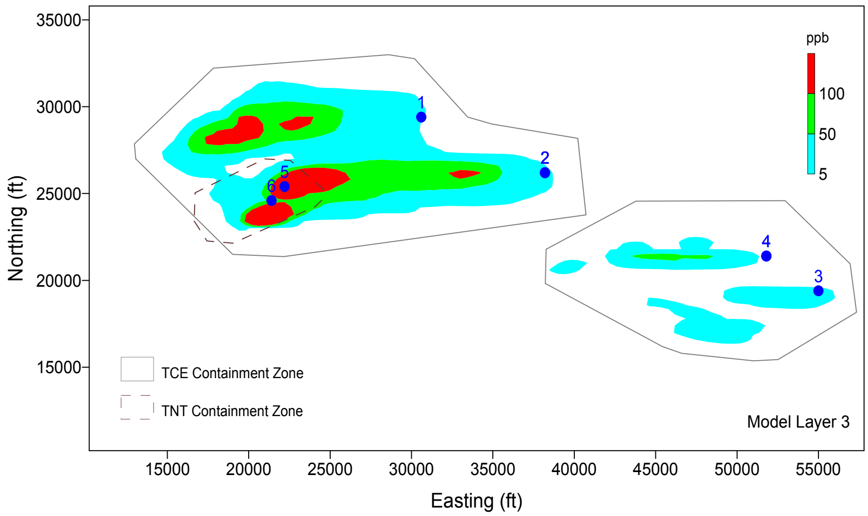
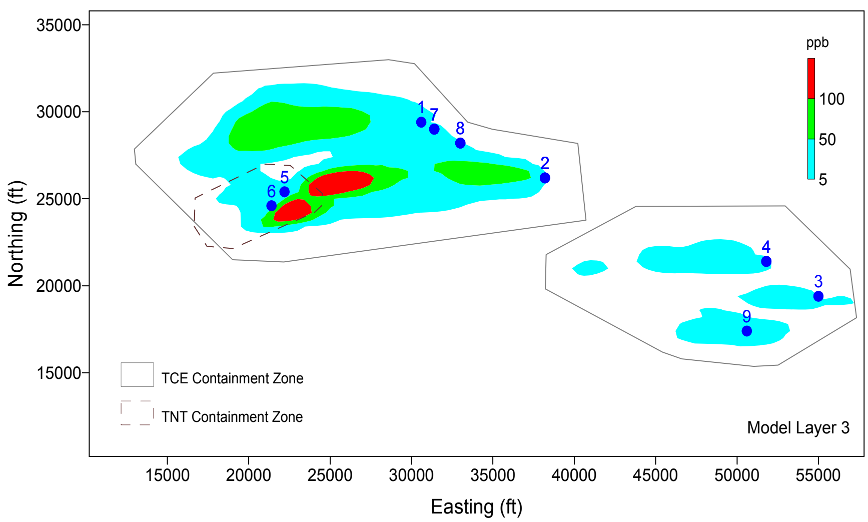


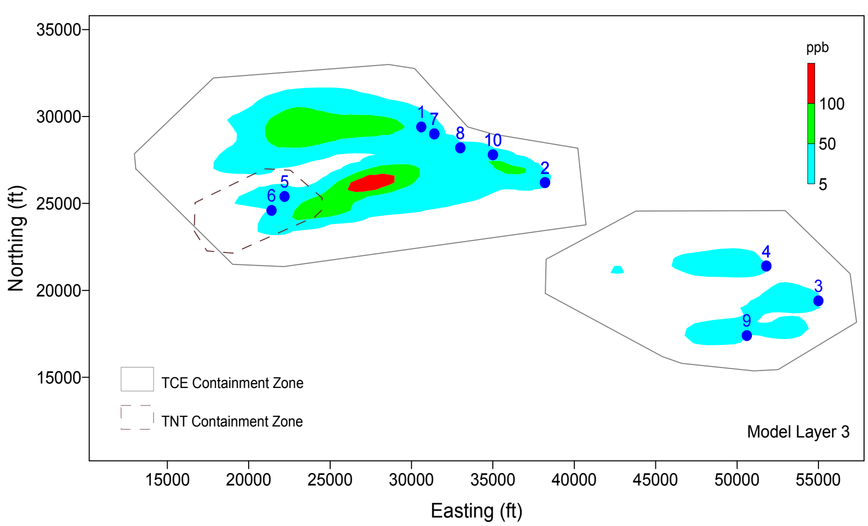
Figure 2.2. Distribution of three major cost categories for the optimal solution of Formulation 1.



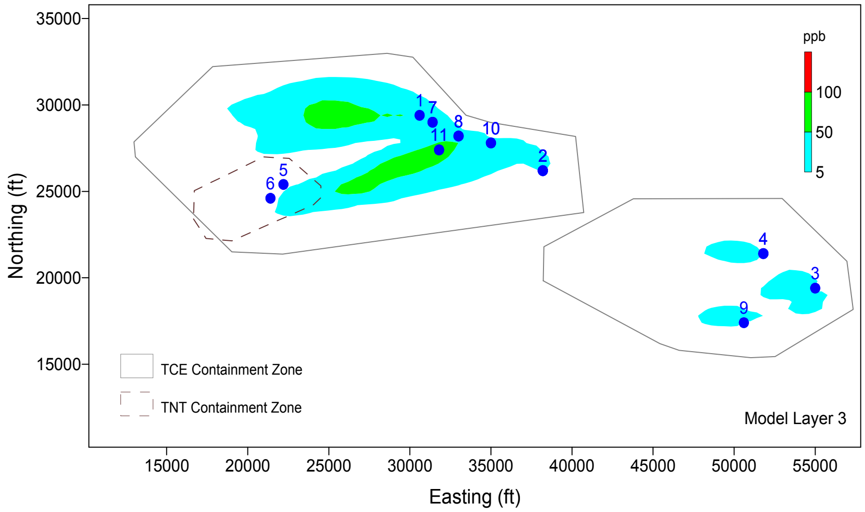
(a) Management period 1 (2003-08)



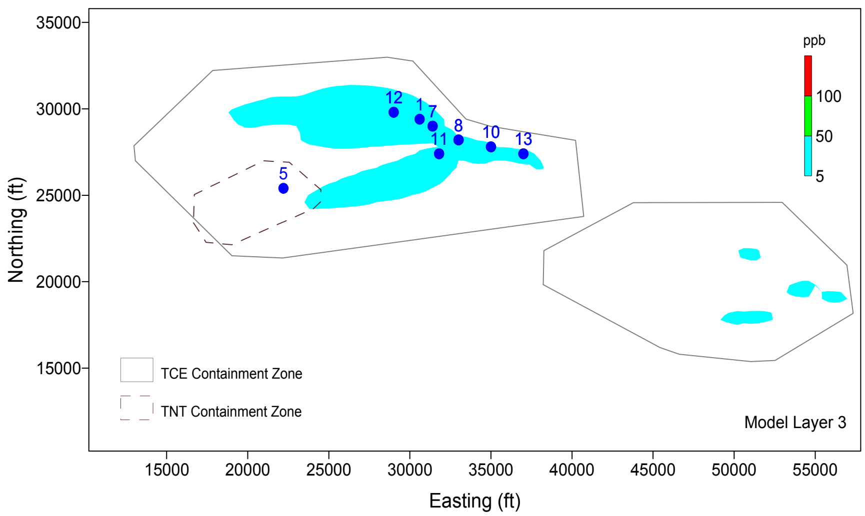
(b) Management period 2 (2008-13)



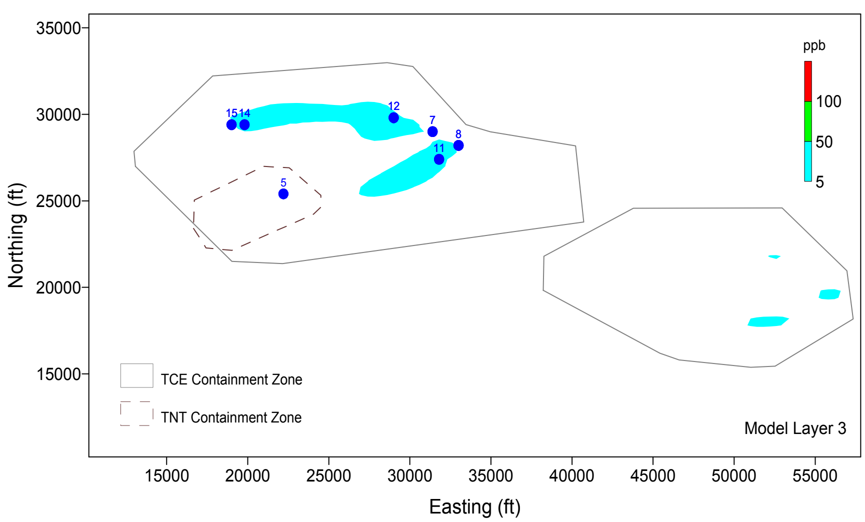
(c) Management period 3 (2013-18)



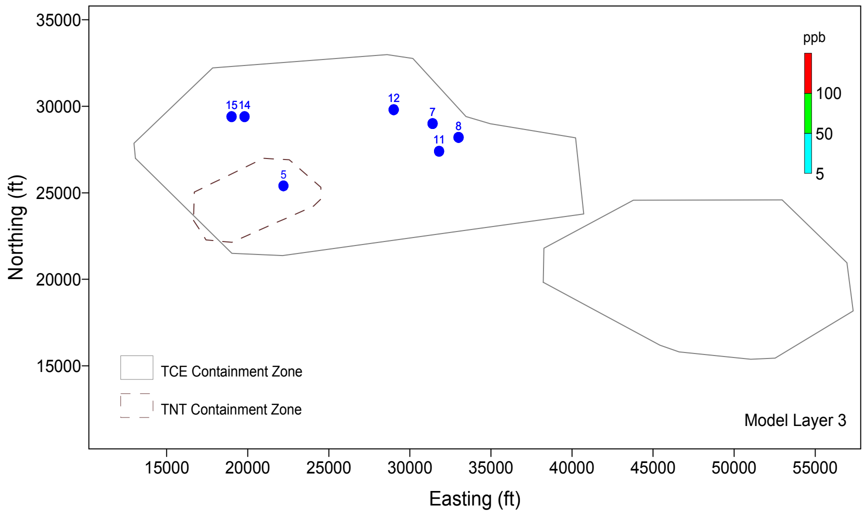
(d) Management period 4 (2018-23)



(e) Management period 5 (2023-28)

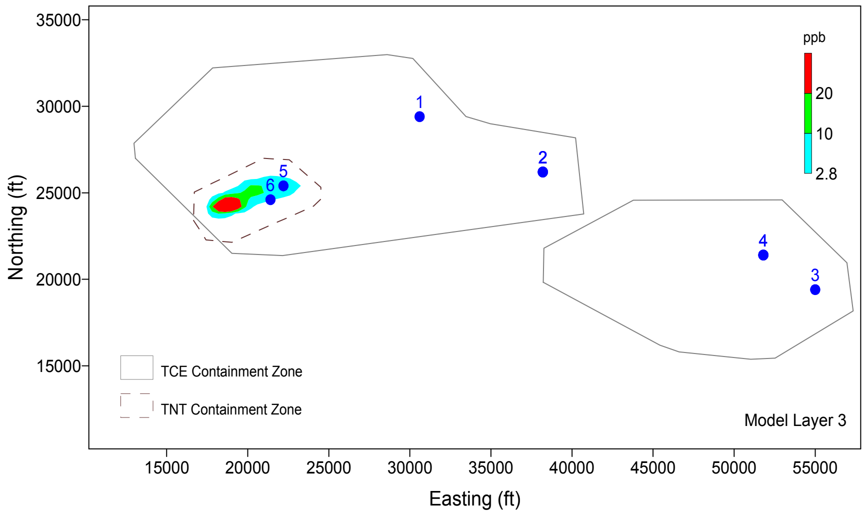


(f) Management period 6 (2028-2033)

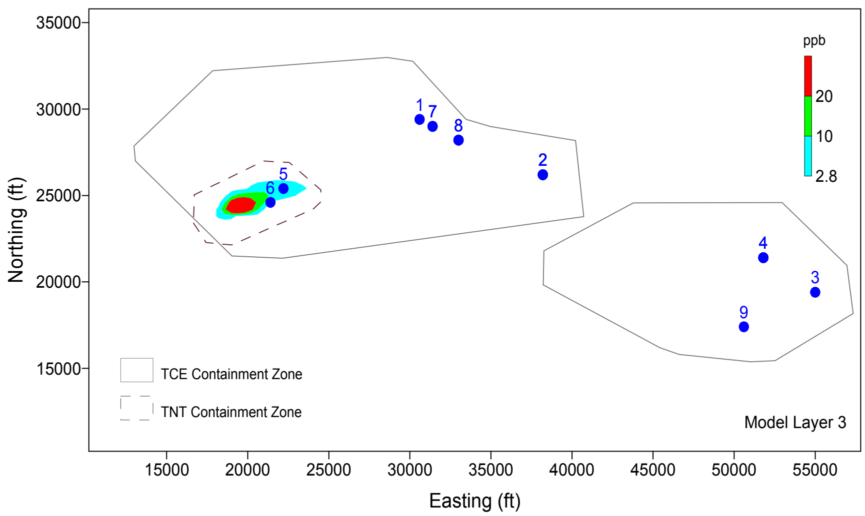


(g) End of the project horizon (2033)

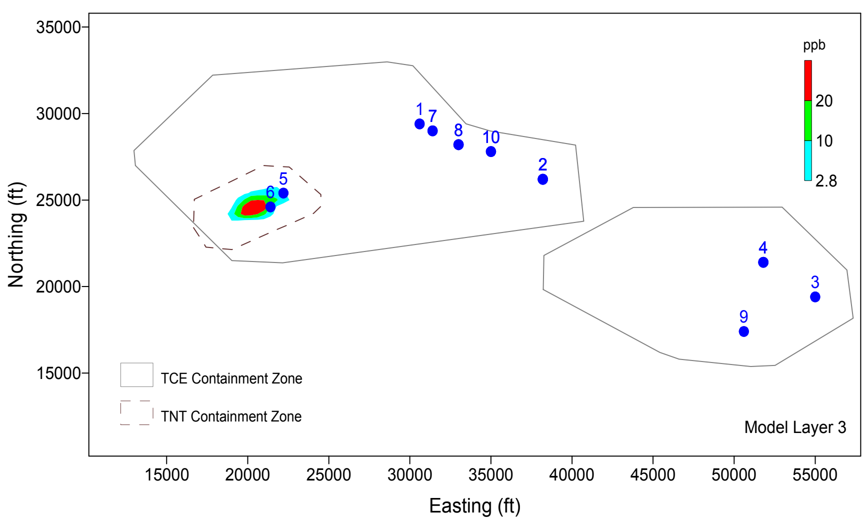
Figure 2.3. Calculated TCE plumes in model layer 3 at the start of six management periods (a) –(f) and at the end of the 30-year project horizon (g). The dots indicate the locations of pumping wells that are active during the management period in which the wells are shown.



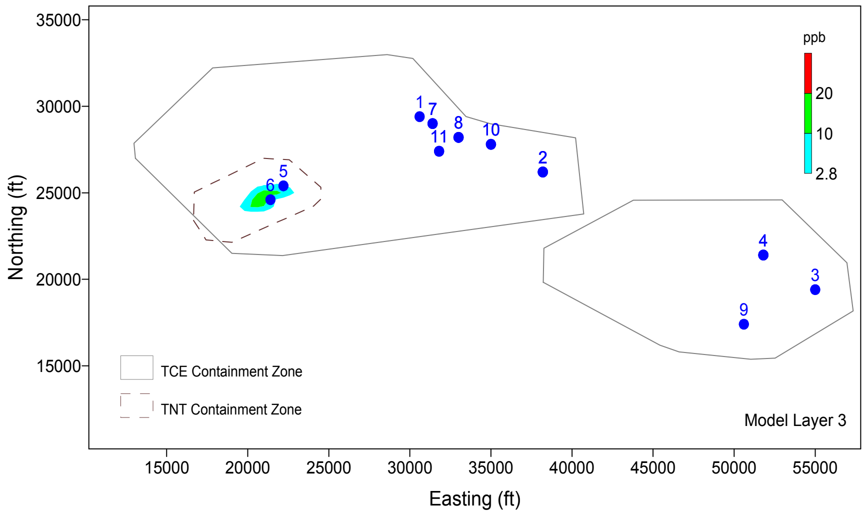
(a) Management period 1 (2003-08)



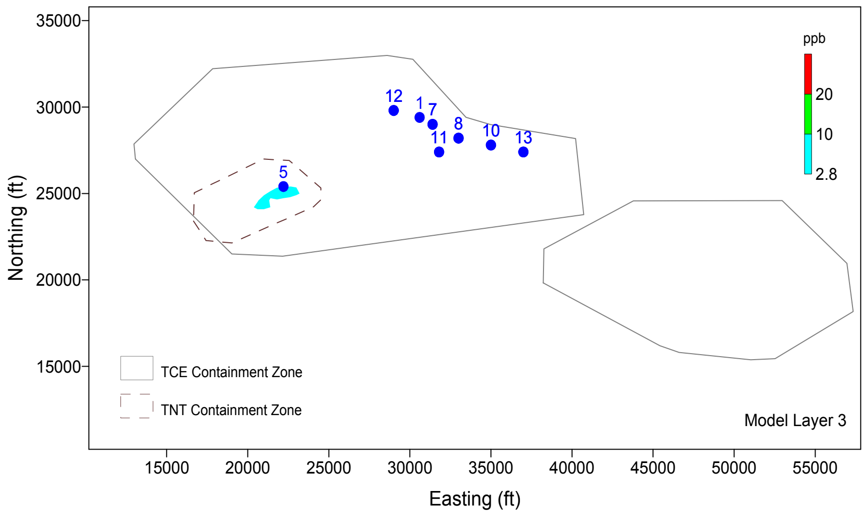
(b) Management period 2 (2008-13)



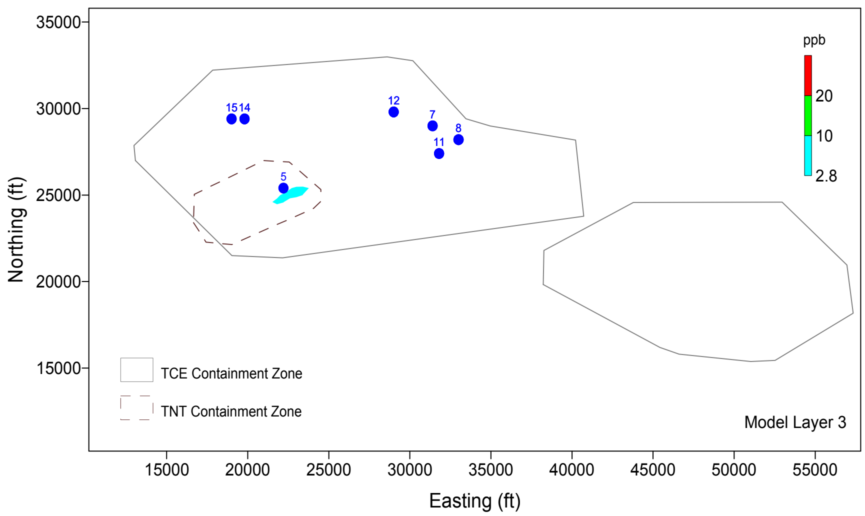
(c) Management period 3 (2013-18)



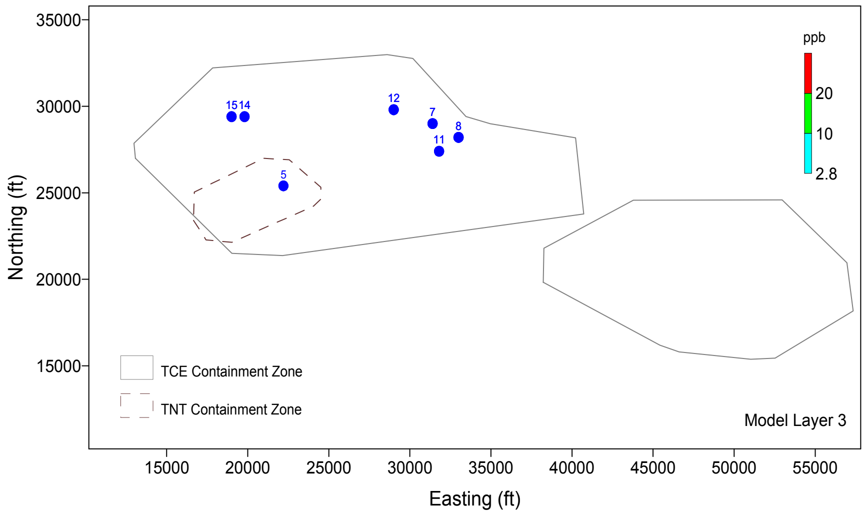
(d) Management period 4 (2018-23)



(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).

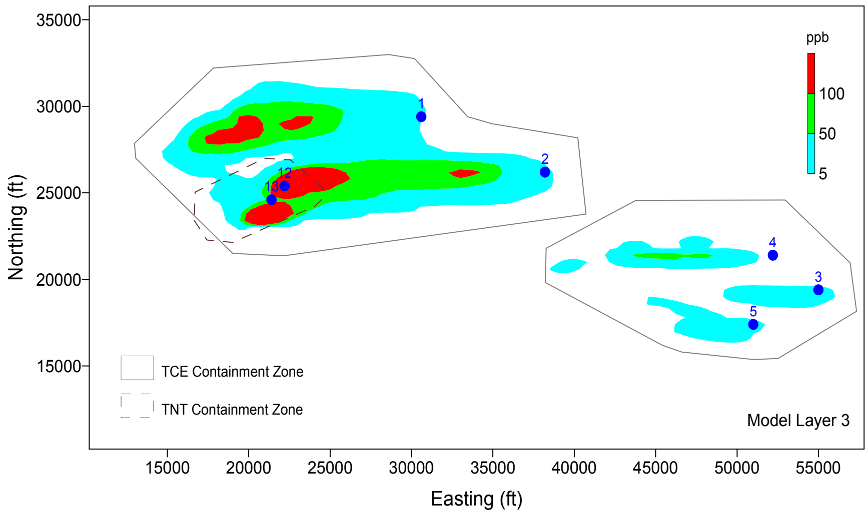
4.3 OPTIMAL SOLUTION

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.

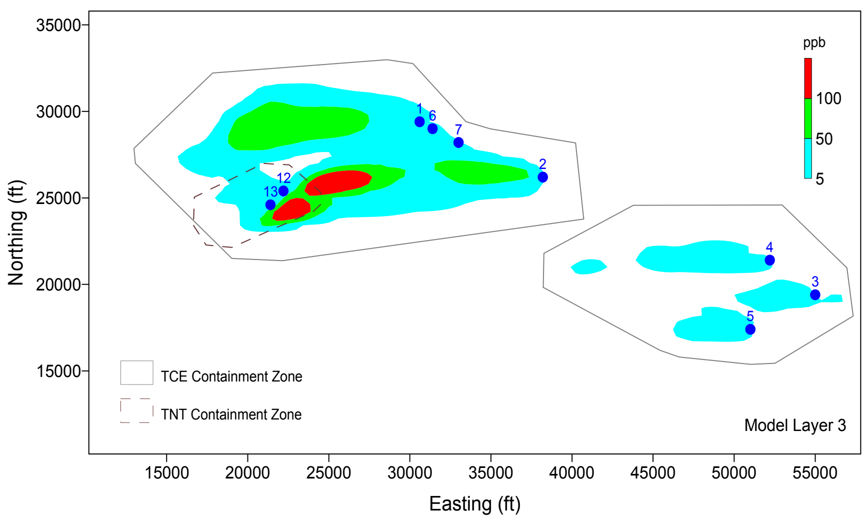
Figures 4.1(a) – (g) show the TCE plumes in model layer 3 and locations of active pumping wells at the start or end of each management period. Figures 4.2(a) – (g) show the same illustrations for TNT plumes. It can be seen that the containment constraints are satisfied at the end of each management period (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.

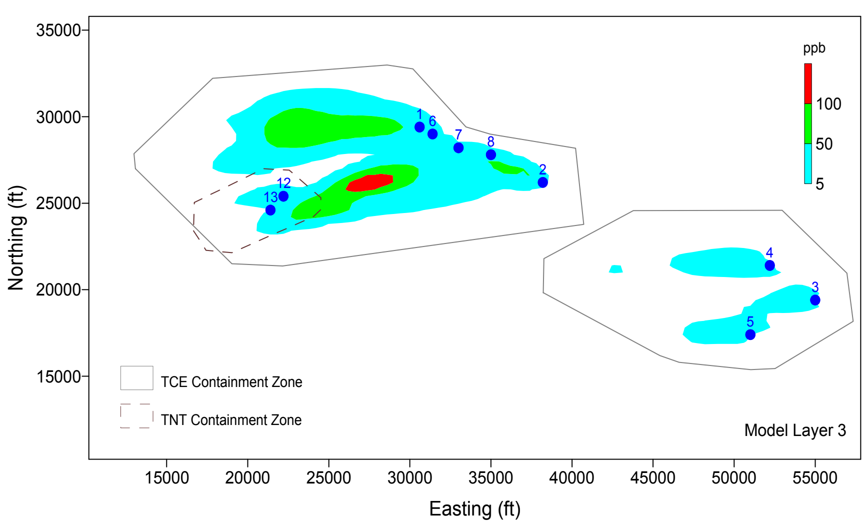
Well ID	Location (K	I	J)	P1 2003-2008	P2 2013	P3 2018	P4 2023	P5 2028	P6 2033
1	3	27	59	-350	-15	-50			-95
2	3	35	78	-290	-170	-180	-200	-310	-120
	4	35	78	-290	-170	-180	-200	-310	-120
	5	35	78	-290	-170	-180	-200	-310	-120
3	3	52	120	-290	-240	-265	-350		
4	3	47	113	-320	-195	-165	-230		
	4	47	113	-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**



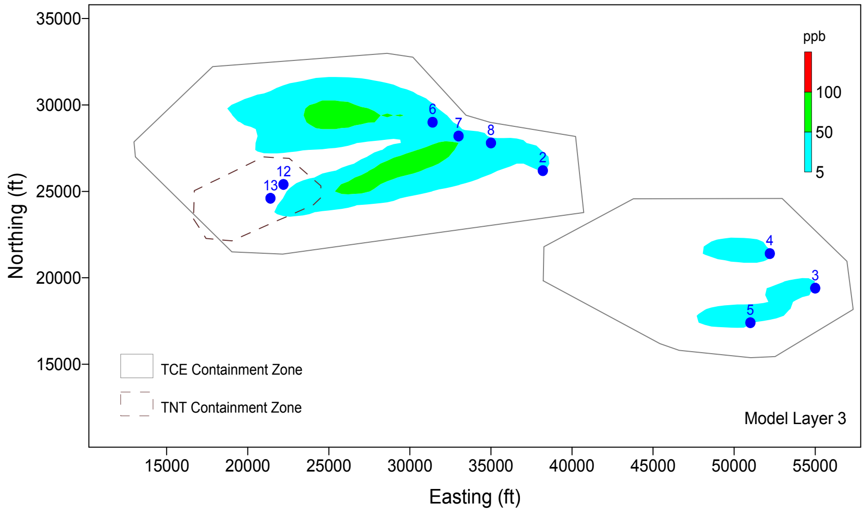
(a) Management period 1 (2003-08)



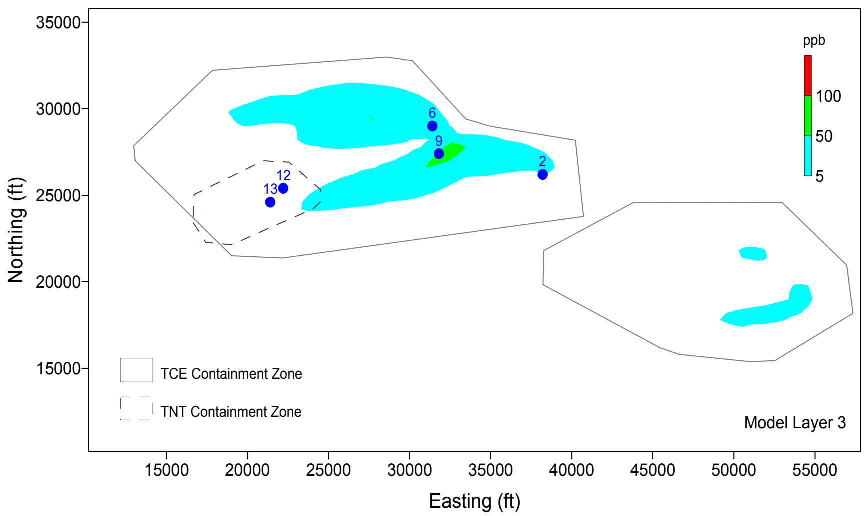
(b) Management period 2 (2008-13)



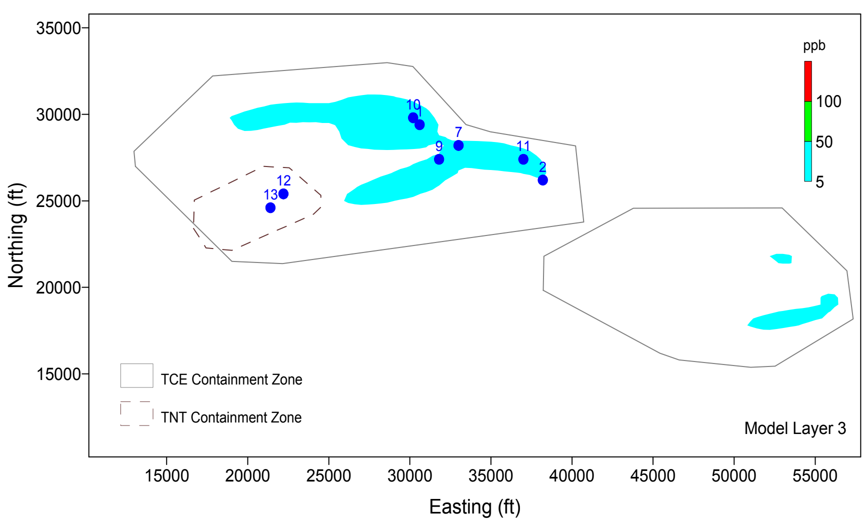
(c) Management period 3 (2013-18)



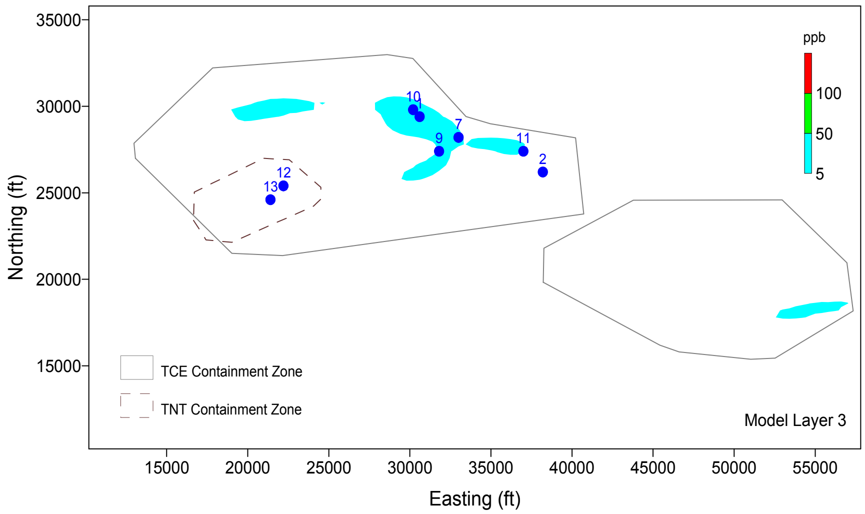
(d) Management period 4 (2018-23)



(e) Management period 5 (2023-28)

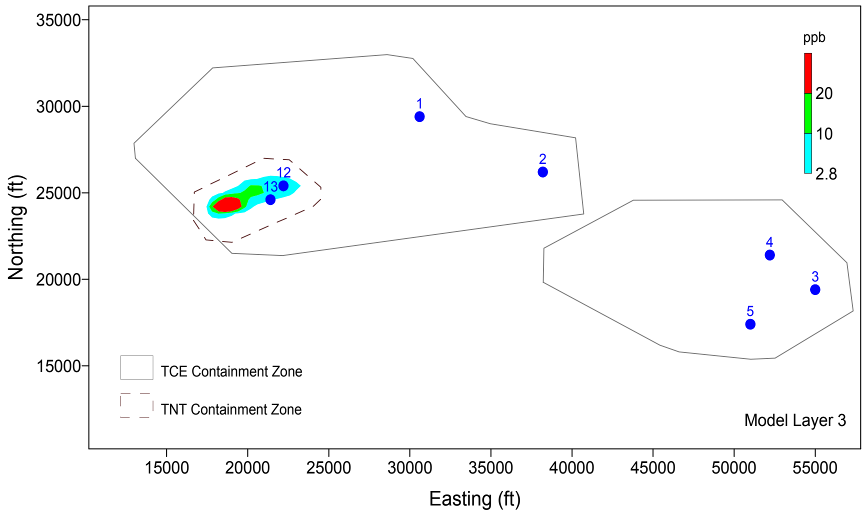


(f) Management period 6 (2028-2033)

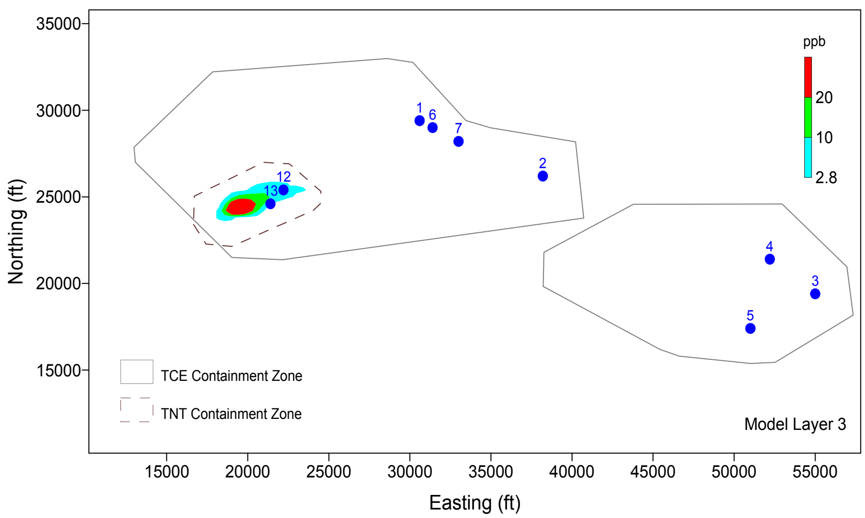


(g) End of the project horizon (2033)

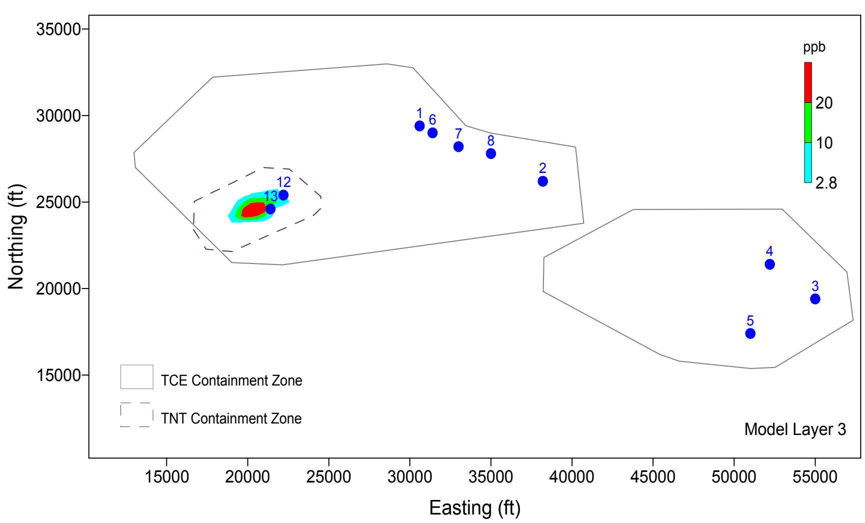
Figure 4.1. Calculated TCE plumes in model layer 3 at the start of six management periods (a) –(f) and at the end of the 30-year project horizon (g). The dots indicate the locations of pumping wells that are active during the management period in which the wells are shown.



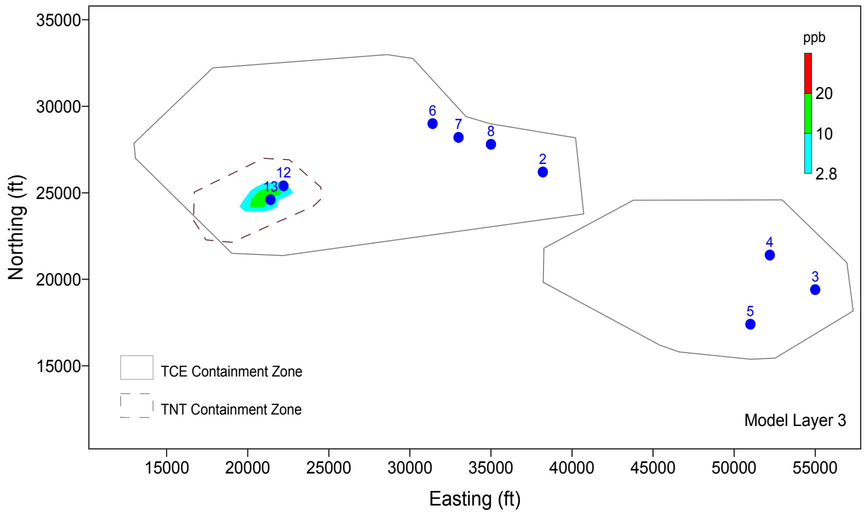
(a) Management period 1 (2003-08)



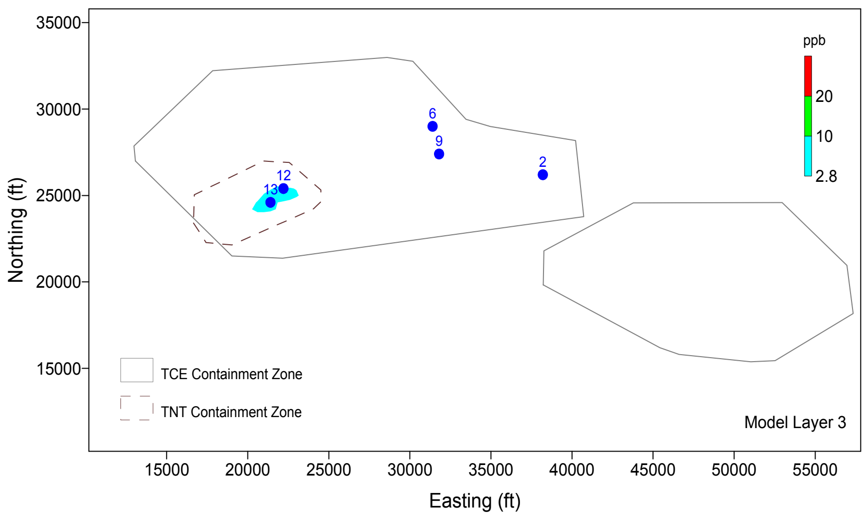
(b) Management period 2 (2008-13)



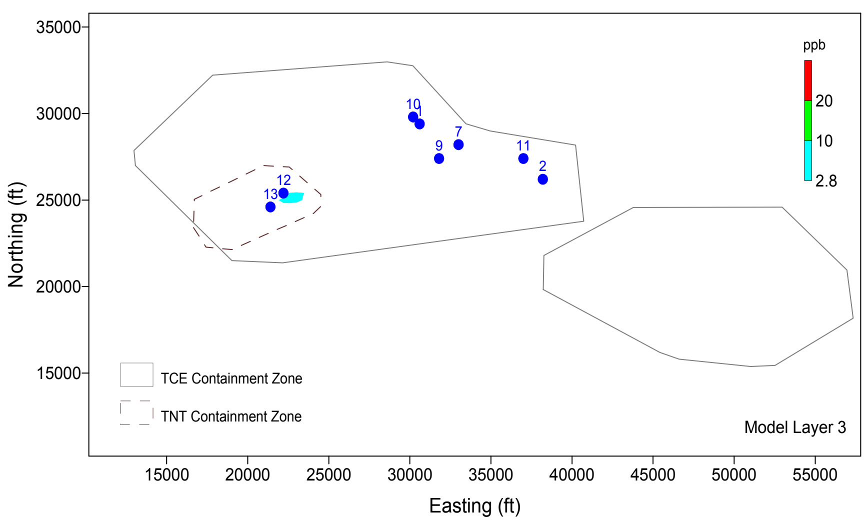
(c) Management period 3 (2013-2018)



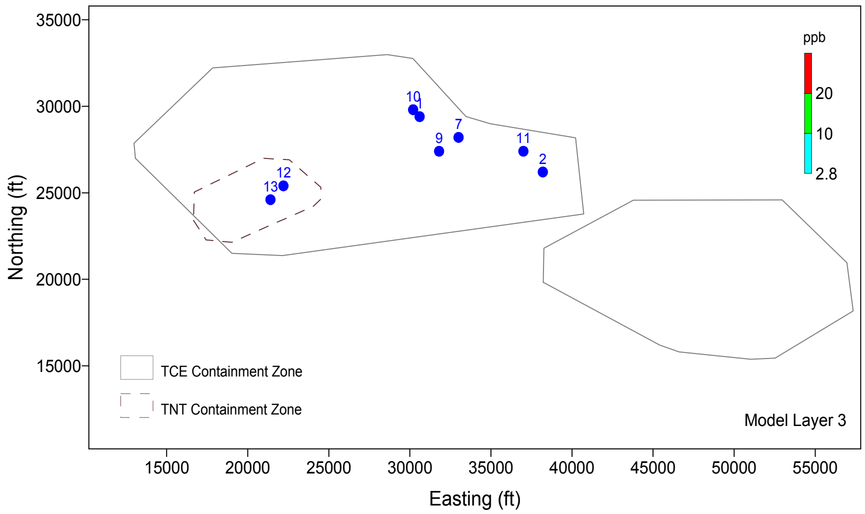
(d) Management period 4 (2018-23)



(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

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USU Report on Blaine

FINAL

OPTIMAL PUMPING STRATEGIES FOR TCE AND TNT PLUMES AT BLAINE NAVAL AMMUNITION DEPOT, HASTINGS, NEBRASKA

Presented to

Navy Facilities Engineering Command
NAVFACENGCOMDET-SLC

Per

Contract No. N47408-00-C-7153

Prepared by

Systems Simulation/Optimization Laboratory
Dept. of Biological and Irrigation Engineering
Bldg EC-216
Utah State University
Logan, UT 84322-4105

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APPENDICES

Executive Summary

We present optimal pumping strategies to address TCE and TNT plumes at Blaine Naval Ammunition Depot (NAD). We provide strategies for three optimization problem formulations (Tables 1 and 2). Each strategy employs multiple five-year management periods (MPs). Each MP consists of 10 periods of time-varying background pumping, two per year. We completed these designs by the September 16 deadline. Per our contract, we performed some additional work on September 17, which is before a second deadline—the date of formally presenting results. We identify that additional work when discussing it.

The Formulation 1 problem is to minimize the present value of containing TCE and TNT plumes, and reducing them to cleanup levels (CLs) within thirty years. CLs are 5.0 ppb for TCE and 2.8 ppb for TNT. Presented Strategy USU1 costs $40.82M. Pumping rates gradually increase with time. USU1 requires constructing ten extraction wells -- 8 wells in the first management period (MP1), and two wells in period five (MP5). Of the ten wells, seven are in the northwestern contamination area and three are in the southeastern area. USU1 achieves CLs at year 30 for TCE and year 29 for TNT. Strategies that achieved cleanup within 20 years or less cost more than USU1, because they required more wells and higher pumping rates. The same is true for Formulation 2 strategies.

The Formulation 2 optimization problem is the same as Formulation 1, except that 2400 gpm of extracted water will not require treatment. Therefore, the cost will be less. Strategy USU2 is the same as USU1, and costs $18.88M.

The Formulation 3 goal is to minimize the maximum MP total pumping rate needed to contain all water contaminated at values exceeding the CLs. Containment must be achieved for 30 years. By the first deadline (September 16) USU developed strategy USU3A. USU3A satisfies Formulation 3 constraints, has time-varying pumping rates with a 2139 gpm maximum. The next day that strategy improved to 2123 gpm (termed strategy USU3A').

During September 17 we also reported preliminary draft strategies for alternative formulations 3B' and 3C'. These differ from Formulation 3 in the size of the containment area. In essence, Formulation 3 uses precisely the containment constraints posed by NAD. Formulation 3B' reduces the size of the area within which the plumes are to be contained by one cell in all directions. Thus Formulation 3B' is a more restrictive or constrained problem than Formulation 3. Formulation 3C' is even more restrictive. It lets the plume expand by a maximum of one cell in any direction. Strategies USU3B' and USU3C' require successively more pumping than USU3A, but were not vigorously optimized. USU reported all strategies mentioned above in its first draft report (SSOL, 2002).

For optimization, we used our SOMOS (Simulation/Optimization Modeling System) software. Employed SOMOS heuristic optimization methods include genetic algorithm (GA) and simulated annealing (SA), augmented by tabu search (TS) procedures. We also used SOMOS' coupled GA and artificial neural networks (ANN). We used the different techniques for different situations in the project.

Introduction

Blaine Naval Ammunition Depot (NAD), in Hastings, Nebraska, has significant contamination of groundwater by volatile hydrocarbons. Figure 1 shows the finite difference grid of flow and transport simulation models of the contaminated aquifer. Figures 2-4 and Figure 5, respectively, show TCE and TNT plumes as they are simulated to exist in January 2003.

NAD posed three optimization problem formulations. Each formulation consists of an objective function and a set of bounds and constraints. The objective function is an equation, the value of which is to be minimized, while satisfying all posed constraints. The objective function equations are functions of pumping and well construction in time. Contractee personnel that will later evaluate any developed pumping strategies indicated that evaluation would only include consideration of how good the objective function value is, and whether constraints are satisfied. Therefore, for this site, USU did not significantly include other considerations in creating the optimal pumping strategies.

We developed optimal groundwater extraction strategies using our SOMOS simulation/optimization model (SSOL and HGS, 2002). Procedures utilized in this project include genetic algorithm (GA), simulated annealing (SA), tabu search (TS) and artificial neural networks (ANN). SOMOS GA and SA codes include TS internally. When GA and SA are referred to below, the included use of TS should be assumed. Others have described procedures for GA (Aly and Peralta, 1999), SA (Shieh and Peralta, 1997), TS (Glover and Laguna, 1997), and linked ANN and GA (Aly and Peralta, 1999). SSOL or Hydrogeosystems Group have used a linked ANN-GA in developing pump and treat strategies for several other sites, including Massachusetts Military Reservation (HGS, 2000). The current SOMOS ANN-GA utilizes an innovative moving subspace or spacetube approach (SSOL and HGS, 2002).

Optimization Techniques

Formulations Addressed

We present optimal pumping strategies for three optimization problems posed by NAD, Formulations 1-3, and modifications thereof. NAD-specified requirements of the strategy development process are:

- The 30-year planning period is discretized into 6 five-year management periods (MPs), and 60 simulation model stress periods. There are two unequal stress periods (SPs) per year, corresponding to irrigation and non-irrigation seasons.
- Input data includes 60 SPs of time varying background irrigation pumping rates. These are not subject to optimization.
- To be optimized are timing and installation of extraction wells and pumping rates for each 5-year management period (MP). Remediation well pumping rates must be constant during a MP. New wells can be added only at the beginning of a MP.

A restriction for all formulations is that no developed pumping strategy can allow TCE or TNT to exceed cleanup levels (CLs) in the *forbidden zones* outside their *cleanup zones*. CLs are 5.0 ppb for TCE and 2.8 ppb for TNT. Polygons encircling the plumes in Figures 2-5 delineate the frontier between the *cleanup zones* and the surrounding *forbidden zones.*

The top part of Figure 6 summarizes mathematical constraints imposed in all three optimization problem formulations. The lower part of Figure 6 describes the additional constraint imposed on Formulations 1 and 2--forcing TCE and TNT concentrations to below CLs by the end of 30 years.

The Formulation 1 optimization problem is to minimize the value of the Figure 7a objective function equation, while satisfying all the Figure 6 constraints. The Figure 7a objective function is the sum of the present value of all manageable remediation costs.

Formulations 1 and 2 differ in how the extracted groundwater is managed. Hence, they differ in how the cost of treating or discharging the extracted water is computed. Formulation 2 does not incur treatment cost or discharge cost for up to 2400 gpm of extracted water. Figure 7b shows the Formulation 2 objective function.

Formulation 3 involves developing a pumping strategy that minimizes the maximum total remediation pumping rate in any management period over a 30-year simulation (Fig. 8). Cleanup need not be achieved within 30 years, but containment constraints must be satisfied (for TCE and TNT) at the end of each of the management periods. A Formulation 3 strategy cannot use more than 25 extraction wells. Since no cost is assigned to the wells, an optimization model will tend to use as many wells as possible. (Theoretically, in an absolute mathematical sense, reducing the number of wells cannot improve the objective function value. Therefore, optimization will tend to maximize the number of number of wells subject to restrictions.)

Between September 16 and September 17, we developed other strategies for the Formulation 3 family. These include USU3A', USU3B' and USU3C'. USU3A' resulted from continuing optimization of strategy USU3A. USU3B' and USU3C' are for alternative optimization problem formulations that restrict plume growth more than USU3 (A or A'). Figure 9 shows the USU3B' and USU3C' *forbidden zones* that prevent the contamination from migrating as far before capture as in the NAD-posed Formulation 3 optimization problem.

Optimization Process and Results

Overview

USU Formulation 1 results are supported by Figures 10-12, Appendix A, and Tables 1 and 3. USU proposes the same strategy for Formulation 2 as for Formulation 1. Therefore, USU Formulation 2 results are supported by the same figures, and also Appendix B and Tables 1 and 4. Formulation 3A is supported by Figures 13-16, Appendix C, and Tables 1 and 5. The Appendices are GeoTrans postprocessor outputs for the respective strategies.

USU developed additional strategies USU3A', USU3B' and USU3C' on September 17, the day between the above work was completed and the day we formally presented results. Strategy USU3A' is supported by Tables 2 and 6, and Appendix D. Formulation 3B' is supported by Figures 17-19, Table 2 and Appendix E. Formulation 3C' is supported by Figures 20-22, Appendix F and Table 2.

Tables 7-9 provide representative optimization solver input parameters. For Formulations 1 and 2 we primarily used the SOMOS GA and SA optimization solvers. For Formulation 3 we used the GA, SA and ANN-GA.

We began the optimization process by exploring candidate well locations for Formulation 3. That yielded a preliminary steady pumping strategy that would satisfy plume containment constraints, and the rest of those in the top part of Figure 6. Then, we pursued developing strategies for Formulations 1 and 3 simultaneously, on different computers.

Formulation 1 and least cost strategy USU1

Beginning with candidate wells and rates that could achieve plume containment, we identified candidate well locations that would likely also help achieve cleanup while satisfying the full set of Formulation 1 constraints (Figure 6). We made preliminary simulations in which we assumed that the managed (candidate) wells would pump steadily for 30 years (60 stress periods). The background (unmanaged) wells pumped at the NAD-specified unsteady rates.

After identifying reasonable sets of candidate wells we used GA to develop steady and transient 30-year pumping strategies. Table 7 shows representative GA input parameters.

We also used GA to develop 20-year pumping strategies that achieved cleanup within 20 years. However, pumping rates required to achieve 20-year cleanup were so great that it was unlikely that a 20-year strategy would be less costly than a 30-year strategy.

We continued Formulation 1 optimization for 30 years. Table 8 shows sample SA input parameters. Time-varying pumping strategy USU1 (Tables 1 and 3) yields the least cost, $40,824,320. It requires constructing 10 wells – eight initially and two at the beginning of management period 5. The GeoTrans post-processor shows the present value cost (Appendix A).

Figures 10-12 show TCE and TNT plumes at year 25. TCE cleanup is achieved in year 30. TNT cleanup is achieved in year 29.

Formulation 2 and least cost strategy USU2

Evaluating the objective function showed that a least-cost strategy for Formulation 1 would also be a least-cost strategy for Formulation 2. Therefore our best Formulation 1 strategy, USU1 is also our best strategy for Formulation 2.

The Formulation 2 optimization problem differs from that of Formulation 1 in the objective function. Therefore, even though the pumping rates are the same for USU1 and USU2, their objective function values differ. Tables 1 and 4 and Appendix B show strategy USU2 and its results.

Formulation 3 mimimax management period pumping strategy USU3A

Formulation 3 deals with minimizing the maximum total pumping rate that occurs in any management period (Figure 8), subject to the containment and other constraints of the top part of Figure 6. Formulation 3 differs from the previous problem formulations in its objective function and because it has no cleanup constraint.

We initially addressed the 30-year problem by assuming steady pumping and using GA. Table 7 shows representative inputs. For different groups of candidate wells, SOMOS developed different pumping strategies that satisfied the constraints. These required constructing different numbers of wells and had different total steady pumping rates. Examples included: 2551 gpm and 11 wells; 2305 gpm and 13 wells. However, we felt we could develop strategies having a better objective function value.

We optimized time-varying pumping using GA, SA, and GA linked with ANN. Tables 7-9 show representative respective inputs. Strategy USU3A had the lowest objective function value (Tables 1 and 5). The USU3A maximum period pumping rate is 2139 gpm. USU3A requires constructing 25 wells. Appendix C shows post-processor output. Figures 13-16 show concentrations predicted to result after 30 years of pumping.

Next Day Strategies USU3A', USU3B' and USU3C'

Within less than 24 hours of the time we reported strategy USU3A, a slightly better strategy (USU3A') evolved. USU3A' uses the same wells as USU1A, but different transient pumping rates to yield an improved objective function value of 2123 gpm. During the same period, preliminary draft strategies USU3B' and USU3C' evolved. These use fewer wells than USU3A and larger forbidden zones.

Strategy USU3B' assumes an alternative forbidden zone for TCE. The forbidden zone boundary is located 1 cell inside the forbidden zone posed by NAD (Figure 9). This is a more restrictive problem than that of USU3A because the contamination is not allowed to move as far. We used GA and SA to develop feasible solutions for the more restrictive optimization problem, but only did a little optimization. The best of those strategies, only partially optimized, is strategy USU3B'. USU3B' steadily pumps 2697 gpm using 24 wells (Appendix E).

Figures 17-19 show the plumes resulting after 30 years pumping per USU3B'. These show that the contamination stays at least 1 cell away from the NAD-posed containment zone.

Strategy USU3C' is a no-plume-growth scenario. In it, the containment zone is only one cell beyond the initial plume. The zone is identical in all layers. GA and SA were used to develop feasible solutions for this problem. The resulting slightly optimized strategy USU3C' uses 3237 gpm of steady pumping. Relaxing the containment constraint a little can allow significantly less pumping.

Summary and Observations

Table 1 summarizes results from the pumping strategies developed during the primary modeling period for the several optimization problem formulations. Strategies USU1 and USU2, for Formulations 1 and 2 respectively, are identical transient pumping strategies. These yield least cost objective function values of $40.8M and $18.9M, respectively. Strategy USU3A has a mini-max pumping rate of 2139 gpm. Representative strategies USU developed for Formulation 3 employed from 11 to 25 wells and from 2551 to 2139 gpm, respectively.

During computational optimization, a solution might not improve for a while, and then might suddenly improve. By the day after we reported strategy USU3A, the objective function pumping rate had improved to the 2123 gpm of strategy USU3A'. From that same 24-hour period we also report strategies (USU3B' and USU3C') developed for problems using larger (more restrictive) forbidden zones. USU3B' and USU3C' were not intensely optimized, but nevertheless demonstrate the general trend of objective function value worsening as a constraint is tightened. Theoretically, as restrictions (constraints) are tightened, globally optimal solutions cannot improve.

This project is intended to demonstrate the power of using optimization techniques for plume remediation design. We believe it does so. Our contract specified that we were to address the three posed optimization problem formulations using only PC computers and without interacting with the client (NAD).

Normally, when using optimization to design a pumping strategy for a client, the developer and the client interact even after the optimization has begun (Peralta and Aly, 1994, 1995, 1996; Hegazy and Peralta, 1997; Peralta, 2001a,b). Interaction is helpful in refining a strategy so that it considers additional factors useful for design and construction.

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Table 1. Strategy summary for three formulations.

Formulation #	1 (Strategy USU1)	2 (Strategy USU2)	3a (Strategy USU3a)
Objective Function Value ($M or gpm)	40.824320	18.879953	2138.7
Number of New Extraction Wells Installed	10	10	25
Cleanup Time for TCE	30	30	N/A
Cleanup Time for TNT	29	29	N/A

Table 2. Executive summary of optimal strategies developed during the day after the primary modeling period.

Base Formulation	3		
Strategy Option	USU3A'	USU3B'	USU3C'
Containment Zone	As posed	Smaller	Smallest
Objective Function Value (gpm)	2123	2692	3237
Number of New Extraction Wells Installed	25	24	24
Elapsed Years Until Cleanup	N/A		

*** Notes:**
- **3A' is designed for the posed optimization problem.**
- **3B' is designed for a containment zone that is one cell smaller in all directions than the posed containment zone. It was not thoroughly optimized.**
- **3C' is designed for the smallest containment zone—a no-plume growth scenario. The containment zone was one cell beyond the initial plume. This design was not thoroughly optimized.**

Table 3. Thirty-year transient pumping strategy USU1 and results.

	Strategy name:	USU1					
		Strategy Pumping Rates (GPM) for each management period (MP)					
	Well Location (K,I,J)	MP1	MP2	MP3	MP4	MP5	MP6
1	(3,26,32), (4,26,32)	0	0	0	0	423	696
2	(3,26,52), (4,26,52)	0	0	0	0	198	147
3	(3,37,39)	299	297	295	350	350	350
4	(3,34,58), (4,34,58)	306	340	379	344	407	344
5	(3,35,81), (4,35,81)	502	476	471	482	482	570
6	(3,28,57), (4,28,57)	506	554	523	564	398	690
7	(3,48,117), (4,48,117)	281	287	285	270	278	183
8	(3,52,122)	257	258	265	242	257	0
9	(3,56,111)	107	140	119	107	135	0
10	(3,33,66), (4,33,66)	226	277	306	392	377	397
	Total extraction (gpm)	2486	2632	2644	2752	3306	3378
	Cleanup time for TCE (years)	30					
	Cleanup time for TNT (years)	29					
	Total cost present value ($M)	**40.82**					

Table 4. Thirty-year transient pumping strategy USU2 and results.

	Strategy name:	USU2					
		Strategy Pumping Rates (gpm) for each management period (MP)					
	Well Location (K,I,J)	MP1	MP2	MP3	MP4	MP5	MP6
1	(3,26,32), (4,26,32)	0	0	0	0	423	696
2	(3,26,52), (4,26,52)	0	0	0	0	198	147
3	(3,37,39)	299	297	295	350	350	350
4	(3,34,58), (4,34,58)	306	340	379	344	407	344
5	(3,35,81), (4,35,81)	502	476	471	482	482	570
6	(3,28,57), (4,28,57)	506	554	523	564	398	690
7	(3,48,117), (4,48,117)	281	287	285	270	278	183
8	(3,52,122)	257	258	265	242	257	0
9	(3,56,111)	107	140	119	107	135	0
10	(3,33,66), (4,33,66)	226	277	306	392	377	397
	Total extraction (gpm)	2486	2632	2644	2752	3306	3378
	Cleanup time for TCE (years)	30					
	Cleanup time for TNT (years)	29					
	Total cost present value ($M)	**18.88**					

Table 5. Thirty-year transient pumping strategy USU3A and results.

	Strategy name:	USU3A					
		Strategy Pumping Rates (gpm) for each management period (MP)					
	Well Location (K,I,J)	MP1	MP2	MP3	MP4	MP5	MP6
1	(4,48,114)	190	190	190	190	190	156
2	(3,47,110)	76	76	76	76	65	0
3	(3,53,116)	145	145	145	145	145	145
4	(3,53,121)	157	157	157	157	157	157
5	(3,57,111)	51	51	51	51	51	51
6	(3,37,39)	277	277	277	277	277	277
7	(4,26,58)	23	23	23	23	23	23
8	(4,27,59)	22	22	22	22	22	22
9	(4,28,60)	18	18	18	18	18	18
10	(4,29,61)	15	15	15	15	15	15
11	(3,30,62), (4,30,62)	53	53	53	53	53	53
12	(3,31,63), (4,31,63)	56	56	56	56	56	56
13	(3,32,64), (4,32,64)	128	128	128	128	128	128
14	(4,34,81)	146	146	146	146	146	146
15	(3,35,81), (4,35,81)	167	167	167	167	167	174
16	(3,36,81)	65	65	65	65	65	65
17	(4,36,81)	70	70	70	70	68	68
18	(3,25,58), (4,25,58)	87	87	87	87	88	114
19	(3,32,68), (4,32,68)	56	56	56	56	57	57
20	(4,33,81)	88	88	88	88	88	88
21	(3,28,60)	73	73	73	73	73	83
22	(3,29,61)	62	62	62	62	62	83
23	(3,26,58)	57	57	57	57	57	57
24	(3,27,59)	57	57	57	57	57	57
25	(3,28,65)	0	0	0	0	10	34
	Total extraction (gpm)	2139	2139	2139	2139	2139	2129
	Minimum maximum pumping rate (gpm)	**2139**					

Table 6. Thirty-year transient pumping strategy USU3A' and results.

	Strategy name:	USU3A'					
		Strategy Pumping Rates (gpm) for each management period (MP)					
	Well Location (K,I,J)	MP1	MP2	MP3	MP4	MP5	MP6
1	(4,48,114)	190	190	190	190	190	0
2	(3,47,110)	76	76	76	76	65	0
3	(3,53,116)	145	145	145	145	145	145
4	(3,53,121)	157	157	157	157	157	157
5	(3,57,111)	51	51	51	51	51	51
6	(3,37,39)	272	272	272	272	272	281
7	(4,26,58)	16	16	16	16	16	16
8	(4,27,59)	15	15	15	15	15	15
9	(4,28,60)	13	13	13	13	13	13
10	(4,29,61)	13	13	13	13	13	13
11	(3,30,62), (4,30,62)	58	58	58	58	58	58
12	(3,31,63), (4,31,63)	56	56	56	56	56	67
13	(3,32,64), (4,32,64)	102	102	102	102	102	102
14	(4,34,81)	146	146	146	146	146	146
15	(3,35,81), (4,35,81)	177	177	177	177	177	271
16	(3,36,81)	65	65	65	65	65	65
17	(4,36,81)	68	68	68	68	68	68
18	(3,25,58), (4,25,58)	84	84	84	84	84	134
19	(3,32,68), (4,32,68)	57	57	57	57	57	98
20	(4,33,81)	88	88	88	88	88	88
21	(3,28,60)	78	78	78	78	78	83
22	(3,29,61)	77	77	77	77	77	94
23	(3,26,58)	57	57	57	57	57	57
24	(3,27,59)	57	57	57	57	57	57
25	(3,28,65)	5	5	5	5	16	44
	Total extraction (gpm)	2123	2123	2123	2123	2123	2123
	Minimum maximum pumping rate (gpm)	**2123**					

Table 7. Representative GA input parameters.

1. Total number of simulations	800
2. Total number of generations	100
3. Generation size	8
4. Penalty coefficient	10
5. Crossover probability	0.8
6. Mutation probability	0.04

Notes:

1. Total number of simulations performed by end of the number of generations specified in item 2.
2. Total number of generations used in a GA optimization.
3. The number of individuals in a generation.
4. Within the objective function, this is the coefficient used to weight unit violations of constraints. The resulting penalty makes the objective function less desirable proportionally with respect to the degree of constraint violation.
5. Probability that a pair of individuals will mate. Usually, one maintains a high probability (i.e. 0.7 ~ 0.9), since without mating, only mutation will change a strategy. Aly and Peralta (1999) report that a probability less than 0.7 produces inferior results.
6. Probability that each bit of a chromosome will mutate. The rate of mutation should generally be low (smaller than 0.1). Mutation is performed after crossover.

Table 8. Representative SA input parameters.

1. Number of moves	6
2. Number of trials	15
3. Initial temperature	400
4. Adjustment parameter	0.01
5. Initial step length	500
6. Initial penalty coefficient	10

Notes:

1. The number of simulations (moves) within a trial.
2. The total number of trials. Within a trial, a particular temperature, penalty coefficient, and moving step size are used. After each trial the temperature is cooled.
3. Initial temperature. The temperature controls the probability that the code will accept a worse strategy.
4. The adjustment parameter for the movement generation function (Corana et. At, 1987). This is a value between 0 and 1.0. The product of the adjustment factor and the decision variable range is the maximum change in decision variable in a movement.
5. Initial step length (expressed in decision variable units). It is the largest step size of moves in the first trial.
6. Initial penalty coefficient used in the first trial. This is the largest penalty coefficient used in a run.

Table 9. Representative ANN-GA input parameters**.**

ANN input parameters	
1. number of cycles	4
2. min. no. of simulations per cycle	10
3. Number of ANN training sessions	4
4. Number of iterations per training session	4000
5. number of nodes in hidden layer	16
6. kappa	0.1
7. phi	0.5
8. theta	0.7
9. Initial learning rate	0.05
GA input parameters	
10. population size	50
11. number of generations	1500
12. crossover probability	0.8
13. mutation probability	0.04
14. penalty coefficient	10

Notes:

1. The number of cycles. A cycle is one process of developing strategies, training ANNs and optimizing. The ANNs represent substitute simulators or response surfaces. The process is continued untill the total number of cycles are completed.
2. The minimum number of real model simulations per cycle. Included within these simulations is the best strategy from the previous cycle.
3. The number of training sessions usually is less than 10, but more is possible. A larger number will require more time to train the ANN, but might improve the training and yield a more accurate ANN.
4. The number of iterations for each ANN training session. This is usually between 500 and 10000.
5. The number of nodes (neurons) in the hidden layer. This number determines the number of weights between the input and hidden layer and hidden layer and output layer. Increasing the number of nodes causes the ANN architecture to become more complex, and increases run time. The more nodes, possibly the better the ANN-prediction abilities—up to a point. Too many nodes can cause an ANN to memorize all inputs and reduce its ability to recognize new patterns.
6. Kappa parameter. Used internally to determine a learning rate. Kappa should have a value between 0 and 1. Normally kappa is 0.1. ANN performance is not very sensitive to this.
7. Phi parameter. Used internally to help determine a learning rate. Phi should have a value between 0 and 1. Normally phi ranges from 0.5 to 0.7.
8. Theta parameter. Used in the adaptive learning algorithm. Theta should have a value between 0 and 1. Normally, we use a theta of 0.1.
9. The initial learning rate. This usually ranges from 0.15 to 0.5. A frequently used value is 0.5. Higher values could lead to oscillation or saturated processing elements (nodes).

10-14. See Notes of Table 7.

Fig. 1. Blaine Naval Ammunition Depot base map.

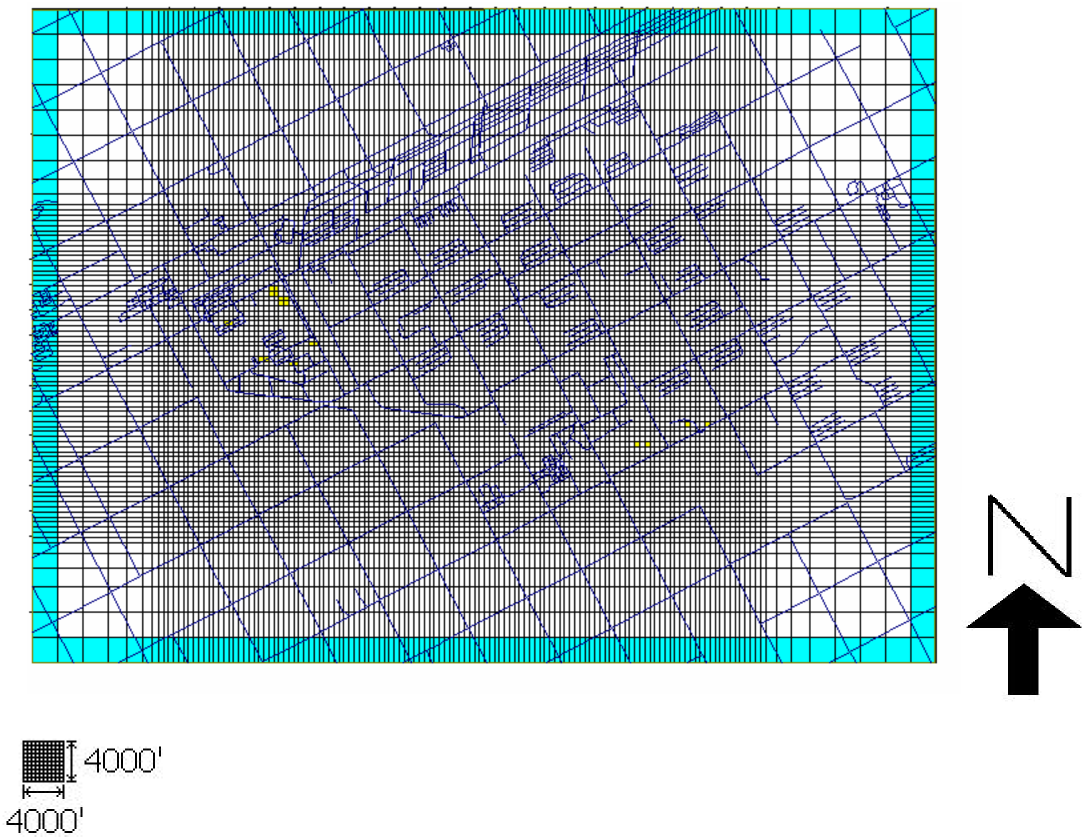


Fig. 2. Initial (Projected 1 Jan 2003) TCE concentrations exceeding 5.0 ppb in Layer 3, and part of finite difference grid with rows and columns numbered.

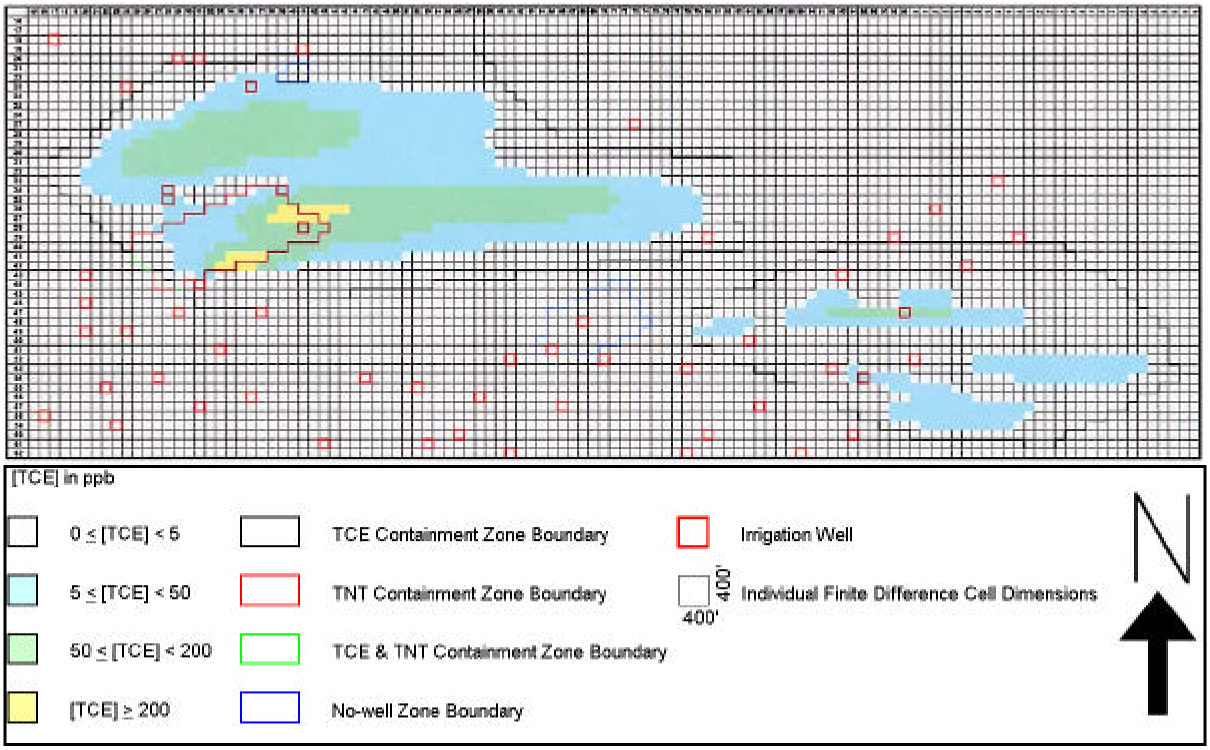


Fig. 3. Initial (Projected 1 Jan 2003) TCE concentrations exceeding 5.0 ppb in Layer 4, and part of finite difference grid with rows and columns numbered.

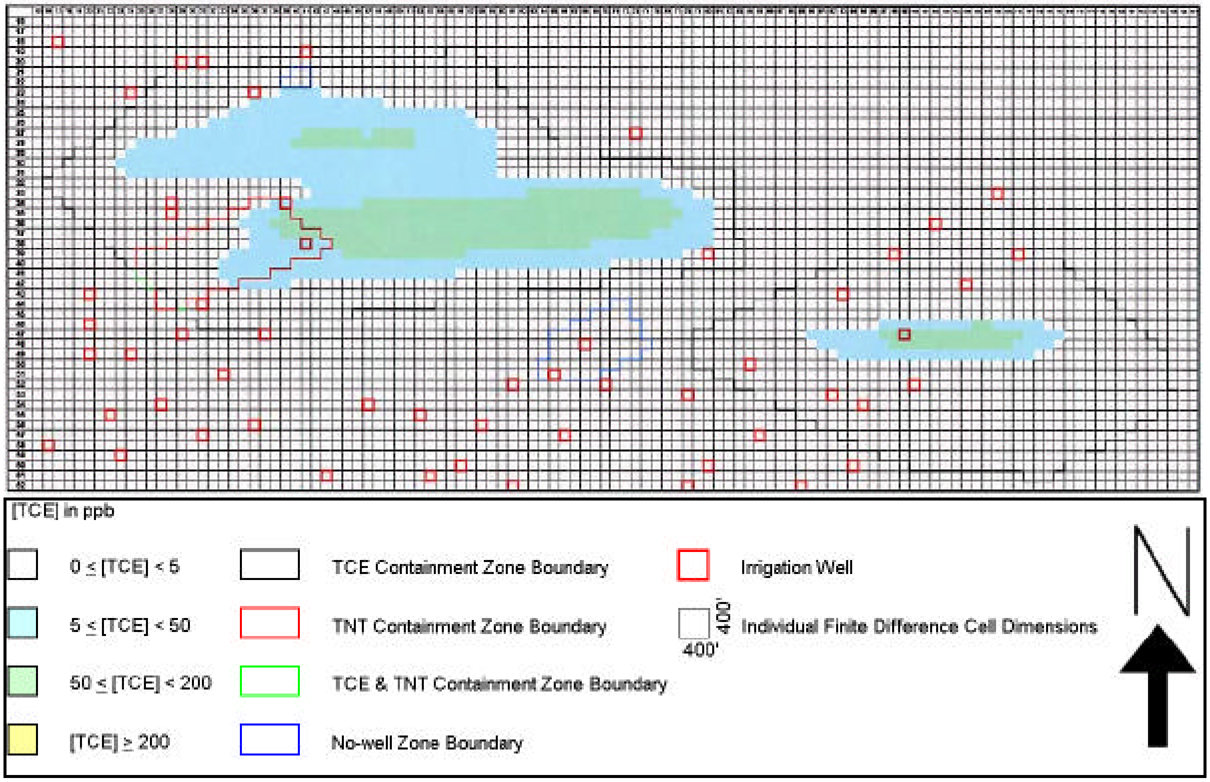


Fig. 4. Initial (Projected 1 Jan 2003) TCE concentrations exceeding 5.0 ppb in Layer 5, and part of finite difference grid with rows and columns numbered.

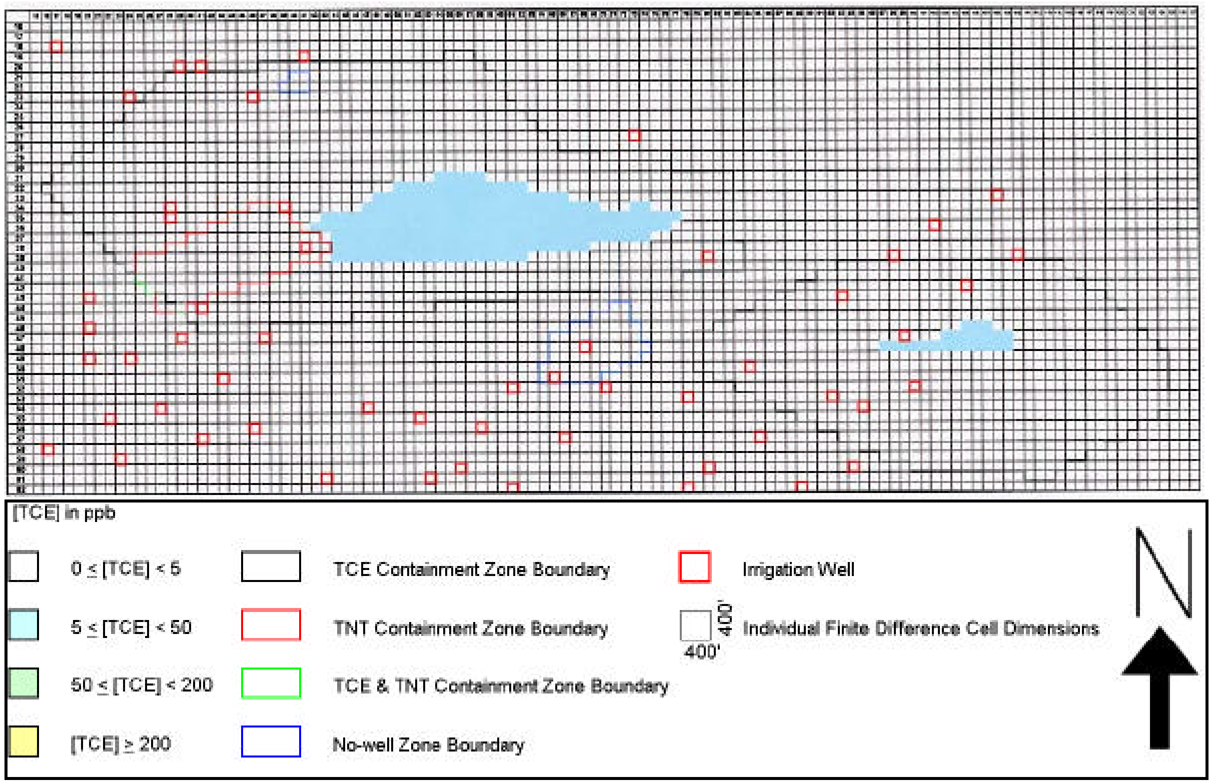


Fig. 5. Initial (Projected 1 Jan 2003) TNT concentrations exceeding 2.8 ppb in layer 3, and part of finite difference grid.

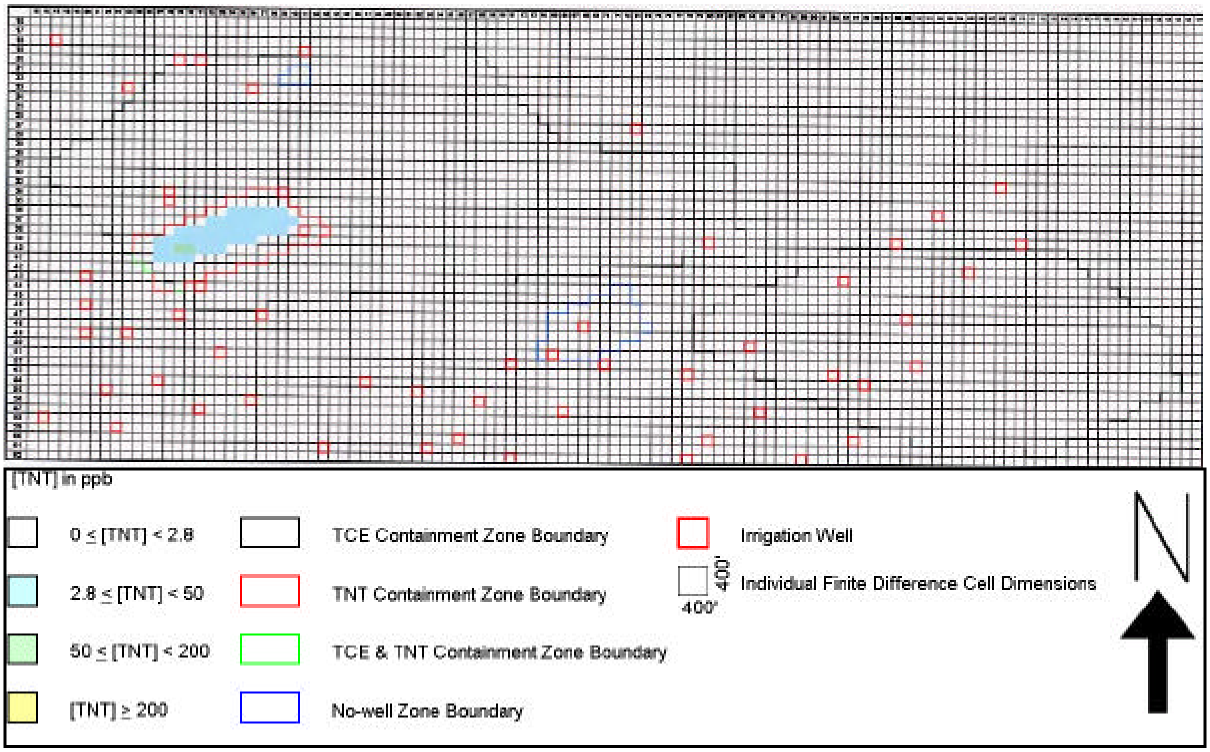


Fig. 6. Constraints for optimization problem formulations.

Constraints for all formulations

- Layer 1 and 2 cells not allowed to become dry
- Use of extraction wells, but no injection
- 350 gpm pumping limit on wells screened in 1 layer
- 700 gpm pumping limit on wells screened in 2 layers
- 1050 gpm pumping limit on wells screened in 3 layers
- No remediation well screening in layer 6
- No remediation wells in restricted areas.
- No remediation wells allowed in irrigation well cells
- Concentrations cannot exceed CLs in forbidden zones at end of any MP (CL_{TCE} = 5ppb, CL_{TNT} = 2.8 ppb)

Additional constraint for Formulations 1 and 2

- Cleanup to CLs within 30 years for Layers 3-6

Fig. 7a. Formulation 1 objective function: minimize present value of cost

MINIMIZE (CCE + CCT + CCD + FCM + FCS + VCE + VCT +VCD)

Evaluated at the end of every year to account for discounting of annual costs:

CCE **=** Capital Costs of new extraction wells($400K)

CCT **=** Capital Cost of Treatment($1.0K per gpm)

CCD **=** Capital Cost of Discharge Piping($1.5K per gpm)

FCM **=** Fixed Cost of Management($115K O&M)

FCS **=** Fixed Cost of Sampling ($300K annual sampling and analysis)

VCE **=** Variable cost of electricity for well operations($0.046K per gpm)

VCT **=** Variable cost of treatment ($0.283K per gpm)

VCD **=** Variable cost of discharge ($0.066K per gpm)

Fig. 7b. Formulation 2 objective function: minimize present value of cost

MINIMIZE (CCE + CCT + CCD + FCM + FCS + VCE + VCT +VCD)

Same as Formulation 1 but assume diversion of 2400 gpm of extracted water:

CCT **=** Capital Cost of Treatment

CCD **=** Capital Cost of Discharge Piping

VCT **=** Variable cost of treatment

VCD **=** Variable cost of discharge

If Qmax = 2400 then

$CCT = CCD = CT_i = CD_i = 0$

Else $CCT = 1.0x[Qmax-2400]$

$CCD = 1.5x[Qmax-2400]$

$CT_i = 0.2863x[Q_i-2400]$

$CD_i = 0.066x[Q_i-2400]$

Fig. 8. Formulation 3 objective function: minimizing maximum total pumping rate in any management period.

MINIMIZE MAXIMUM TOTAL PUMPING RATE IN ANY MANAGEMENT PERIOD

MINIMIZE (Q_{max})

Q_{max} is the maximum total pumping at remediation wells (Layers 3-6) in any management period over a 30-year simulation.

Fig. 9. Formulation 3 surrogate containment zones for Strategies USU3B' and USU3C'.

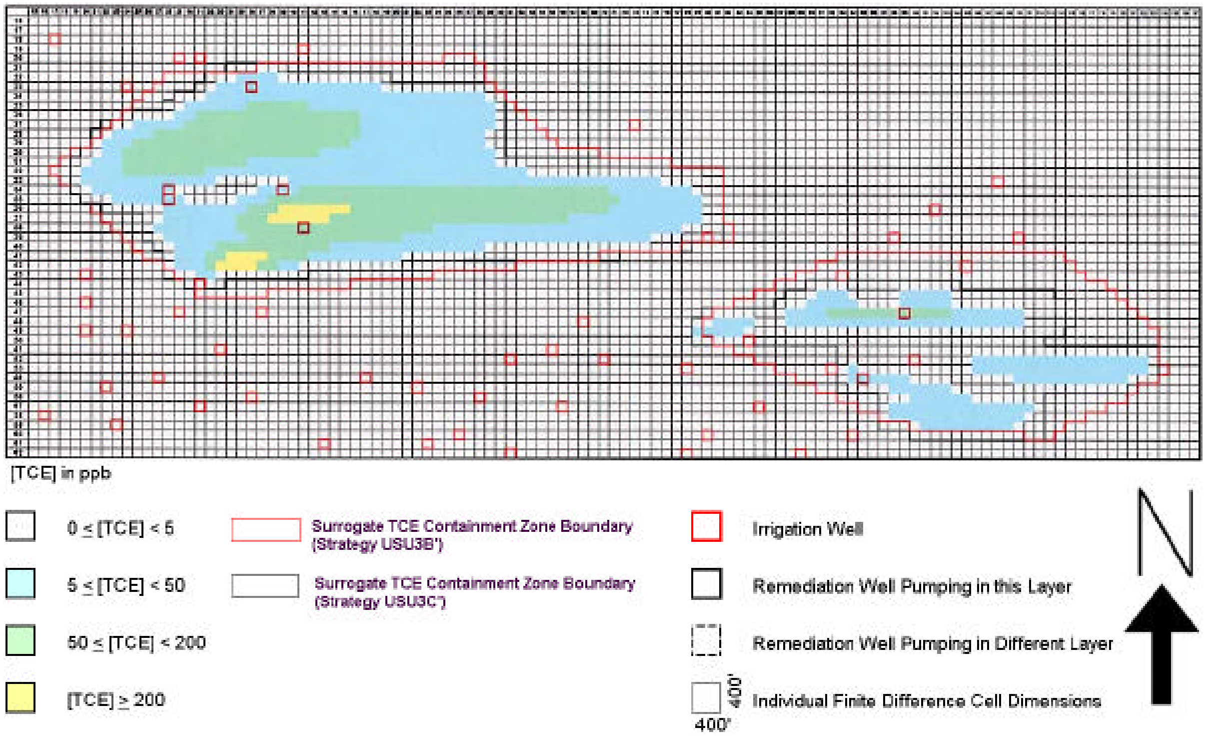


Fig. 10. Strategy USU1: TCE concentrations ≥ 5.0 ppb in Layer 3 after 25 years of pumping.

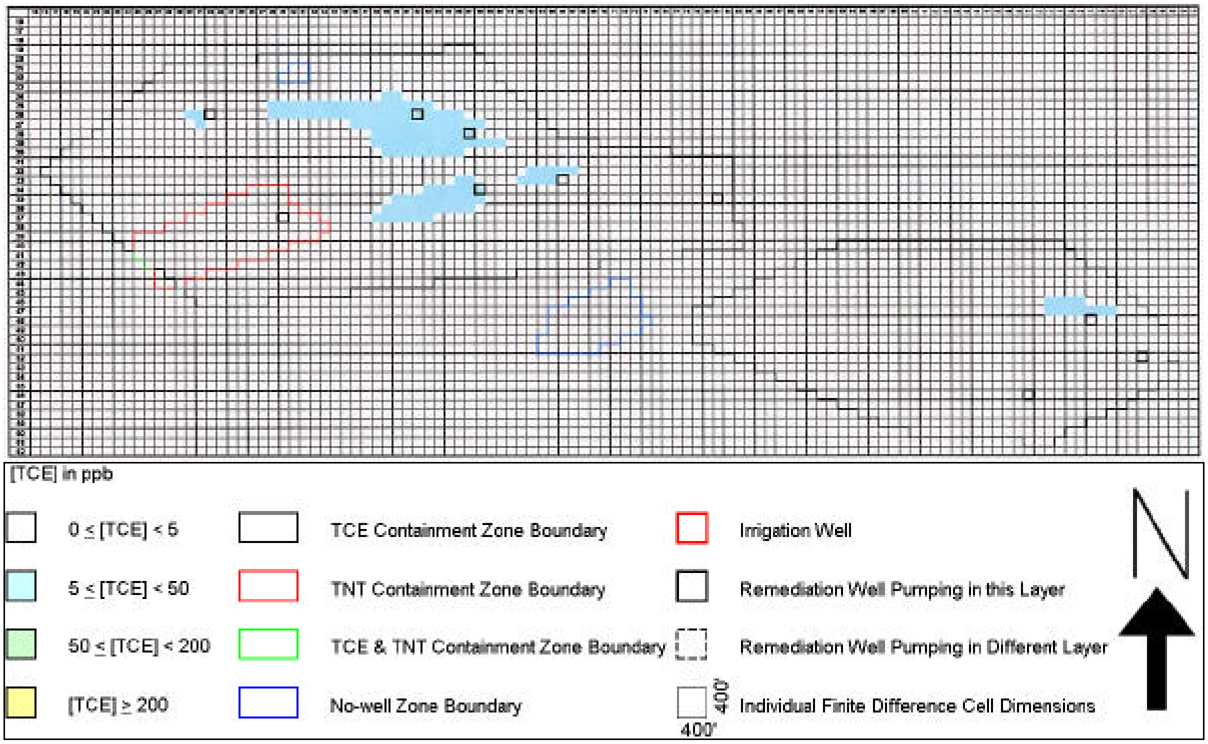


Fig. 11. Strategy USU1: TCE concentrations ≥ 5.0 ppb in Layer 4 after 25 years of pumping.

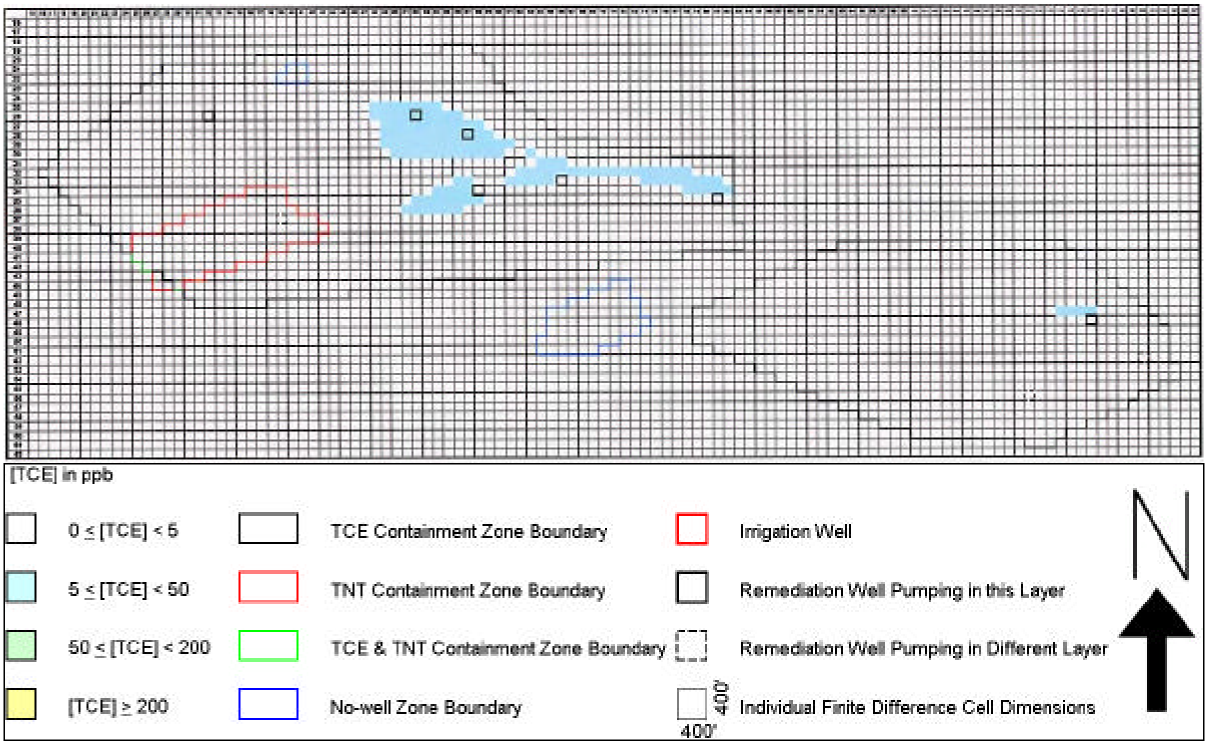


Fig. 12. Strategy USU1: TNT concentrations ≥ 2.8 ppb in Layer 3 after 25 years of pumping.

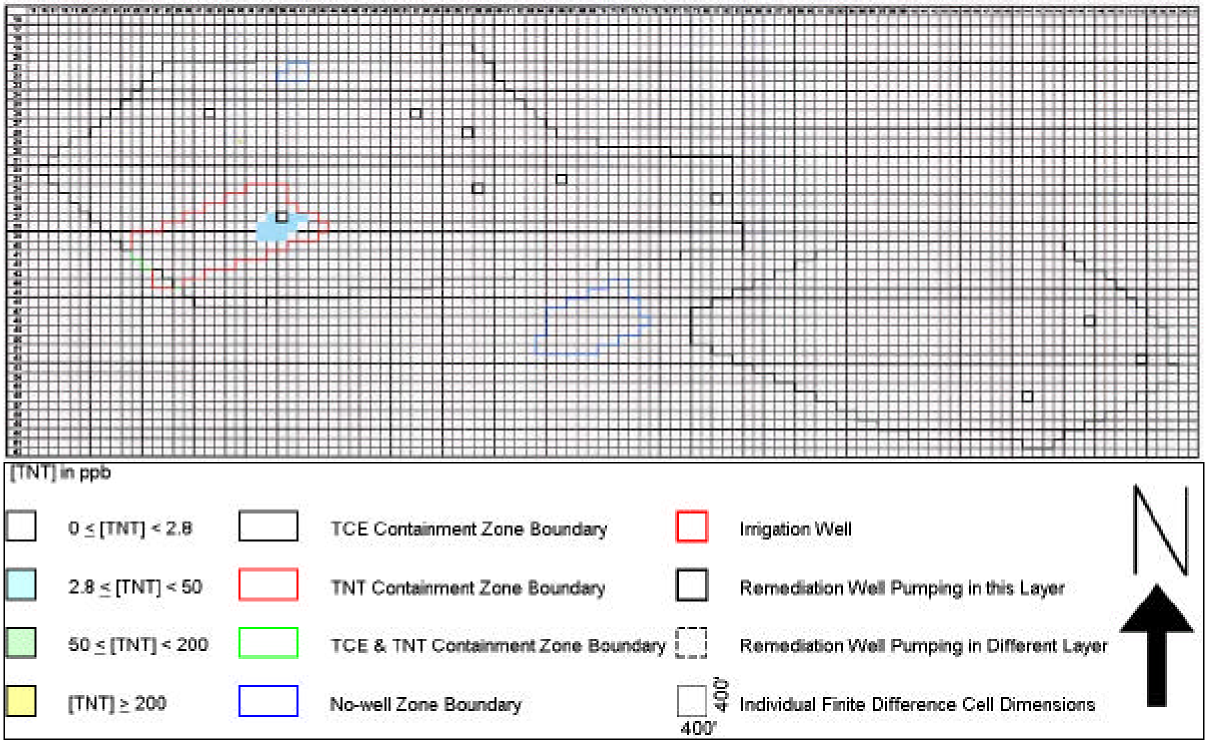


Fig. 13. Strategy USU3A: TCE concentrations ≥ 5.0 ppb in Layer 3 after 30 years of pumping.

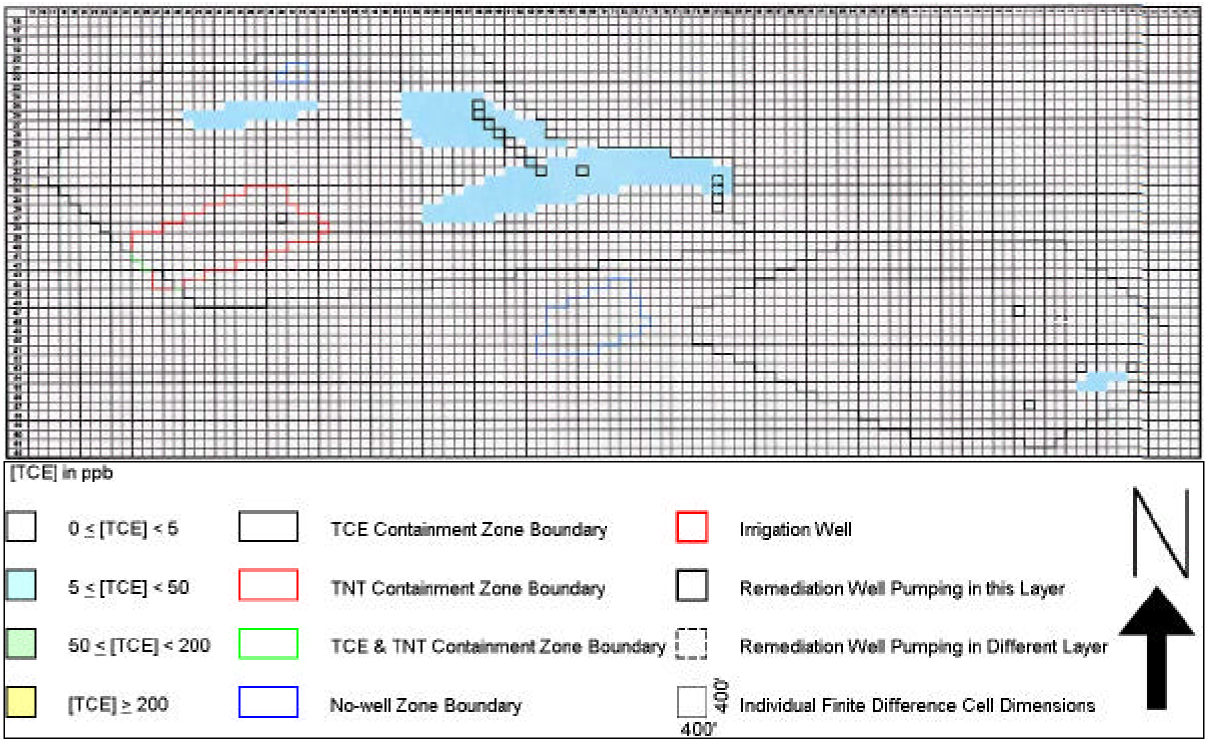


Fig. 14. Strategy USU3A: TCE concentrations ≥ 5.0 ppb in Layer 4 after 30 years of pumping.

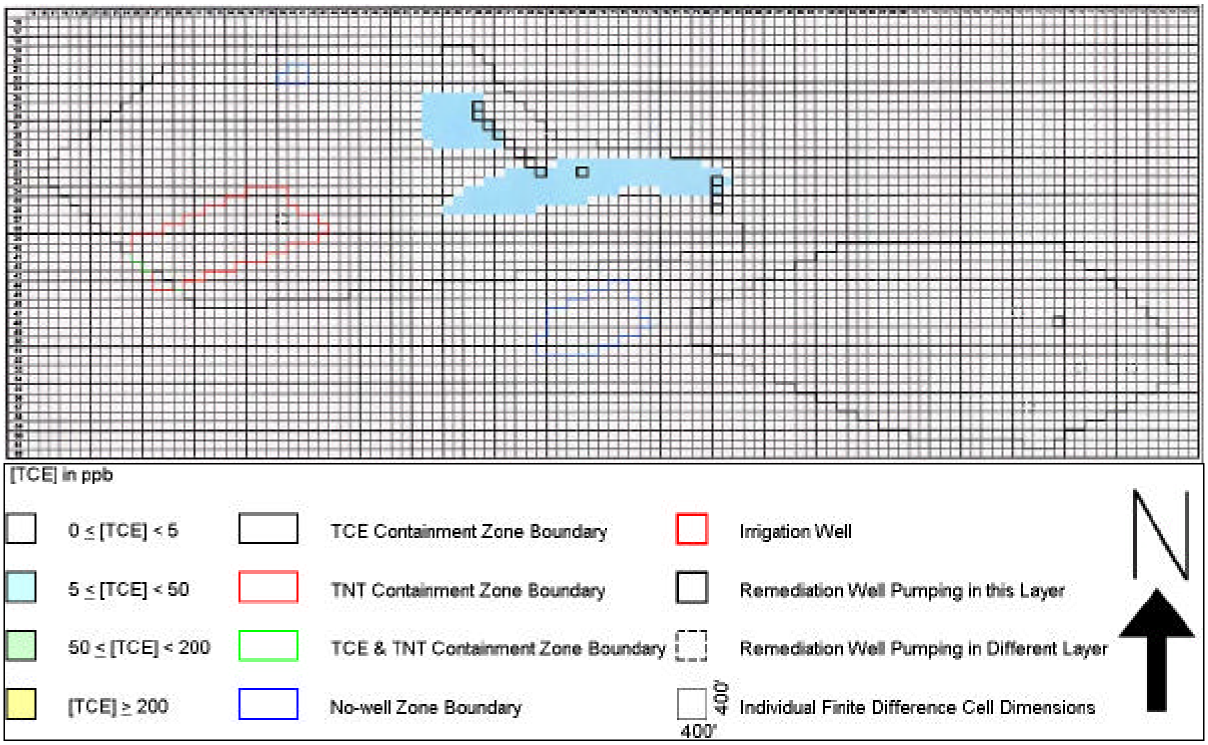


Fig. 15. Strategy USU3A: TCE concentrations ≥ 5.0 ppb in Layer 5 after 30 years of pumping.

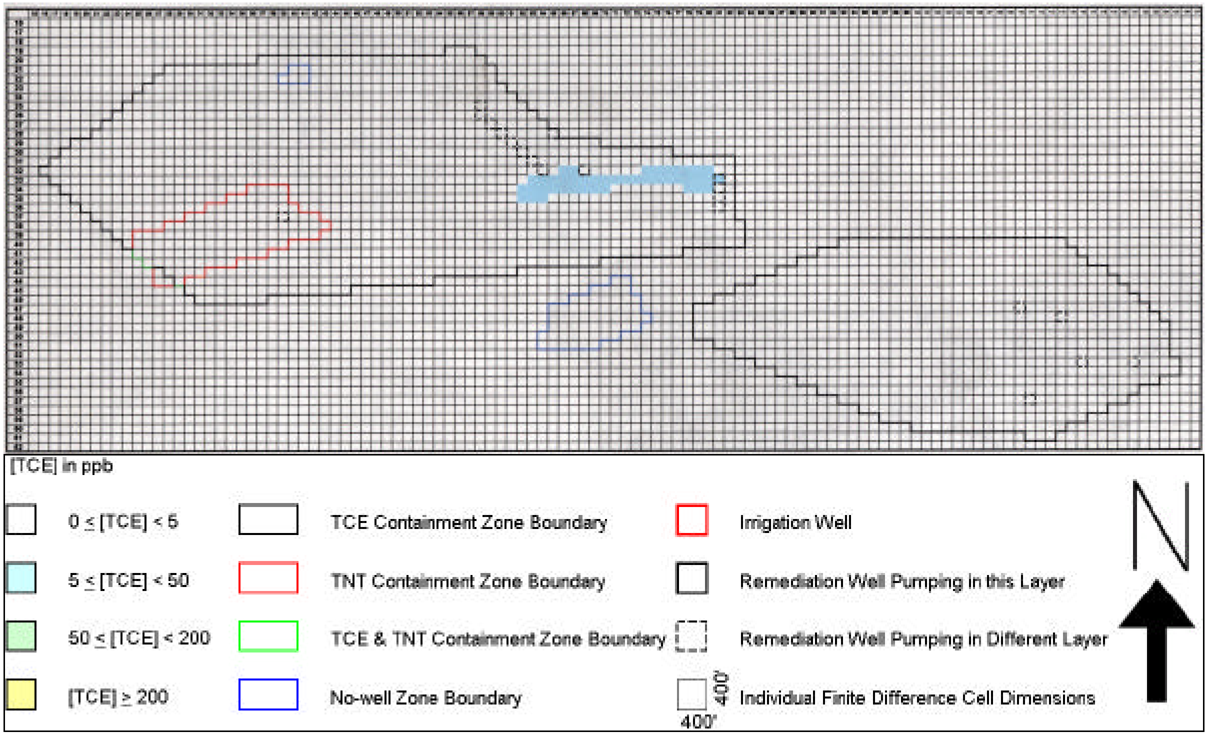


Fig. 16. Strategy USU3A: TNT concentrations > 2.8 ppb in Layer 3 after 30 years of pumping.

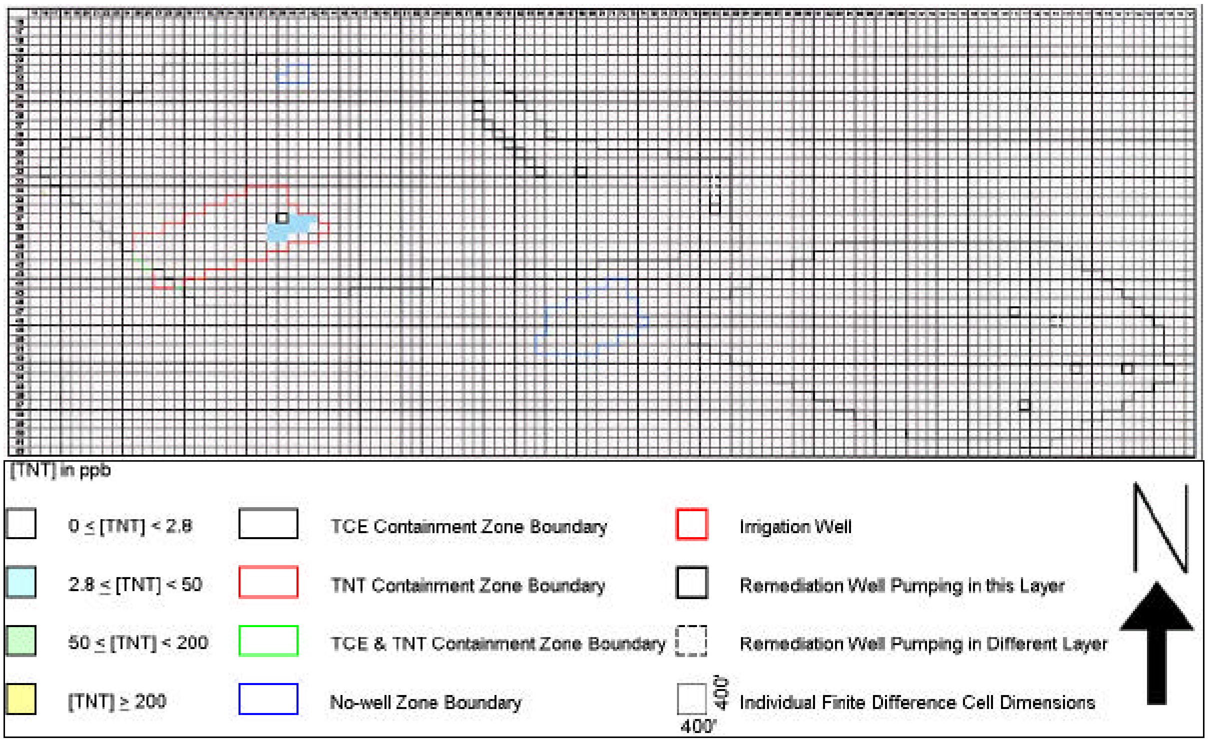


Fig. 17. Strategy USU3B': TCE concentrations ≥ 5.0 ppb in Layer 3 after 30 years of pumping.

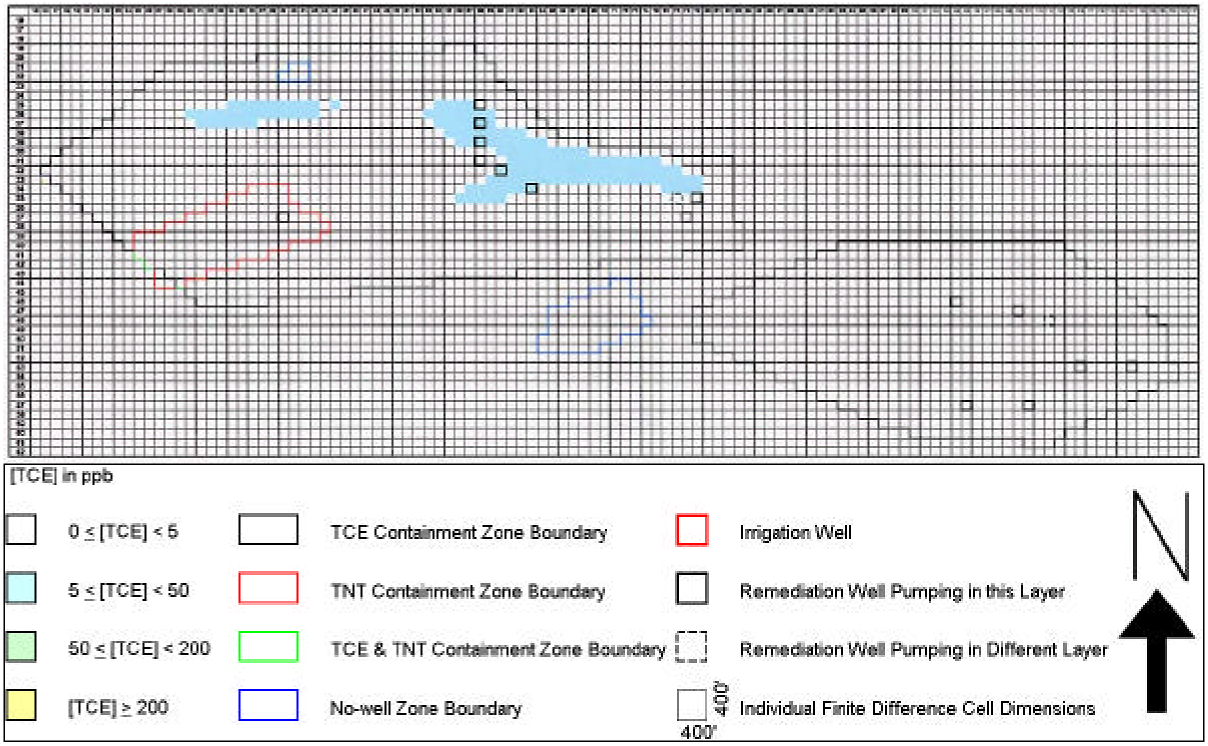


Fig. 18. Strategy USU3B': TCE concentrations ≥ 5.0 ppb in Layer 4 after 30 years of pumping.

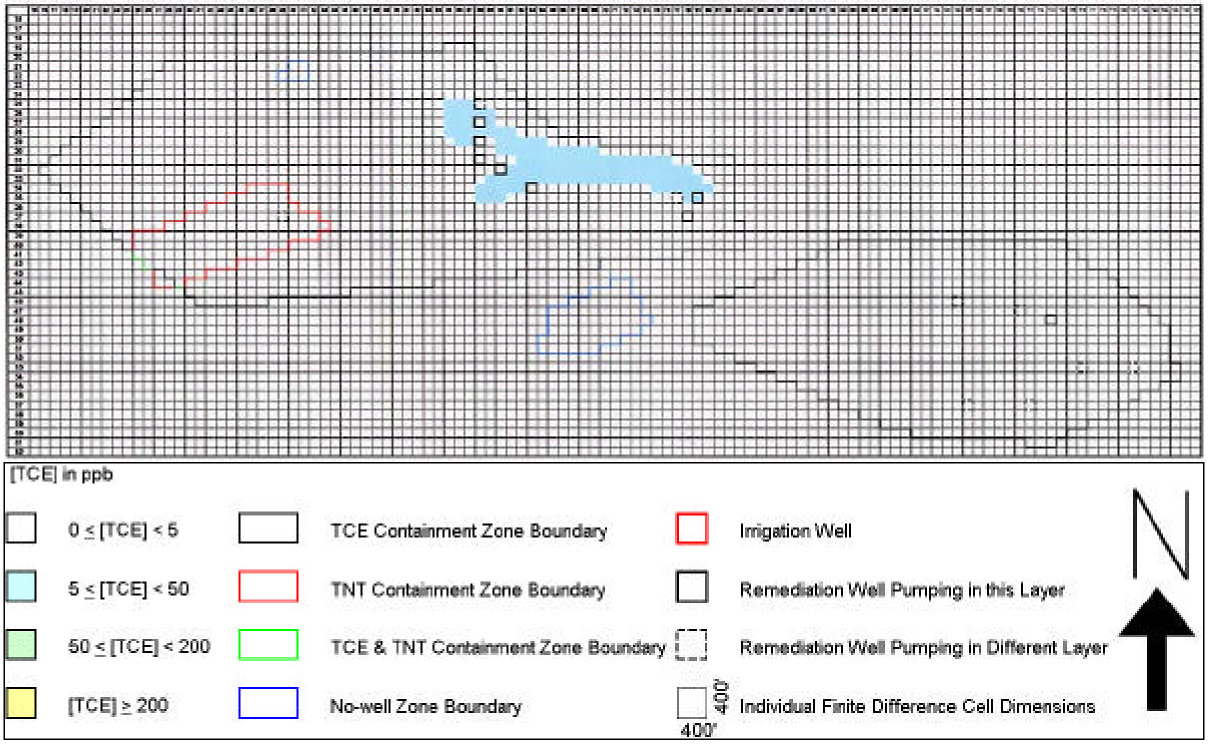


Fig. 19. Strategy USU3B’: TNT concentrations ≥ 2.8 ppb in Layer 3 after 30 years of pumping.

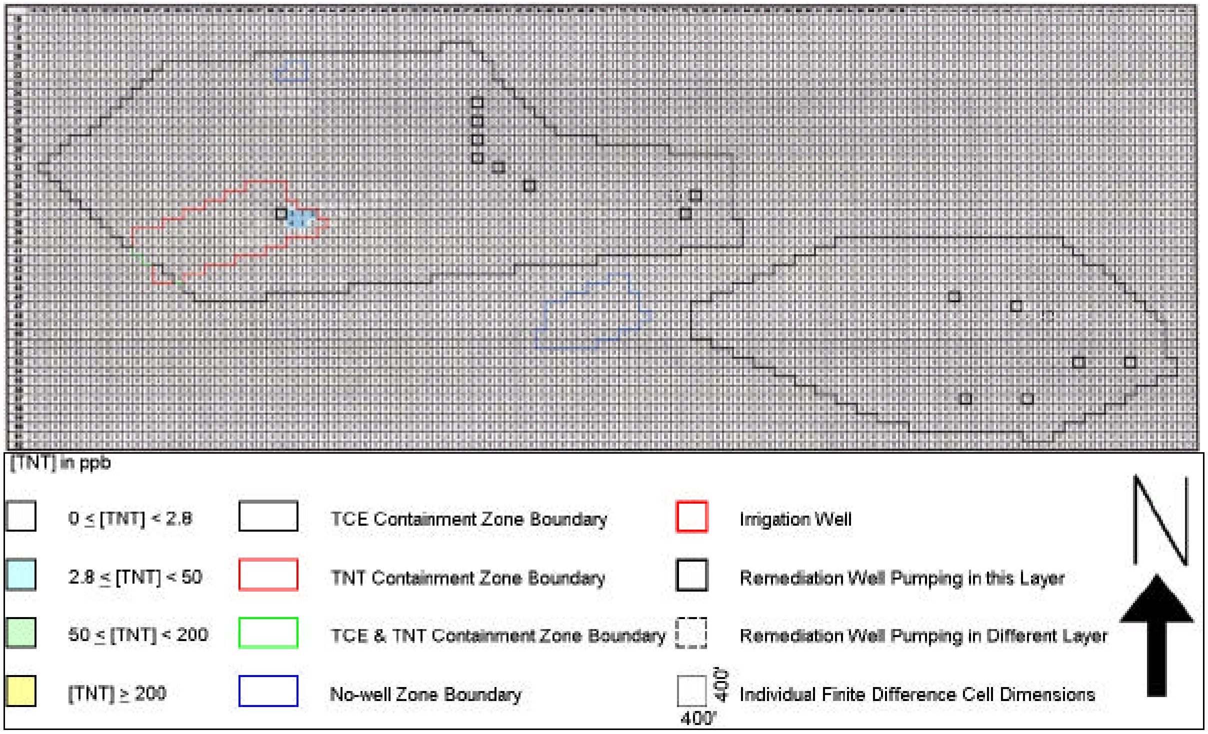


Fig. 20. Strategy USU3C’: TCE concentrations ≥ 5.0 ppb in Layer 3 after 30 years of pumping.

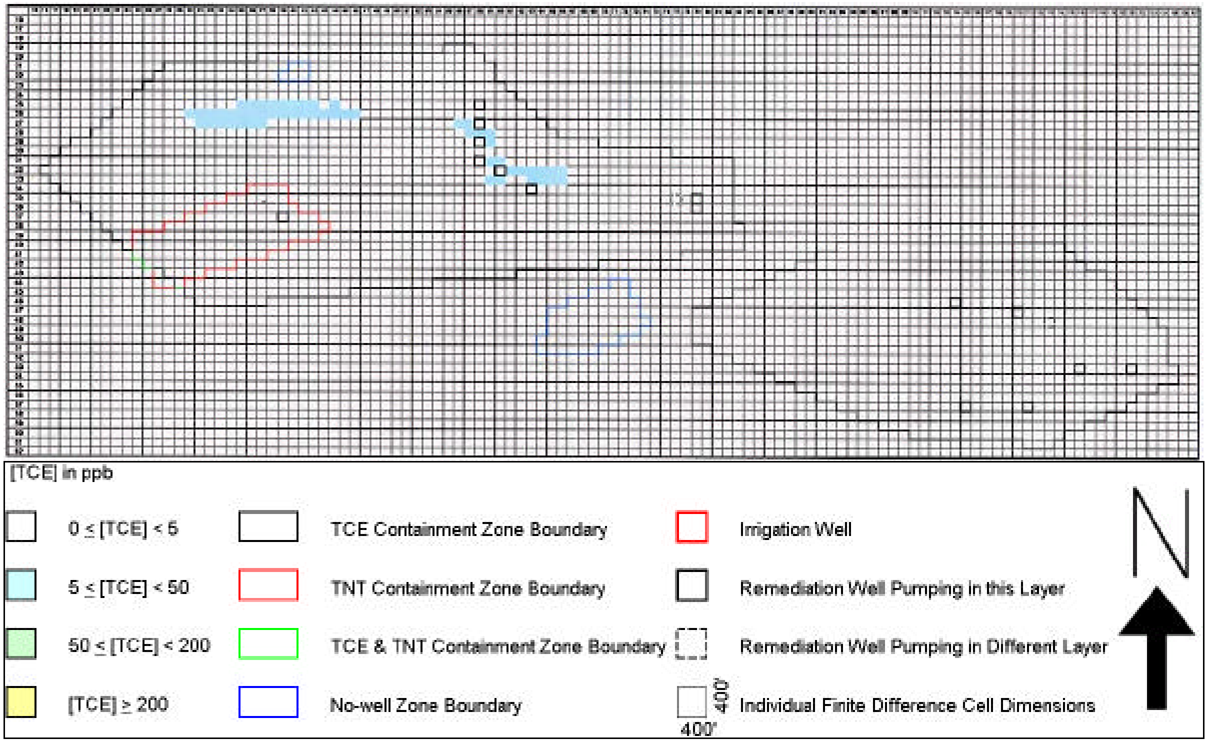


Fig. 21. Strategy USU3C’: TCE concentrations ≥ 5.0 ppb in Layer 4 after 30 years of pumping.

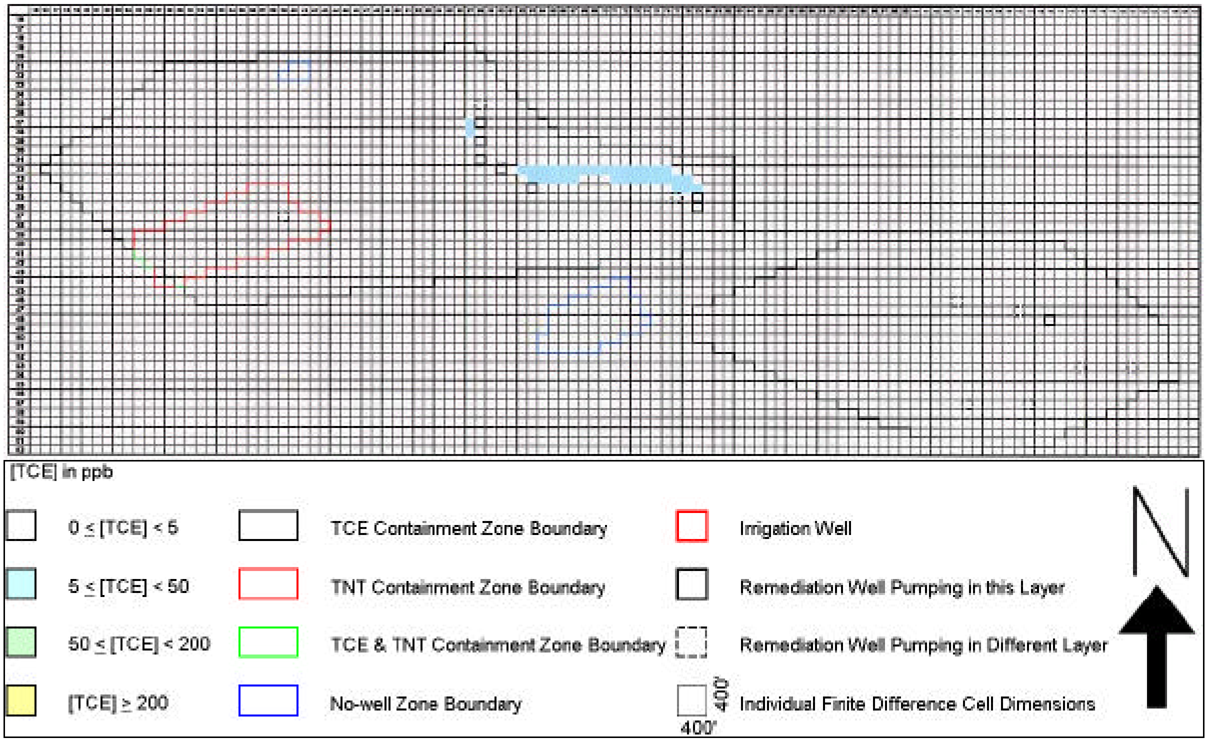
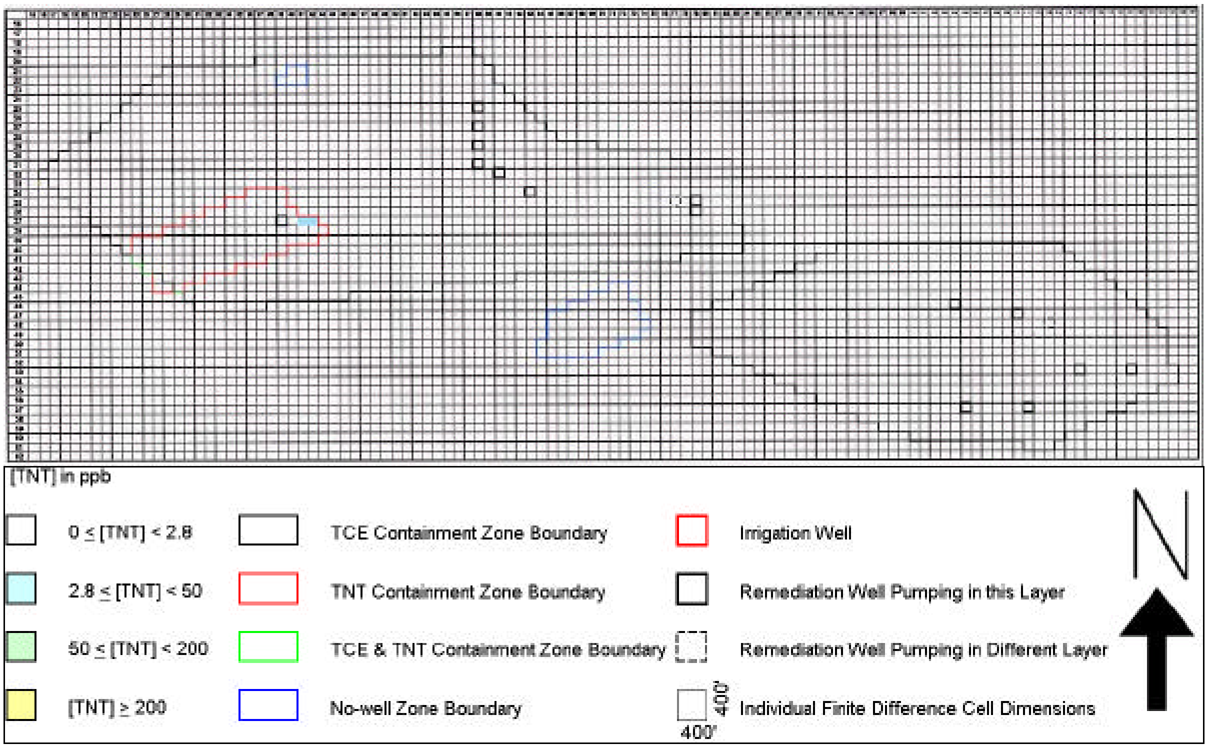


Fig. 22. Strategy USU3C’: TNT concentrations ≥ 2.8 ppb in Layer 3 after 30 years of pumping.



Appendix A. Post processor evaluation of Strategy USU1.

```
                      Intermediate Variables Calculation
                      ----------------------------------

     Cleanup Year for TCE
             30
     Cleanup Year for TNT
             29
     Cleanup Year for Formulation  1
             30

     Number of Irrigation Wells and Total Rates
          Season          Number of Wells          Total Rate (gpm)
          ------          ---------------          ----------------
              1                 12                      2100.000
              2                951                     54298.152

     Total Number of Wells In Each Stress Period
          Stress Period
          -------------
              1                   8
              2                   8
              3                   8
              4                   8
              5                  10
              6                   8

     Extraction Well Rates (Combining Multi-Aquifer Wells)
          Well Index        Well Rate (gpm)        Screen Layers
          ----------        ---------------        -------------
          Stress Period:   1
              3                301.293                   1
              5                305.995                   2
              6                501.766                   2
              7                506.161                   2
              8                280.873                   2
             10                257.029                   1
             11                106.675                   1
             12                226.452                   2
          Stress Period:   2
              3                299.906                   1
              5                340.447                   2
              6                476.291                   2
              7                553.506                   2
              8                287.169                   2
             10                258.369                   1
             11                139.636                   1
```

```
         12                276.945                 2
      Stress Period:   3
          3                296.473                 1
          5                378.909                 2
          6                471.190                 2
          7                522.951                 2
          8                285.247                 2
         10                264.722                 1
         11                118.956                 1
         12                305.694                 2
      Stress Period:   4
          3                350.000                 1
          5                344.374                 2
          6                481.870                 2
          7                563.751                 2
          8                270.223                 2
         10                242.447                 1
         11                107.055                 1
         12                392.073                 2
      Stress Period:   5
          1                423.055                 2
          2                198.286                 2
          3                350.000                 1
          5                407.335                 2
          6                482.275                 2
          7                397.610                 2
          8                277.517                 2
         10                257.210                 1
         11                134.971                 1
         12                377.257                 2
      Stress Period:   6
          1                696.104                 2
          2                147.429                 2
          3                350.000                 1
          5                344.031                 2
          6                569.756                 2
          7                690.192                 2
          8                183.397                 2
         12                397.195                 2

 Number of New Extraction Wells in Each Stress Period
          8
          0
          0
          0
          2
          0

 Total Pumping Rate in Each Stress Period (gpm)
      Pumping Rate
      ------------
        2486.244
```

```
            2632.270
            2644.140
            2751.792
            3305.517
            3378.104


                           Objective Function Calculation
                           ------------------------------

     The Capital Costs of New Wells (thousand of dollars)
          3602.053

     The Capital Costs of Treatment Plant (thousand of dollars)
          3378.104

     The Capital Costs of Discharge Piping (thousand of dollars)
          5067.156

     The Fixed Costs of O&M (thousand of dollars)
          2189.114

     The Fixed Costs of Sampling (thousand of dollars)
          5710.732

     The Variable Costs of Electricity for Operating Wells (thousand
of dollars)
          2431.264

     The Variable Costs of Treatment (thousand of dollars)
         14957.560

     The Variable Costs of Discharge (thousand of dollars)
          3488.336

     The Objective Function Value (thousands of dollars) for
Formulation #  1
         40824.320


                           Constraints Check-Out
                           ---------------------


     --- Modification Occurrence Constraint ---

     The Modification Occurrence Constraint Satisfied


     --- Cleanup Year Constraint ---

     The Cleanup Year
```

```
          30
The Cleanup Year Constraint Satisfied


--- Plume Containment Constraint ---

The Plume Containment Constraint Satisfied


--- Pumping Limit Constraint ---

The Pumping Limit Constraint Satisfied


--- Well Restricted Areas Constraint ---

The Well Restricted Areas Constraint Satisfied


--- Remediation Well Location Constraint ---

The Remediation Well Location Constraint Satisfied


--- Dry Cell Constraint ---

The Dry Cell Constraint Satisfied


--- Irrigation Well Constraint ---

The Irrigation Well Constraint Satisfied


--- Well Screen Constraint ---

The Well Screen Constraint Satisfied


Number of Constraints Not Satisfied
           0
```

Appendix B. Post processor evaluation of Strategy USU2.

```
                         Intermediate Variables Calculation
                         ----------------------------------

     Cleanup Year for TCE
             30
     Cleanup Year for TNT
             29
     Cleanup Year for Formulation  2
             30

     Number of Irrigation Wells and Total Rates
          Season          Number of Wells          Total Rate (gpm)
          ------          ---------------          ----------------
              1                 12                       2100.000
              2                951                      54298.152

     Total Number of Wells In Each Stress Period
          Stress Period
          -------------
              1                    8
              2                    8
              3                    8
              4                    8
              5                   10
              6                    8

     Extraction Well Rates (Combining Multi-Aquifer Wells)
          Well Index        Well Rate (gpm)         Screen Layers
          ----------        ---------------         -------------
          Stress Period:   1
              3                301.293                    1
              5                305.995                    2
              6                501.766                    2
              7                506.161                    2
              8                280.873                    2
             10                257.029                    1
             11                106.675                    1
             12                226.452                    2
          Stress Period:   2
              3                299.906                    1
              5                340.447                    2
              6                476.291                    2
              7                553.506                    2
              8                287.169                    2
             10                258.369                    1
             11                139.636                    1
             12                276.945                    2
          Stress Period:   3
```

```
            3                296.473                   1
            5                378.909                   2
            6                471.190                   2
            7                522.951                   2
            8                285.247                   2
           10                264.722                   1
           11                118.956                   1
           12                305.694                   2
        Stress Period:   4
            3                350.000                   1
            5                344.374                   2
            6                481.870                   2
            7                563.751                   2
            8                270.223                   2
           10                242.447                   1
           11                107.055                   1
           12                392.073                   2
        Stress Period:   5
            1                423.055                   2
            2                198.286                   2
            3                350.000                   1
            5                407.335                   2
            6                482.275                   2
            7                397.610                   2
            8                277.517                   2
           10                257.210                   1
           11                134.971                   1
           12                377.257                   2
        Stress Period:   6
            1                696.104                   2
            2                147.429                   2
            3                350.000                   1
            5                344.031                   2
            6                569.756                   2
            7                690.192                   2
            8                183.397                   2
           12                397.195                   2

   Number of New Extraction Wells in Each Stress Period
            8
            0
            0
            0
            2
            0

   Total Pumping Rate in Each Stress Period (gpm)
        Pumping Rate
        ------------
          2486.244
          2632.270
          2644.140
```

```
            2751.792
            3305.517
            3378.104


                           Objective Function Calculation
                           ------------------------------

     The Capital Costs of New Wells (thousand of dollars)
          3602.053

     The Capital Costs of Treatment Plant (thousand of dollars)
           978.104

     The Capital Costs of Discharge Piping (thousand of dollars)
          1467.156

     The Fixed Costs of O&M (thousand of dollars)
          2189.114

     The Fixed Costs of Sampling (thousand of dollars)
          5710.732

     The Variable Costs of Electricity for Operating Wells (thousand
of dollars)
          2431.264

     The Variable Costs of Treatment (thousand of dollars)
          2028.462

     The Variable Costs of Discharge (thousand of dollars)
           473.069

     The Objective Function Value (thousands of dollars) for
Formulation #  2
         18879.953


                           Constraints Check-Out
                           ---------------------


     --- Modification Occurrence Constraint ---

     The Modification Occurrence Constraint Satisfied


     --- Cleanup Year Constraint ---

     The Cleanup Year
             30
     The Cleanup Year Constraint Satisfied
```

```
--- Plume Containment Constraint ---

The Plume Containment Constraint Satisfied

--- Pumping Limit Constraint ---

The Pumping Limit Constraint Satisfied

--- Well Restricted Areas Constraint ---

The Well Restricted Areas Constraint Satisfied

--- Remediation Well Location Constraint ---

The Remediation Well Location Constraint Satisfied

--- Dry Cell Constraint ---

The Dry Cell Constraint Satisfied

--- Irrigation Well Constraint ---

The Irrigation Well Constraint Satisfied

--- Well Screen Constraint ---

The Well Screen Constraint Satisfied

Number of Constraints Not Satisfied
         0
```

Appendix C. Post processor evaluation of Strategy USU3A.

```
                    Intermediate Variables Calculation
                    ----------------------------------

     Cleanup Year for TCE
          > 30 years
     Cleanup Year for TNT
           > 30 years
     Cleanup Year for Formulation  3
           > 30 years

     Number of Irrigation Wells and Total Rates
          Season          Number of Wells          Total Rate (gpm)
          ------          ---------------          ----------------
              1                12                        2100.000
              2               951                       54298.152

     Total Number of Wells In Each Stress Period
          Stress Period
          -------------
              1                  24
              2                  24
              3                  24
              4                  24
              5                  25
              6                  24

     Extraction Well Rates (Combining Multi-Aquifer Wells)
          Well Index        Well Rate (gpm)        Screen Layers
          ----------        ---------------        -------------
          Stress Period:   1
              1                189.616                   1
              2                 75.740                   1
              3                145.091                   1
              4                156.800                   1
              5                 51.434                   1
              6                277.403                   1
              7                 23.444                   1
              8                 21.652                   1
              9                 17.657                   1
             10                 15.361                   1
             11                 52.592                   2
             12                 56.395                   2
             13                128.197                   2
             14                146.213                   1
             15                166.629                   2
             16                 65.164                   1
             17                 69.896                   1
             18                 86.691                   2
```

19	56.104	2
20	87.730	1
21	72.727	1
22	61.647	1
23	57.377	1
24	57.065	1
Stress Period: 2		
1	189.616	1
2	75.740	1
3	145.091	1
4	156.800	1
5	51.434	1
6	277.403	1
7	23.444	1
8	21.652	1
9	17.657	1
10	15.361	1
11	52.592	2
12	56.395	2
13	128.197	2
14	146.213	1
15	166.629	2
16	65.164	1
17	68.083	1
18	87.730	2
19	56.925	2
20	87.730	1
21	72.727	1
22	61.647	1
23	57.377	1
24	57.065	1
Stress Period: 3		
1	189.616	1
2	75.740	1
3	145.091	1
4	156.800	1
5	51.434	1
6	277.403	1
7	23.444	1
8	21.652	1
9	17.657	1
10	15.361	1
11	52.592	2
12	56.395	2
13	128.197	2
14	146.213	1
15	166.629	2
16	65.164	1
17	68.083	1
18	87.730	2
19	56.925	2
20	87.730	1

21	72.727	1
22	61.647	1
23	57.377	1
24	57.065	1
Stress Period: 4		
1	189.616	1
2	75.740	1
3	145.091	1
4	156.800	1
5	51.434	1
6	277.403	1
7	23.444	1
8	21.652	1
9	17.657	1
10	15.361	1
11	52.592	2
12	56.395	2
13	128.197	2
14	146.213	1
15	166.629	2
16	65.164	1
17	68.083	1
18	87.730	2
19	56.925	2
20	87.730	1
21	72.727	1
22	61.647	1
23	57.377	1
24	57.065	1
Stress Period: 5		
1	189.616	1
2	65.294	1
3	145.091	1
4	156.800	1
5	51.434	1
6	277.403	1
7	23.444	1
8	21.652	1
9	17.657	1
10	15.361	1
11	52.592	2
12	56.395	2
13	128.197	2
14	146.213	1
15	166.629	2
16	65.164	1
17	68.083	1
18	87.730	2
19	56.925	2
20	87.730	1
21	72.727	1
22	61.647	1

23	57.377	1
24	57.065	1
25	10.447	1
Stress Period: 6		
1	155.870	1
3	145.091	1
4	156.800	1
5	51.434	1
6	277.403	1
7	23.444	1
8	21.652	1
9	17.657	1
10	15.361	1
11	52.592	2
12	56.395	2
13	128.197	2
14	146.213	1
15	174.421	2
16	65.164	1
17	68.083	1
18	113.704	2
19	56.925	2
20	87.730	1
21	83.117	1
22	83.143	1
23	57.377	1
24	57.065	1
25	33.704	1

Number of New Extraction Wells in Each Stress Period

24
0
0
0
1
0

Total Pumping Rate in Each Stress Period (gpm)

Pumping Rate
2138.623
2138.670
2138.670
2138.670
2138.670
2128.540

Objective Function Calculation

The Objective Function Value (gpm) for Formulation # 3

```
      2138.670

                  Constraints Check-Out
                  ---------------------

 --- Modification Occurrence Constraint ---

 The Modification Occurrence Constraint Satisfied

 --- Plume Containment Constraint ---

 The Plume Containment Constraint Satisfied

 --- Pumping Limit Constraint ---

 The Pumping Limit Constraint Satisfied

 --- Well Restricted Areas Constraint ---

 The Well Restricted Areas Constraint Satisfied

 --- Remediation Well Location Constraint ---

 The Remediation Well Location Constraint Satisfied

 --- Dry Cell Constraint ---

 The Dry Cell Constraint Satisfied

 --- Irrigation Well Constraint ---

 The Irrigation Well Constraint Satisfied

 --- Well Screen Constraint ---

 The Well Screen Constraint Satisfied

 --- Maximum Number of New Wells Constraint ---

 Total Number of New Wells Ever Installed
         25
```

```
The Maximum Number of New Wells Constraint Satisfied


Number of Constraints Not Satisfied
         0
```

Appendix D. Post processor evaluation of Strategy USU3A’.

Intermediate Variables Calculation

Cleanup Year for TCE
> 30 years
Cleanup Year for TNT
> 30 years
Cleanup Year for Formulation 3
> 30 years

Number of Irrigation Wells and Total Rates

Season	Number of Wells	Total Rate (gpm)
1	12	2100.000
2	951	54298.152

Total Number of Wells In Each Stress Period

Stress Period	
1	25
2	25
3	25
4	25
5	25
6	23

Extraction Well Rates (Combining Multi-Aquifer Wells)

Well Index	Well Rate (gpm)	Screen Layers
Stress Period: 1		
1	189.616	1
2	75.740	1
3	145.091	1
4	156.800	1
5	51.434	1
6	272.208	1
7	15.652	1
8	14.899	1
9	13.018	1
10	12.764	1
11	57.787	2
12	56.395	2
13	102.223	2
14	146.213	1
15	177.018	2
16	65.164	1
17	68.083	1

18	83.574	2
19	56.925	2
20	87.730	1
21	77.922	1
22	77.231	1
23	57.377	1
24	57.065	1
25	5.195	1
Stress Period: 2		
1	189.616	1
2	75.740	1
3	145.091	1
4	156.800	1
5	51.434	1
6	272.208	1
7	15.652	1
8	14.899	1
9	13.018	1
10	12.764	1
11	57.787	2
12	56.395	2
13	102.223	2
14	146.213	1
15	177.018	2
16	65.164	1
17	68.083	1
18	83.574	2
19	56.925	2
20	87.730	1
21	77.922	1
22	77.231	1
23	57.377	1
24	57.065	1
25	5.195	1
Stress Period: 3		
1	189.616	1
2	75.740	1
3	145.091	1
4	156.800	1
5	51.434	1
6	272.208	1
7	15.652	1
8	14.899	1
9	13.018	1
10	12.764	1
11	57.787	2
12	56.395	2
13	102.223	2
14	146.213	1
15	177.018	2
16	65.164	1
17	68.083	1

18	83.574	2
19	56.925	2
20	87.730	1
21	77.922	1
22	77.231	1
23	57.377	1
24	57.065	1
25	5.195	1
Stress Period: 4		
1	189.616	1
2	75.740	1
3	145.091	1
4	156.800	1
5	51.434	1
6	272.208	1
7	15.652	1
8	14.899	1
9	13.018	1
10	12.764	1
11	57.787	2
12	56.395	2
13	102.223	2
14	146.213	1
15	177.018	2
16	65.164	1
17	68.083	1
18	83.574	2
19	56.925	2
20	87.730	1
21	77.922	1
22	77.231	1
23	57.377	1
24	57.065	1
25	5.195	1
Stress Period: 5		
1	189.616	1
2	65.294	1
3	145.091	1
4	156.800	1
5	51.434	1
6	272.208	1
7	15.652	1
8	14.899	1
9	13.018	1
10	12.764	1
11	57.787	2
12	56.395	2
13	102.223	2
14	146.213	1
15	177.018	2
16	65.164	1
17	68.083	1

```
         18                   83.574                    2
         19                   56.925                    2
         20                   87.730                    1
         21                   77.922                    1
         22                   77.231                    1
         23                   57.377                    1
         24                   57.065                    1
         25                   15.642                    1
      Stress Period:   6
          3                  145.091                    1
          4                  156.800                    1
          5                   51.434                    1
          6                  280.732                    1
          7                   15.652                    1
          8                   14.899                    1
          9                   13.018                    1
         10                   12.764                    1
         11                   57.787                    2
         12                   66.784                    2
         13                  102.223                    2
         14                  146.213                    1
         15                  270.525                    2
         16                   65.164                    1
         17                   68.083                    1
         18                  134.483                    2
         19                   98.483                    2
         20                   87.730                    1
         21                   83.117                    1
         22                   93.532                    1
         23                   57.377                    1
         24                   57.065                    1
         25                   44.094                    1


 Number of New Extraction Wells in Each Stress Period
         25
          0
          0
          0
          0
          0

 Total Pumping Rate in Each Stress Period (gpm)
      Pumping Rate
      ------------
        2123.122
        2123.122
        2123.122
        2123.122
        2123.122
        2123.049
```

```
                    Objective Function Calculation
                    ------------------------------

    The Objective Function Value (gpm) for Formulation #  3
         2123.122

                    Constraints Check-Out
                    ---------------------


    --- Modification Occurrence Constraint ---

    The Modification Occurrence Constraint Satisfied


    --- Plume Containment Constraint ---

    The Plume Containment Constraint Satisfied


    --- Pumping Limit Constraint ---

    The Pumping Limit Constraint Satisfied


    --- Well Restricted Areas Constraint ---

    The Well Restricted Areas Constraint Satisfied


    --- Remediation Well Location Constraint ---

    The Remediation Well Location Constraint Satisfied


    --- Dry Cell Constraint ---

    The Dry Cell Constraint Satisfied


    --- Irrigation Well Constraint ---

    The Irrigation Well Constraint Satisfied


    --- Well Screen Constraint ---

    The Well Screen Constraint Satisfied
```

```
--- Maximum Number of New Wells Constraint ---

Total Number of New Wells Ever Installed
        25

The Maximum Number of New Wells Constraint Satisfied


Number of Constraints Not Satisfied
         0
```

Appendix E. Post processor evaluation of Strategy USU3B'.

```
                      Intermediate Variables Calculation
                      ----------------------------------

     Cleanup Year for TCE
          > 30 years
     Cleanup Year for TNT
           > 30 years
     Cleanup Year for Formulation  3
           > 30 years

     Number of Irrigation Wells and Total Rates
          Season          Number of Wells          Total Rate (gpm)
          ------          ---------------          ----------------
              1                 12                     2100.000
              2                951                    54298.152

     Total Number of Wells In Each Stress Period
          Stress Period
          -------------
              1                   24
              2                   24
              3                   24
              4                   24
              5                   24
              6                   24

     Extraction Well Rates (Combining Multi-Aquifer Wells)
          Well Index        Well Rate (gpm)        Screen Layers
          ----------        ---------------        -------------
          Stress Period:   1
              1                  98.597                  1
              2                  75.590                  1
              3                  65.517                  1
              4                  93.834                  1
              5                 180.265                  1
              6                  74.244                  1
              7                  73.366                  1
              8                 118.732                  1
              9                  42.494                  1
             10                 245.896                  1
             11                 290.909                  1
             12                  76.686                  1
             13                  61.086                  1
             14                 137.340                  1
             15                 136.888                  1
             16                  88.306                  1
             17                  81.335                  1
```

18	150.831	1
19	198.187	1
20	98.930	1
21	95.610	1
22	72.821	1
23	102.696	1
24	32.203	1
Stress Period: 2		
1	98.597	1
2	75.590	1
3	65.517	1
4	93.834	1
5	180.265	1
6	74.244	1
7	73.366	1
8	118.732	1
9	42.494	1
10	245.896	1
11	290.909	1
12	76.686	1
13	61.086	1
14	137.340	1
15	136.888	1
16	88.306	1
17	81.335	1
18	150.831	1
19	198.187	1
20	98.930	1
21	95.610	1
22	72.821	1
23	102.696	1
24	32.203	1
Stress Period: 3		
1	98.597	1
2	75.590	1
3	65.517	1
4	93.834	1
5	180.265	1
6	74.244	1
7	73.366	1
8	118.732	1
9	42.494	1
10	245.896	1
11	290.909	1
12	76.686	1
13	61.086	1
14	137.340	1
15	136.888	1
16	88.306	1
17	81.335	1
18	150.831	1
19	198.187	1

20	98.930	1
21	95.610	1
22	72.821	1
23	102.696	1
24	32.203	1
Stress Period: 4		
1	98.597	1
2	75.590	1
3	65.517	1
4	93.834	1
5	180.265	1
6	74.244	1
7	73.366	1
8	118.732	1
9	42.494	1
10	245.896	1
11	290.909	1
12	76.686	1
13	61.086	1
14	137.340	1
15	136.888	1
16	88.306	1
17	81.335	1
18	150.831	1
19	198.187	1
20	98.930	1
21	95.610	1
22	72.821	1
23	102.696	1
24	32.203	1
Stress Period: 5		
1	98.597	1
2	75.590	1
3	65.517	1
4	93.834	1
5	180.265	1
6	74.244	1
7	73.366	1
8	118.732	1
9	42.494	1
10	245.896	1
11	290.909	1
12	76.686	1
13	61.086	1
14	137.340	1
15	136.888	1
16	88.306	1
17	81.335	1
18	150.831	1
19	198.187	1
20	98.930	1
21	95.610	1

22	72.821	1
23	102.696	1
24	32.203	1
Stress Period: 6		
1	98.597	1
2	75.590	1
3	65.517	1
4	93.834	1
5	180.265	1
6	74.244	1
7	73.366	1
8	118.732	1
9	42.494	1
10	245.896	1
11	290.909	1
12	76.686	1
13	61.086	1
14	137.340	1
15	136.888	1
16	88.306	1
17	81.335	1
18	150.831	1
19	198.187	1
20	98.930	1
21	95.610	1
22	72.821	1
23	102.696	1
24	32.203	1

Number of New Extraction Wells in Each Stress Period

24
0
0
0
0
0

Total Pumping Rate in Each Stress Period (gpm)

Pumping Rate
2692.364
2692.364
2692.364
2692.364
2692.364
2692.364

Objective Function Calculation

The Objective Function Value (gpm) for Formulation # 3

```
      2692.364

                       Constraints Check-Out
                       ---------------------

   --- Modification Occurrence Constraint ---

   The Modification Occurrence Constraint Satisfied

   --- Plume Containment Constraint ---

   The Plume Containment Constraint Satisfied

   --- Pumping Limit Constraint ---

   The Pumping Limit Constraint Satisfied

   --- Well Restricted Areas Constraint ---

   The Well Restricted Areas Constraint Satisfied

   --- Remediation Well Location Constraint ---

   The Remediation Well Location Constraint Satisfied

   --- Dry Cell Constraint ---

   The Dry Cell Constraint Satisfied

   --- Irrigation Well Constraint ---

   The Irrigation Well Constraint Satisfied

   --- Well Screen Constraint ---

   The Well Screen Constraint Satisfied

   --- Maximum Number of New Wells Constraint ---

   Total Number of New Wells Ever Installed
           24
```

```
The Maximum Number of New Wells Constraint Satisfied


Number of Constraints Not Satisfied
         0
```

Appendix F. Post processor evaluation of Strategy USU3C'.

```
                    Intermediate Variables Calculation
                    ----------------------------------

    Cleanup Year for TCE
         > 30 years
    Cleanup Year for TNT
          > 30 years
    Cleanup Year for Formulation  3
          > 30 years

    Number of Irrigation Wells and Total Rates
         Season          Number of Wells          Total Rate (gpm)
         ------          ---------------          ----------------
             1                 12                       2100.000
             2                951                      54298.152

    Total Number of Wells In Each Stress Period
         Stress Period
         -------------
             1                   24
             2                   24
             3                   24
             4                   24
             5                   24
             6                   24

    Extraction Well Rates (Combining Multi-Aquifer Wells)
         Well Index        Well Rate (gpm)        Screen Layers
         ----------        ---------------        -------------
         Stress Period:   1
             1                145.408                   1
             2                116.665                   1
             3                112.218                   1
             4                 95.455                   1
             5                228.883                   1
             6                 90.665                   1
             7                 79.034                   1
             8                135.829                   1
             9                 71.164                   1
            10                281.855                   1
            11                316.883                   1
            12                 80.213                   1
            13                 75.268                   1
            14                167.647                   1
            15                189.200                   1
            16                102.639                   1
            17                133.429                   1
```

18	155.330	1
19	178.592	1
20	107.771	1
21	132.810	1
22	87.242	1
23	126.587	1
24	26.000	1
Stress Period: 2		
1	145.408	1
2	116.665	1
3	112.218	1
4	95.455	1
5	228.883	1
6	90.665	1
7	79.034	1
8	135.829	1
9	71.164	1
10	281.855	1
11	316.883	1
12	80.213	1
13	75.268	1
14	167.647	1
15	189.200	1
16	102.639	1
17	133.429	1
18	155.330	1
19	178.592	1
20	107.771	1
21	132.810	1
22	87.242	1
23	126.587	1
24	26.000	1
Stress Period: 3		
1	145.408	1
2	116.665	1
3	112.218	1
4	95.455	1
5	228.883	1
6	90.665	1
7	79.034	1
8	135.829	1
9	71.164	1
10	281.855	1
11	316.883	1
12	80.213	1
13	75.268	1
14	167.647	1
15	189.200	1
16	102.639	1
17	133.429	1
18	155.330	1
19	178.592	1

20	107.771	1
21	132.810	1
22	87.242	1
23	126.587	1
24	26.000	1
Stress Period: 4		
1	145.408	1
2	116.665	1
3	112.218	1
4	95.455	1
5	228.883	1
6	90.665	1
7	79.034	1
8	135.829	1
9	71.164	1
10	281.855	1
11	316.883	1
12	80.213	1
13	75.268	1
14	167.647	1
15	189.200	1
16	102.639	1
17	133.429	1
18	155.330	1
19	178.592	1
20	107.771	1
21	132.810	1
22	87.242	1
23	126.587	1
24	26.000	1
Stress Period: 5		
1	145.408	1
2	116.665	1
3	112.218	1
4	95.455	1
5	228.883	1
6	90.665	1
7	79.034	1
8	135.829	1
9	71.164	1
10	281.855	1
11	316.883	1
12	80.213	1
13	75.268	1
14	167.647	1
15	189.200	1
16	102.639	1
17	133.429	1
18	155.330	1
19	178.592	1
20	107.771	1
21	132.810	1

22	87.242	1
23	126.587	1
24	26.000	1
Stress Period: 6		
1	145.408	1
2	116.665	1
3	112.218	1
4	95.455	1
5	228.883	1
6	90.665	1
7	79.034	1
8	135.829	1
9	71.164	1
10	281.855	1
11	316.883	1
12	80.213	1
13	75.268	1
14	167.647	1
15	189.200	1
16	102.639	1
17	133.429	1
18	155.330	1
19	178.592	1
20	107.771	1
21	132.810	1
22	87.242	1
23	126.587	1
24	26.000	1

Number of New Extraction Wells in Each Stress Period

24
0
0
0
0
0

Total Pumping Rate in Each Stress Period (gpm)

Pumping Rate
3236.784
3236.784
3236.784
3236.784
3236.784
3236.784

Objective Function Calculation

The Objective Function Value (gpm) for Formulation # 3

```
        3236.784

                          Constraints Check-Out
                          ---------------------

    --- Modification Occurrence Constraint ---

    The Modification Occurrence Constraint Satisfied

    --- Plume Containment Constraint ---

    The Plume Containment Constraint Satisfied

    --- Pumping Limit Constraint ---

    The Pumping Limit Constraint Satisfied

    --- Well Restricted Areas Constraint ---

    The Well Restricted Areas Constraint Satisfied

    --- Remediation Well Location Constraint ---

    The Remediation Well Location Constraint Satisfied

    --- Dry Cell Constraint ---

    The Dry Cell Constraint Satisfied

    --- Irrigation Well Constraint ---

    The Irrigation Well Constraint Satisfied

    --- Well Screen Constraint ---

    The Well Screen Constraint Satisfied

    --- Maximum Number of New Wells Constraint ---

    Total Number of New Wells Ever Installed
            24
```

```
The Maximum Number of New Wells Constraint Satisfied


Number of Constraints Not Satisfied
         0
```