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)

<u>Formulation 1 -- Important Notes</u>:

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 $ug/l \times ft^3/year$.
- 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

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

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

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

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.

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

where

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

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.
a is a coefficient accounting for 10% system downtime (90% uptime), a=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)

$$CW_{ij} = 1.423\times10^{-7}(Q_{ij}) \quad \text{for} \quad 0\ \text{ft}^3/\text{year} < Q_{ij} \le 2.811\times10^{7}\ \text{ft}^3/\text{year}$$
$$CW_{ij} = 3.556\times10^{-6}(Q_{ij}) - 6 \quad \text{for} \quad 2.811\times10^{7}\ \text{ft}^3/\text{year} < Q_{ij} \le 7.027\times10^{7}\ \text{ft}^3/\text{year}$$

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.

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

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

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 *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

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

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.

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

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,

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

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^{ij}_{RDX} : the concentration of RDX at grid location (i,j)
C^{ij}_{TNT} : 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 $\left(\text{i.e., } 2.832 \times 10^{-8} \dfrac{\mathrm{L \cdot kg}}{\mathrm{ft^3} \cdot m\mathrm{g}}\right)$

$\mathbf{M_{TNT}}$: 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$\times$ft^3 to kg $\left(\text{i.e., } 2.832 \times 10^{-8} \dfrac{\text{L} \cdot \text{kg}}{\text{ft}^3 \cdot m\text{g}}\right)$

Formulation 3 -- Constraints

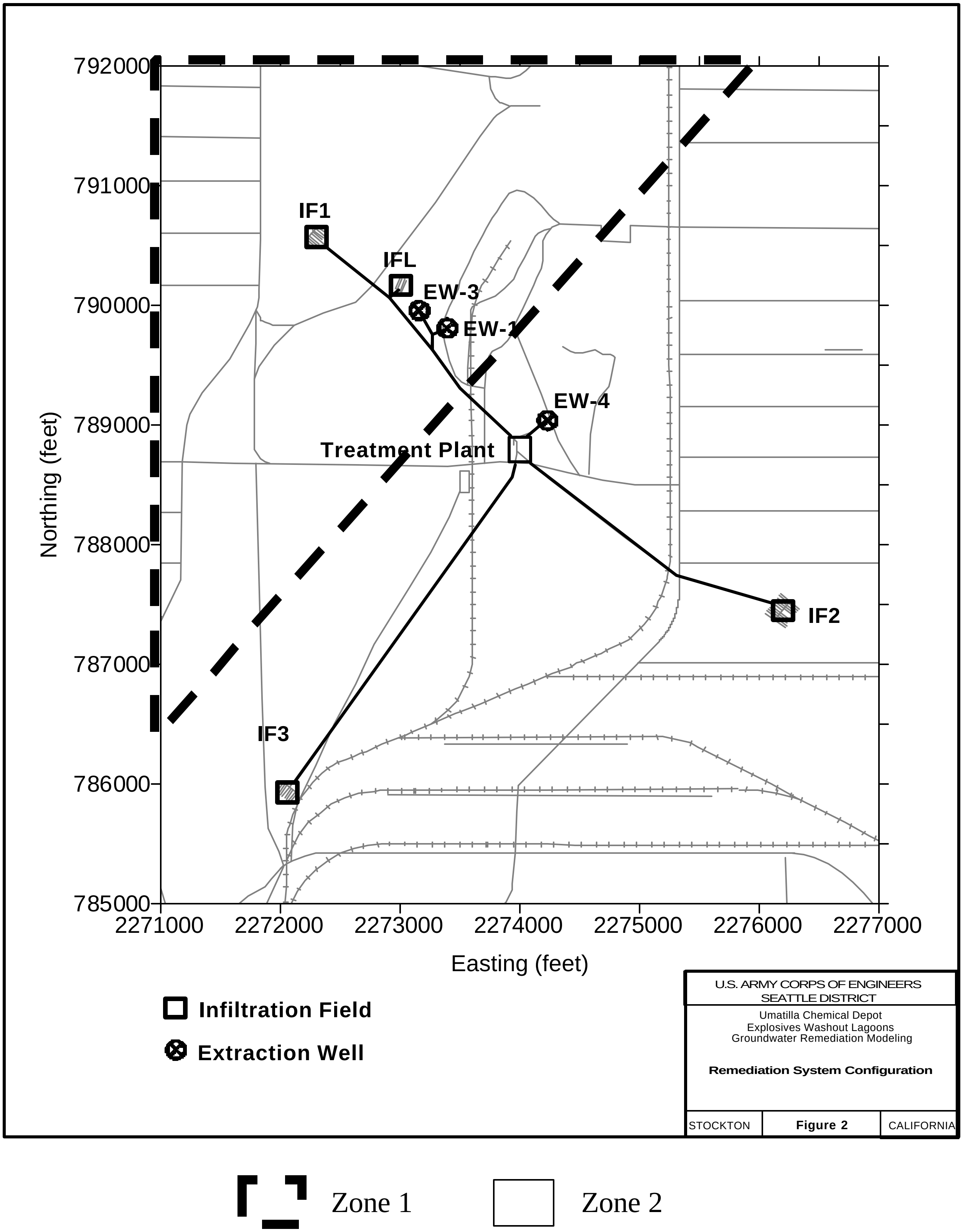
Same as Formulation 1, plus the following constraints:

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



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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

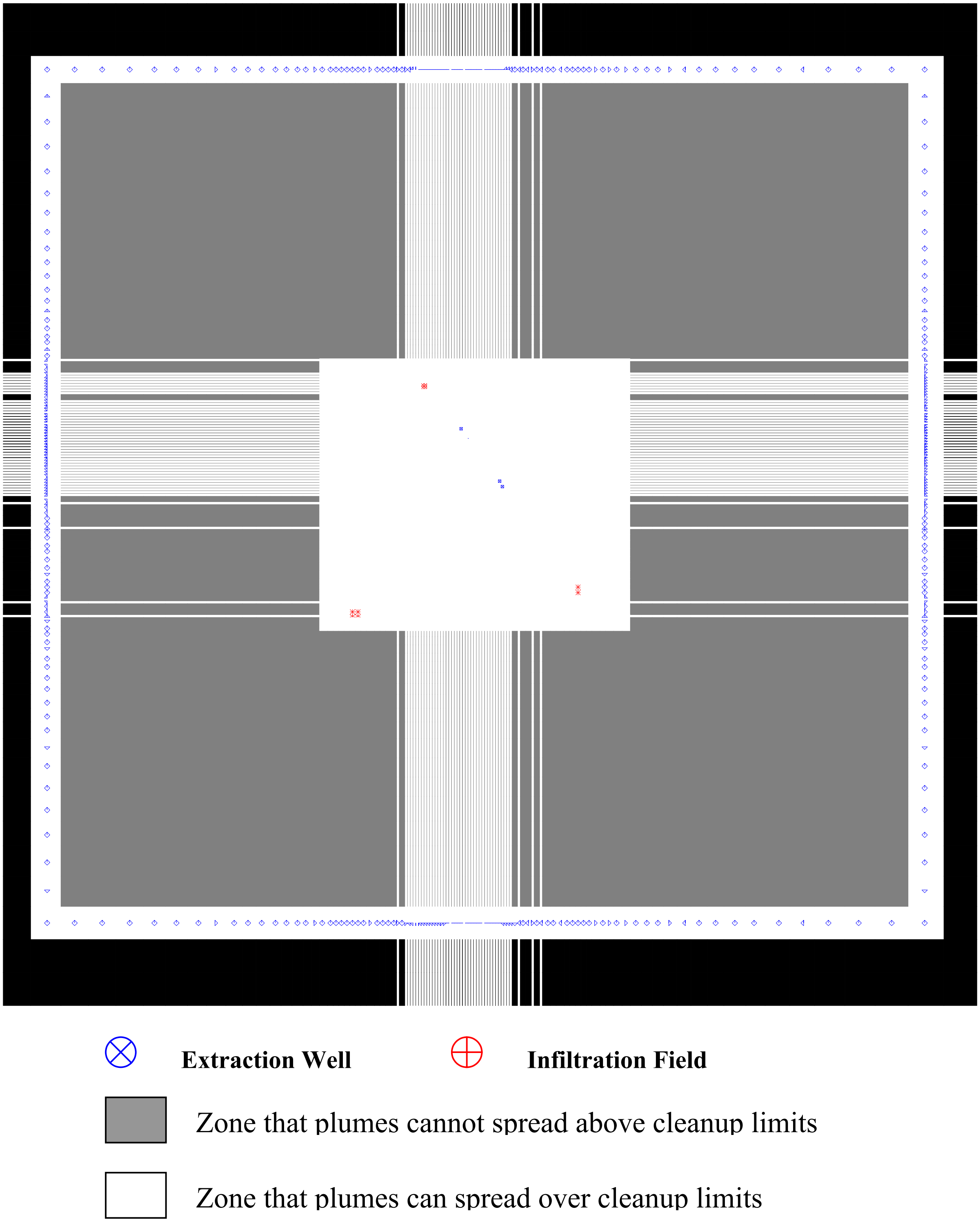
Extraction Well
Infiltration Field
Zone that plumes cannot spread above cleanup limits
Zone that plumes can spread over cleanup limits

Figure 2