

FINAL

**OPTIMAL PUMPING STRATEGIES
FOR
UMATILLA CHEMICAL DEPOT RDX AND TNT PLUMES**

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

31 Dec 2002

TABLE OF CONTENTS

EXECUTIVE SUMMARY	1
INTRODUCTION	3
OPTIMIZATION TECHNIQUE.....	4
FORMULATIONS ADDRESSED.....	4
THE OPTIMIZATION PROCEDURE	5
<i>Preliminaries</i>	5
<i>Formulation 3 process</i>	6
<i>Formulations 1, 2 and 4 processes</i>	6
FORMULATION RESULTS	7
FORMULATION 3.....	8
LEAST COST STRATEGY USU1A.....	8
ALTERNATIVE NEAR-LEAST-COST STRATEGIES USU1B	9
FORMULATION 2.....	11
FORMULATION 4.....	11
SATURATED THICKNESS	12
CONCLUSIONS.....	13
REFERENCES	14

TABLES

Table 1.	Executive summary of optimal strategies for Umatilla Chemical Depot formulations ¹	16
Table 2.	Current, USU1A, & USU1B pumping strategies and results.	17
Table 3.	Twenty-year transient pumping Strategy USU3.....	17
Table 4.	Twenty-year transient pumping Strategy USU4.....	18
Table 5.	Representative example of GA input parameters.	19
Table 6.	Representative example of ANN-GA input parameters.	20

FIGURES

Fig. 1.	Initial (Projected 1 Jan 2002) TNT concentrations exceeding 2.8 ppb, and part of finite difference grid with rows and columns numbered.	21
Fig. 2.	Initial (Projected 1 Jan 2002) RDX concentrations exceeding 2.1 ppb, and part of finite difference grid.	21
Fig. 3.	Preliminary optimization problem: minimize mass remaining after 5 years.	22
Fig. 4.	Production functions for mass removal versus time for current strategy and strategies USU3 and USU4.....	22
Fig. 5.	Marginal functions for mass removal versus time for current strategy and strategies USU3 and USU4.....	23
Fig. 6.	Formulation 1 objective function: minimize present value of cost.....	24

Fig. 7.	Formulation 1 surrogate optimization problem.	24
Fig. 8.	Strategy USU1A: Time series of resulting maximum concentrations.	25
Fig. 9.	Strategy USU1A: RDX concentrations > 2.1 ppb after 1 year of pumping.	26
Fig. 10.	Strategy USU1A: RDX concentrations > 2.1 ppb after 2 years of pumping.	27
Fig. 11.	Strategy USU1A: RDX concentrations > 2.1 ppb after 3 years of pumping.	28
Fig. 12.	Strategy USU1A: TNT concentrations > 2.8 ppb after 1 year of pumping.	29
Fig. 13.	Strategy USU1A: TNT concentrations > 2.8 ppb after 2 years of pumping.	30
Fig. 14.	Strategy USU1A: TNT concentrations > 2.8 ppb after 3 years of pumping.	31
Fig. 15.	Layer 1 hydraulic conductivity distribution (ft/day), and USU4 well locations.	32
Fig. 16.	Some feasible locations of well U-2 and selected robustness ranges.	33
Fig. 17.	Optimization problem addressed by sequential optimization of four 5-year periods: minimize mass remaining after 20 years.	34
Fig. 18.	USU3: heads after five years of pumping, and initial RDX > 2.8 ppb.	34
Fig. 19.	Strategy USU3: time series of mass remaining.	35
Fig. 20.	Formulation 4 optimization problem (minimize cost to reach CL and continued pumping to minimize mass remaining).	36
Fig. 21.	Modified USU4: cost to CLs versus conductivity multiplier.	36
Fig. 22.	Layer 1 bottom elevation and wells U-1, EW-3, and EW-1.	37
Fig. 23.	Row 48, Layers 1-5 bottom elevations (ft MSL).	38
Fig. 24.	Column 57, Layers 1-5, bottom elevations (ft MSL).	38

APPENDICES

Appendix A.	MODFLOW well package of Strategy USU1A.	39
Appendix B.	Post processor evaluation of Strategy USU1A.	40
Appendix C.	MODFLOW well package of Strategy USU1B.	43
Appendix D.	Post processor evaluation of Strategy USU1B and USU4 cost.	44
Appendix E.	MODFLOW well package of Strategy USU3.	47
Appendix F.	Post processor evaluation of Strategy USU3.	49
Appendix G.	MODFLOW well package of Strategy USU4.	52
Appendix H.	Post processor evaluation of Strategy USU4, mass remaining after 20 Years.	53

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 backpropagation 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 ft²/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.

References

Hegazy, M.A. and R.C. Peralta. 1997. Feasibility Considerations of an Optimal Pumping Strategy to Capture TCE/PCE Plume at March AFB, CA. Prepared for Earth Technology Corporation. Report SS/OL 97-1 Systems Simulation/Optimization Laboratory, Dept. of Biological and Irrigation Engineering, Utah State University, Logan, UT, 41 p.

Peralta, R. C. 2001a. Demonstrations in remediation. In Modeling and Management of Emerging Environmental Issues , DuPont Corporation. In press.

Peralta, R. C. 2001b. Remediation simulation/optimization demonstrations. In Proceedings of MODFLOW and Other Modeling Odysseys. 2001. Eds, Seo, Poeter, Zheng and Poeter, Pub. IGWMC. p. 651-657.

Peralta, R.C. and A.H. Aly. 1994. Pumping Strategies Developed to Capture Castle AFB OU-2 TCE Plume. Report SS/OL 96-1 Systems Simulation/Optimization Laboratory, Dept. of Biological and Irrigation Engineering, Utah State University, Logan, UT, 42 p.

Peralta, R.C. and A.H. Aly. 1995. Optimal pumping strategy to capture TCE plume at base boundary, Norton AFB, California, ERC Report No. 1. US Air Force, Air Force Center for Environmental Excellence, Environmental Restoration Directorate. 37 p.

Peralta, R.C. and A.H. *Aly. 1996. Optimal Pumping Strategies for Capturing TCE and DCE Plumes Near Mission Drive, Wurtsmith Air Force Base, Michigan: Feasibility Study. 20 p. Revised version included as section 4 in Basewide Groundwater Flow Model and Simulation/Optimization Modeling for Capture/Cleanup of the Mission Drive Plume. p. 20

Systems Simulation/Optimization Laboratory. 2001. Flow and transport optimization end-of-simulation results: Umatilla Chemical Depot. Interim project completion report and Errata submitted to U. S. Navy. 5 p.

Systems Simulation/Optimization Laboratory and HydroGeoSystems Group. 2001. Simulation/Optimization MOdeling System (SOMOS) users manual. SS/OL, Dept. of Biological and Irrigation Engineering, Utah State University, Logan, Utah. 457 p.

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 Values²					
- Cost to CL	\$1,663,841	≈\$1,664,200	\$1,663,841	N/A	\$1,664,212
- Mass after 20 years	N/A	N/A	N/A	0.2015 kg	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 (K,I,J)	Pumping Rates (GPM) per stress period (SP)			
		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 (K,I,J)	Pumping Rates (GPM) per stress period (SP)			
		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 until 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.

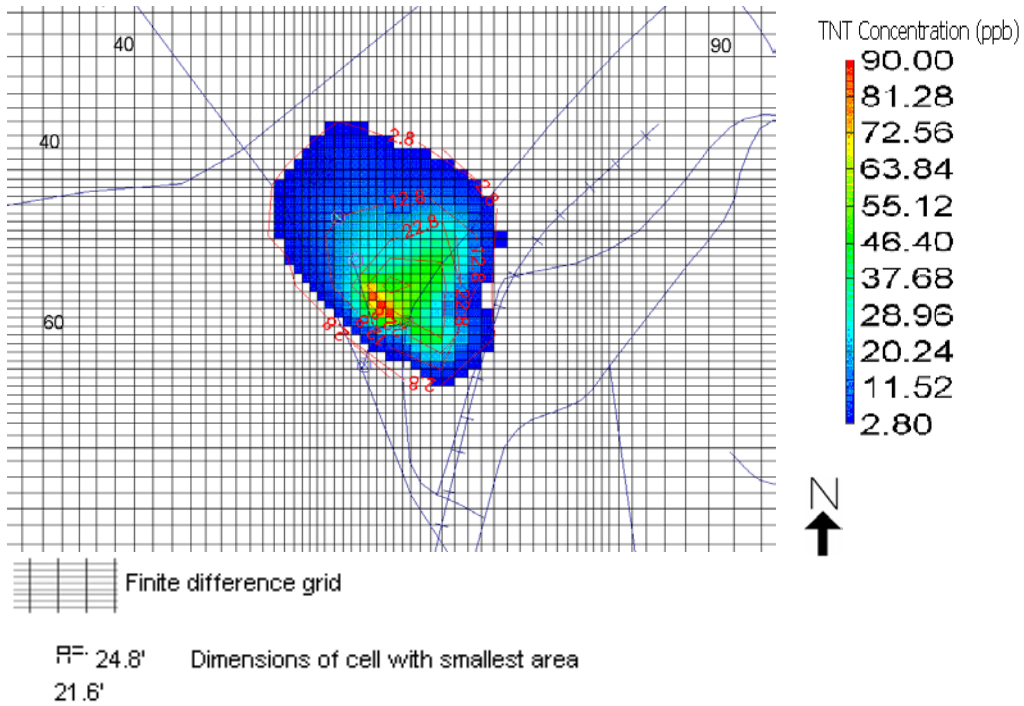


Fig. 2. Initial (Projected 1 Jan 2002) RDX concentrations exceeding 2.1 ppb, and part of finite difference grid.

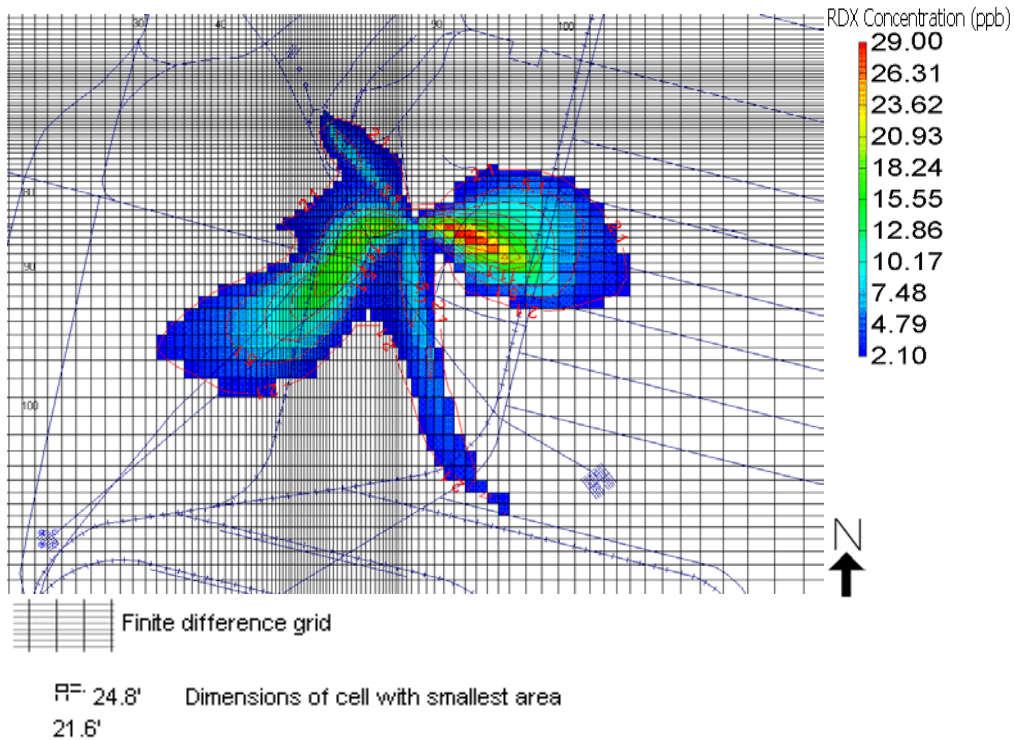


Fig. 3. Preliminary optimization problem: minimize mass remaining after 5 years.

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.

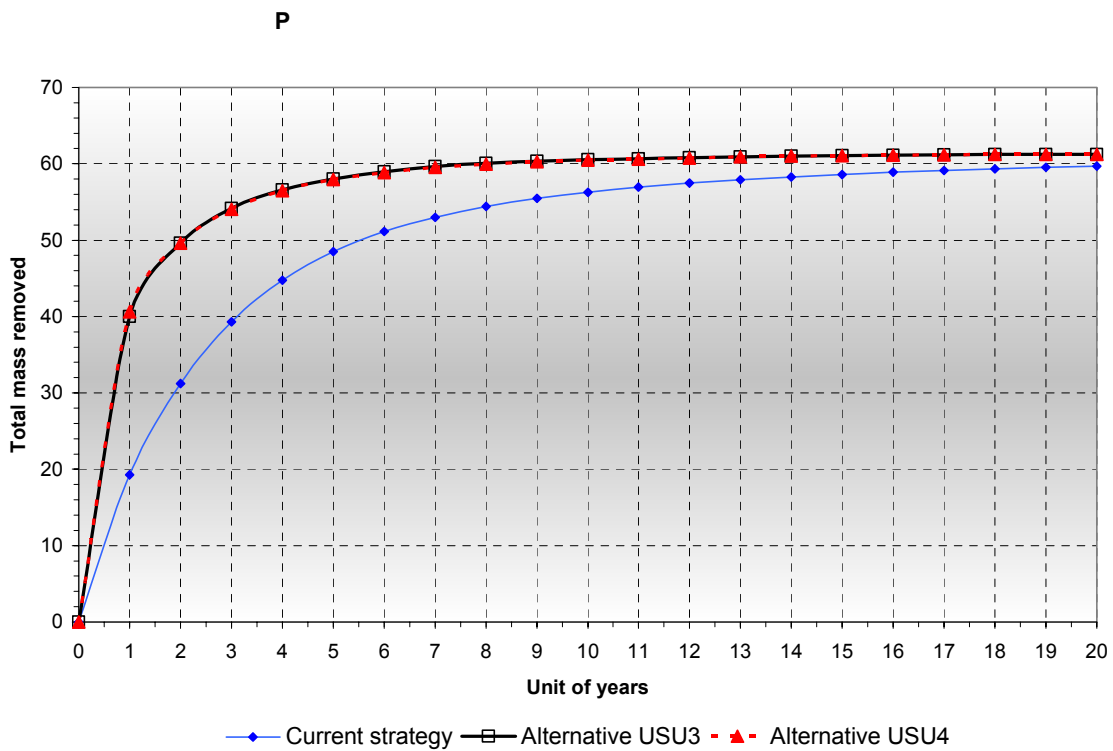


Fig. 5. Marginal functions for mass removal versus time for current strategy and strategies USU3 and USU4.

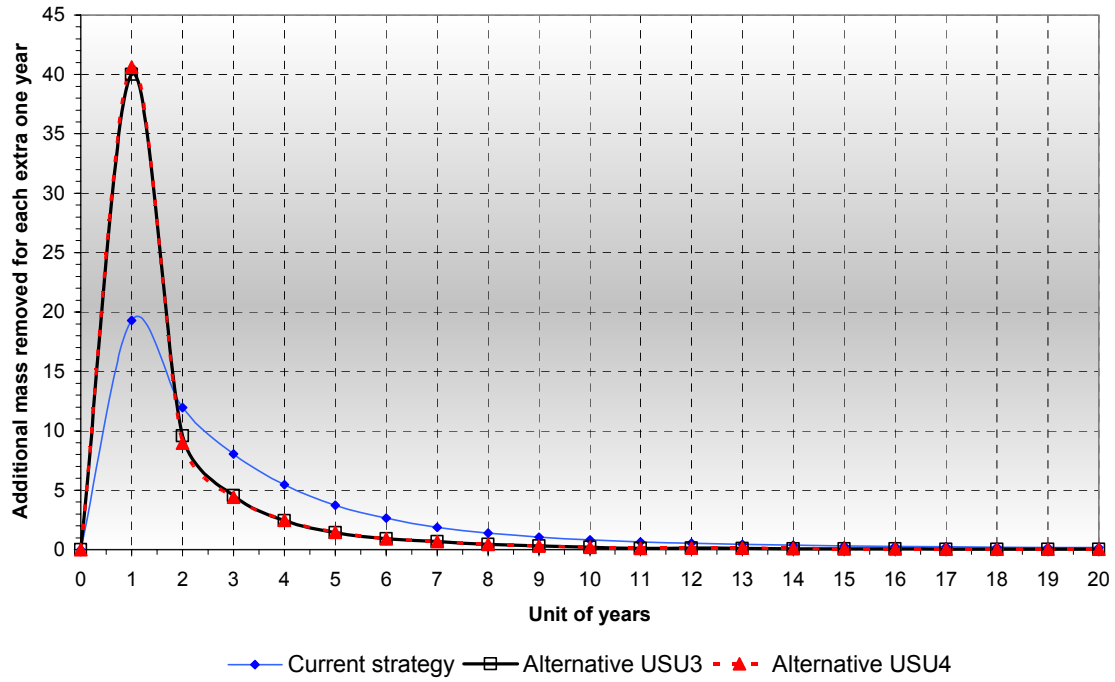


Fig. 6. Formulation 1 objective function: minimize present value of cost.

**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.

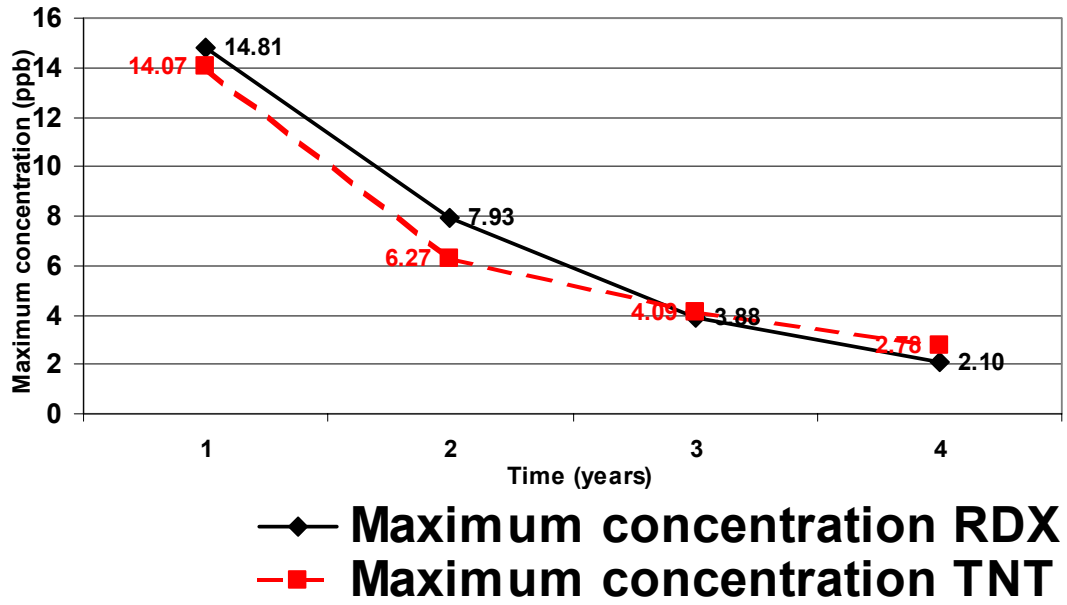


Fig. 9. Strategy USU1A: RDX concentrations ≥ 2.1 ppb after 1 year of pumping.

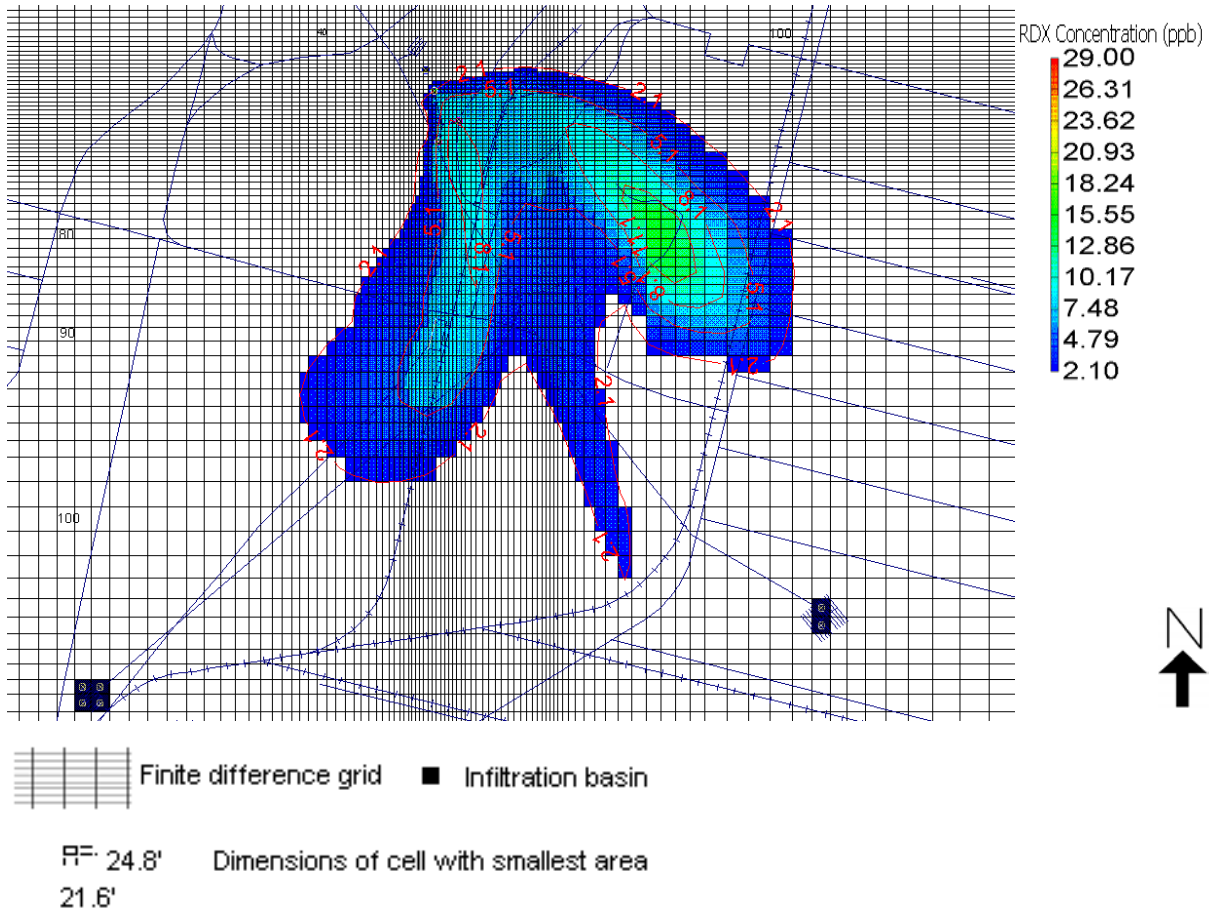


Fig. 10. Strategy USU1A: RDX concentrations ≥ 2.1 ppb after 2 years of pumping.

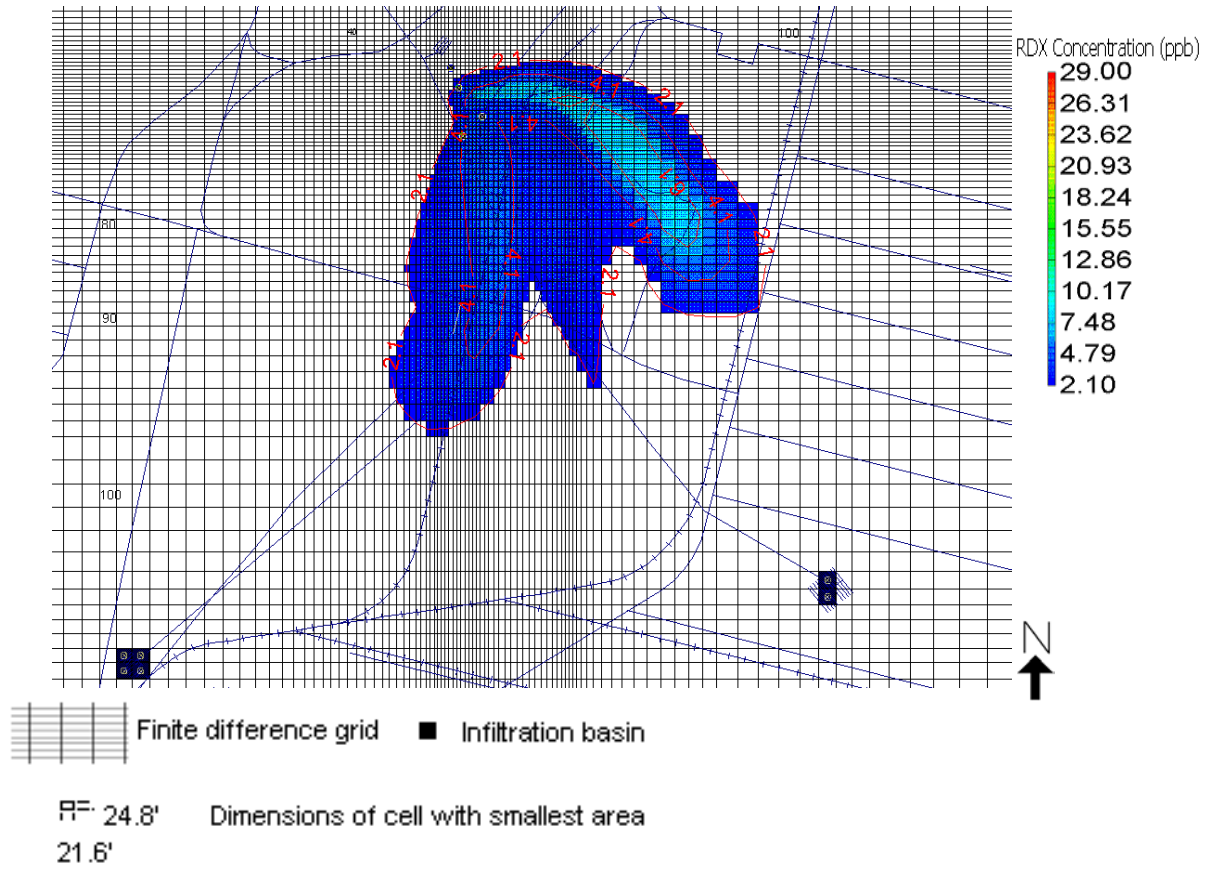


Fig. 11. Strategy USU1A: RDX concentrations ≥ 2.1 ppb after 3 years of pumping.

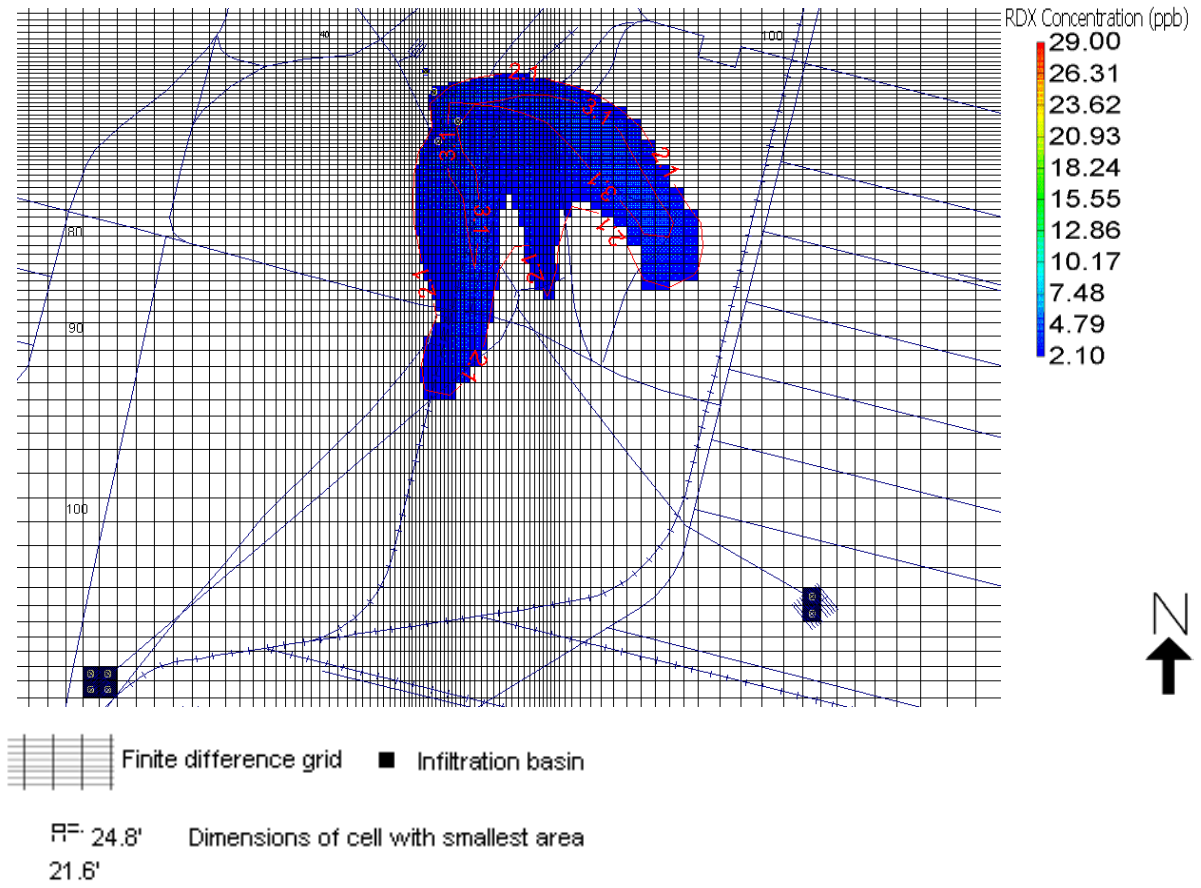


Fig. 12. Strategy USU1A: TNT concentrations ≥ 2.8 ppb after 1 year of pumping.

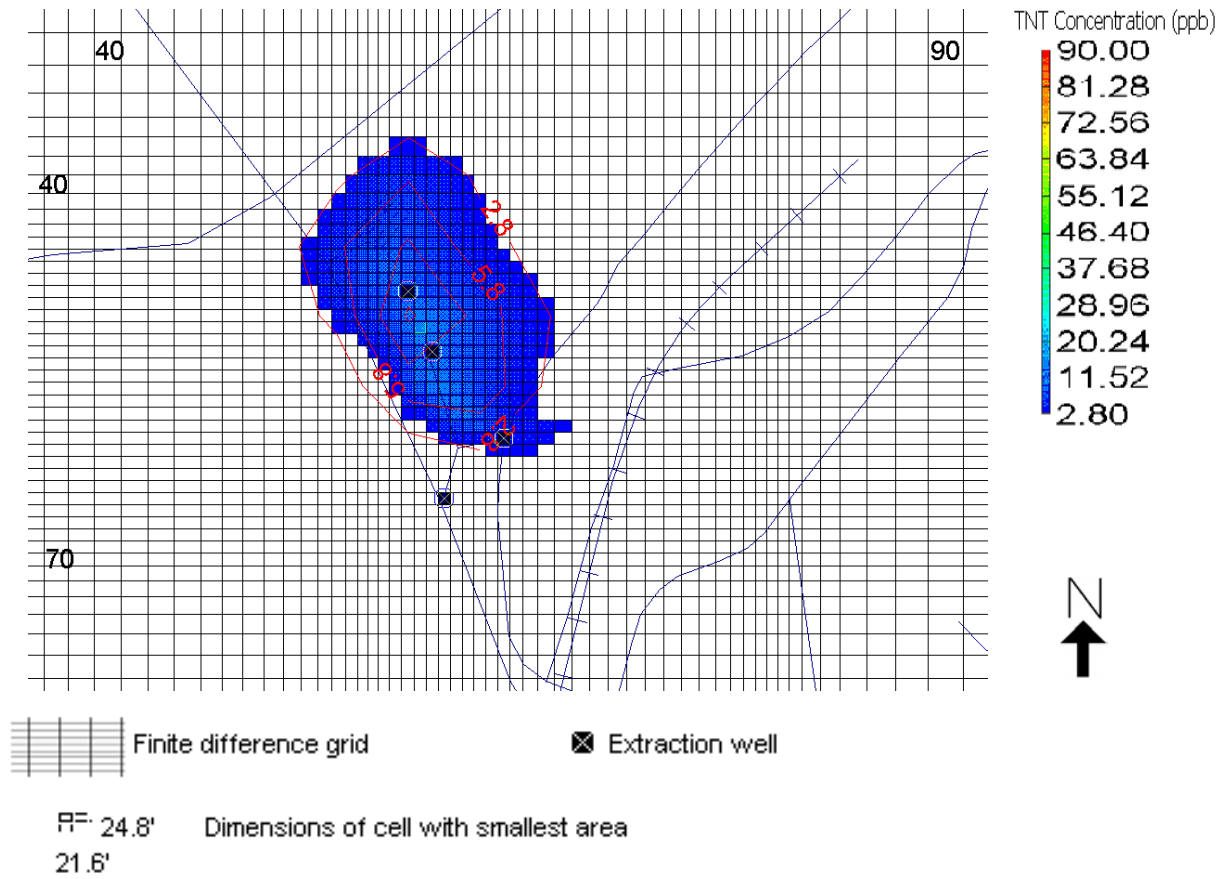


Fig. 13. Strategy USU1A: TNT concentrations ≥ 2.8 ppb after 2 years of pumping.

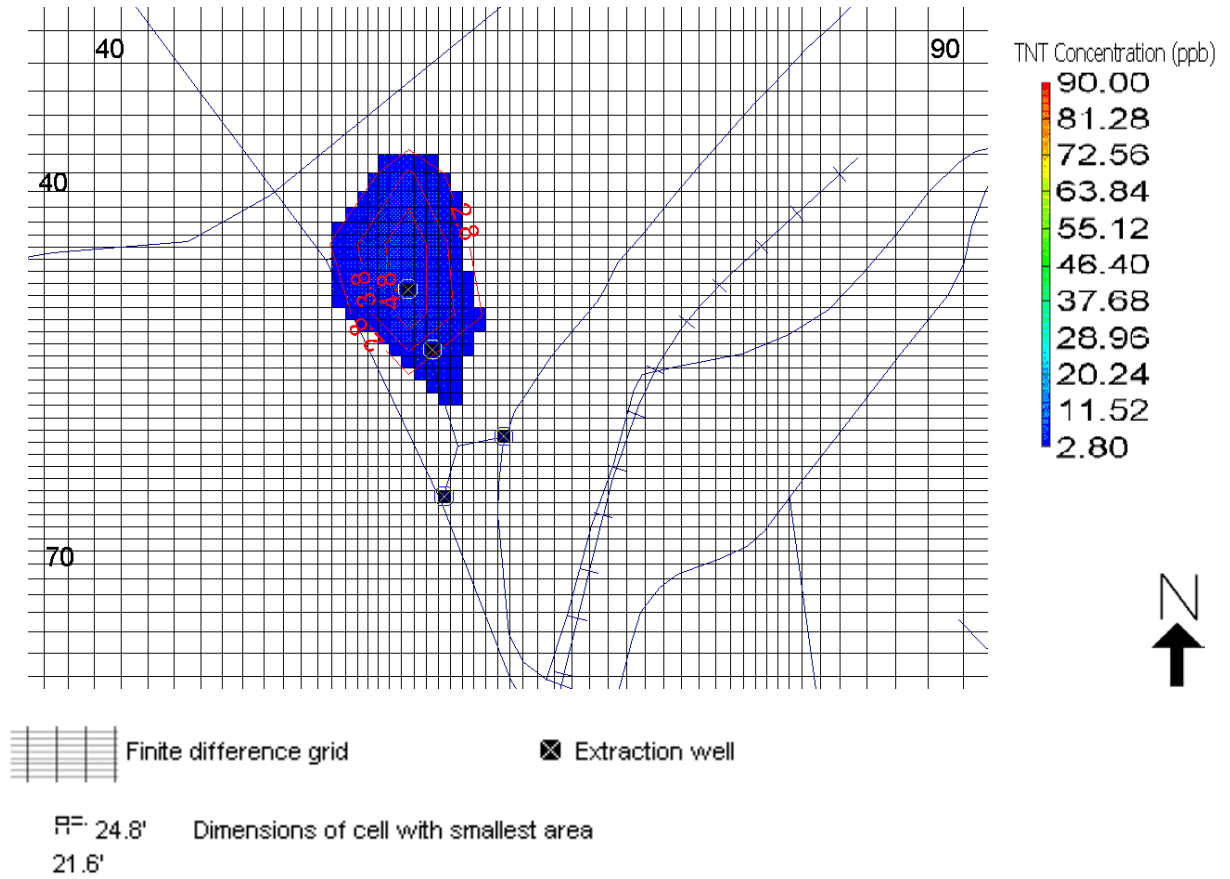


Fig. 14. Strategy USU1A: TNT concentrations ≥ 2.8 ppb after 3 years of pumping.

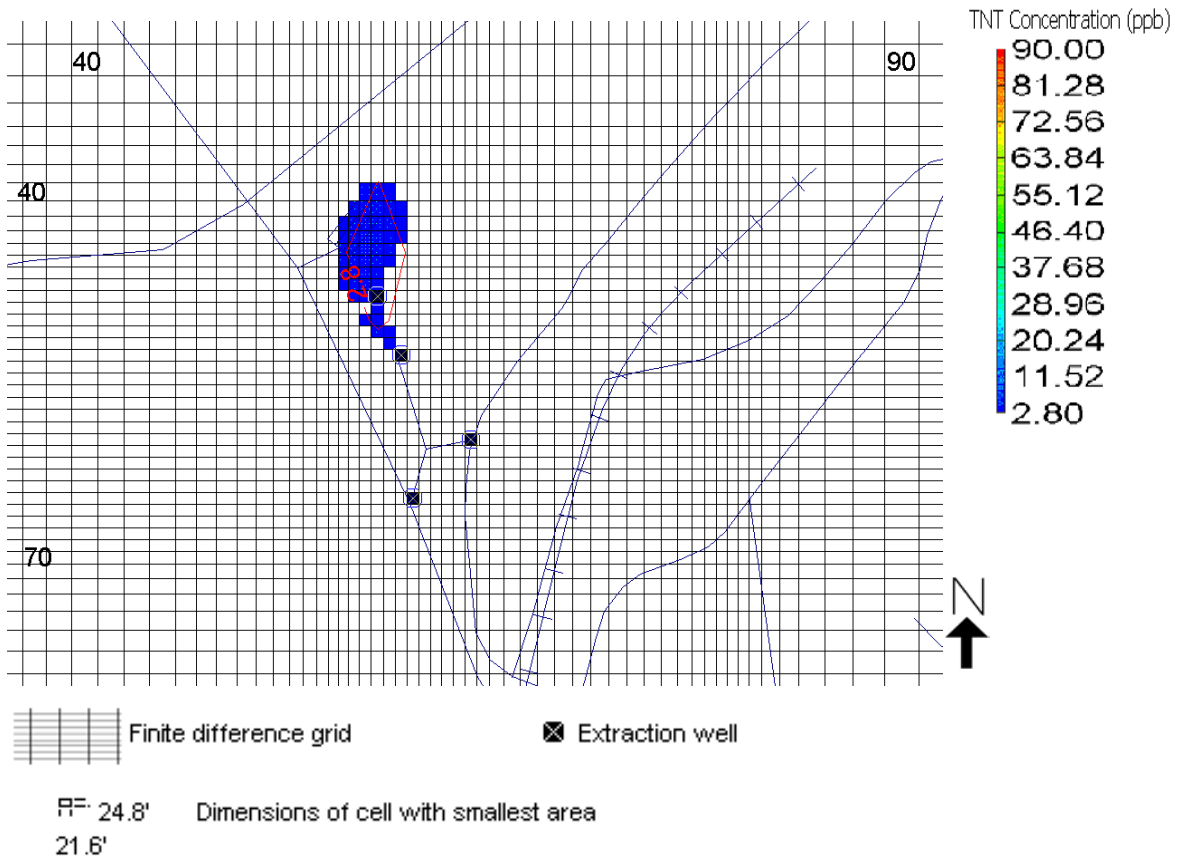


Fig. 15. Layer 1 hydraulic conductivity distribution (ft/day), and USU4 well locations.

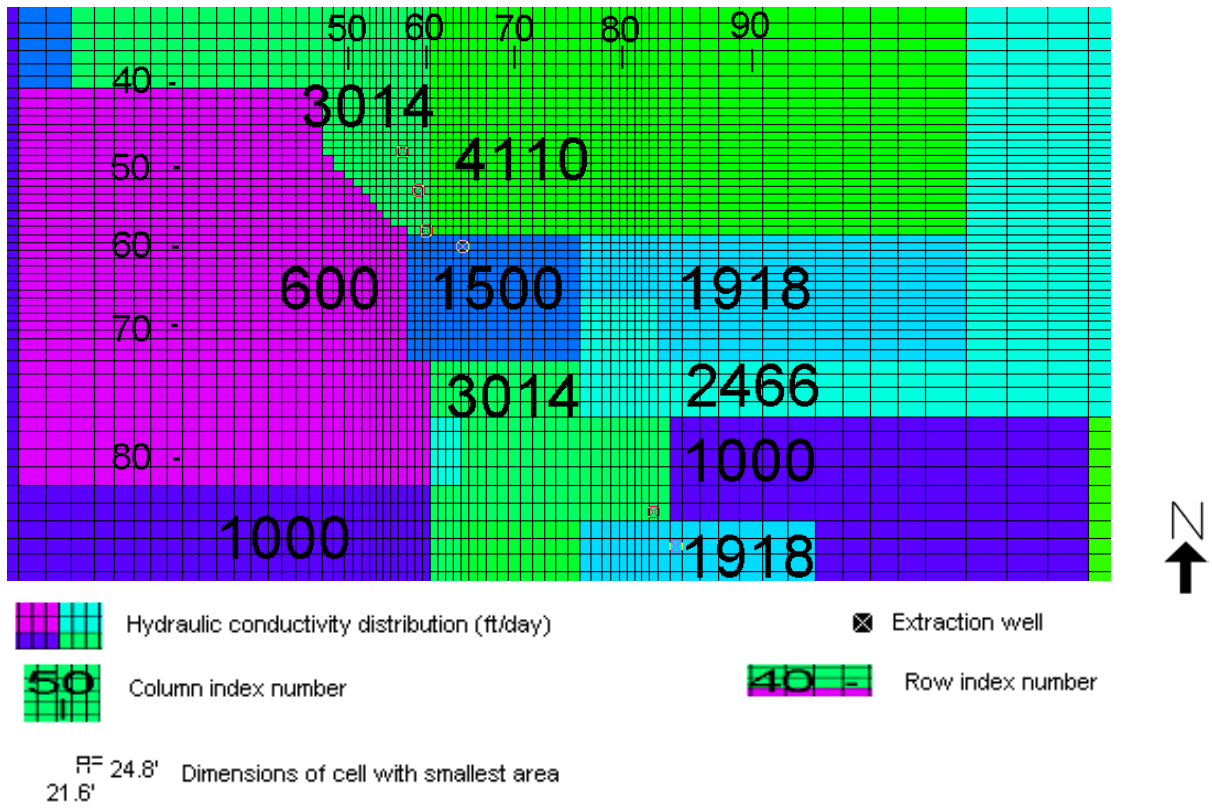
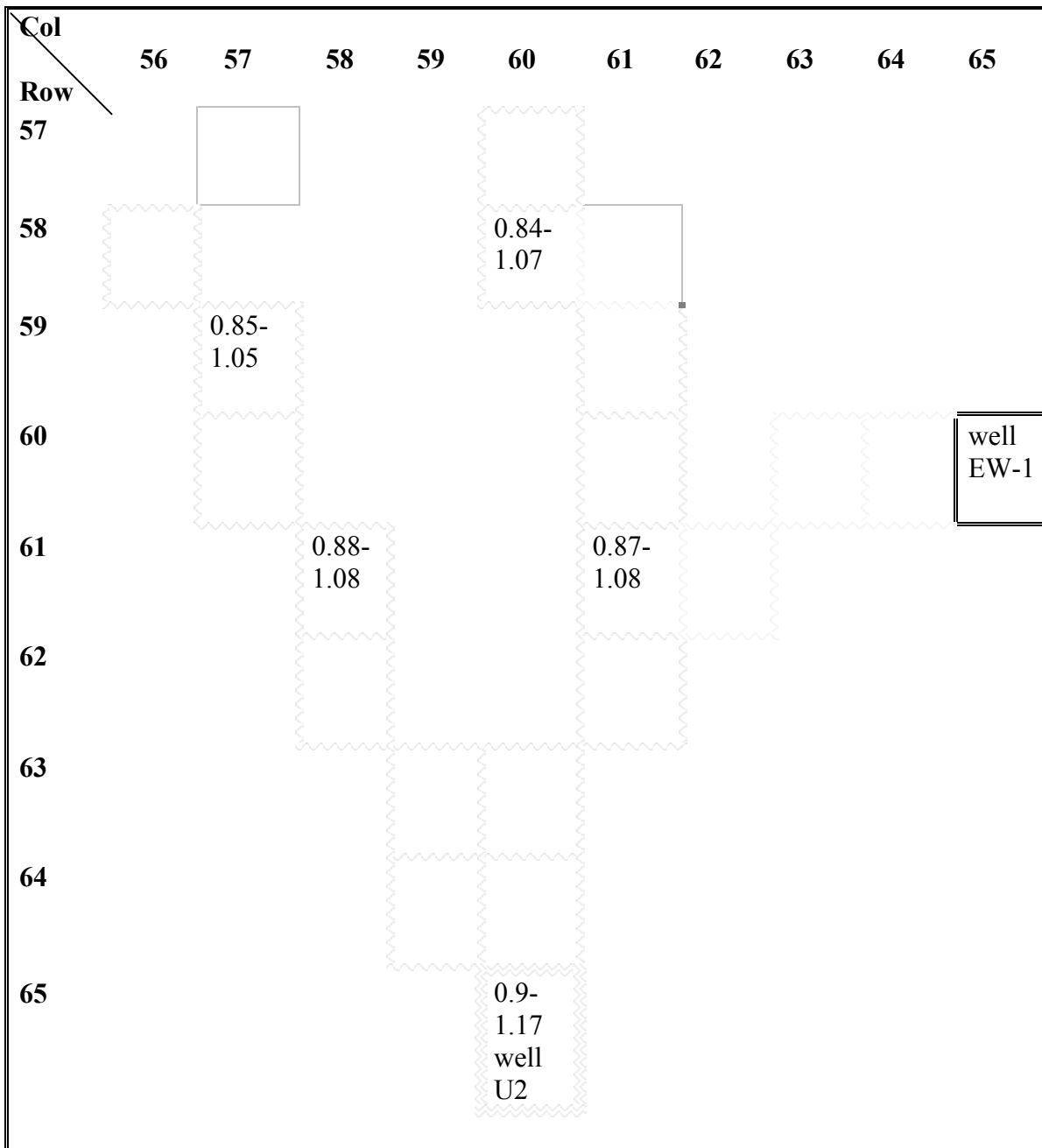


Fig. 16. Some feasible locations of well U-2 and selected robustness ranges.



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.

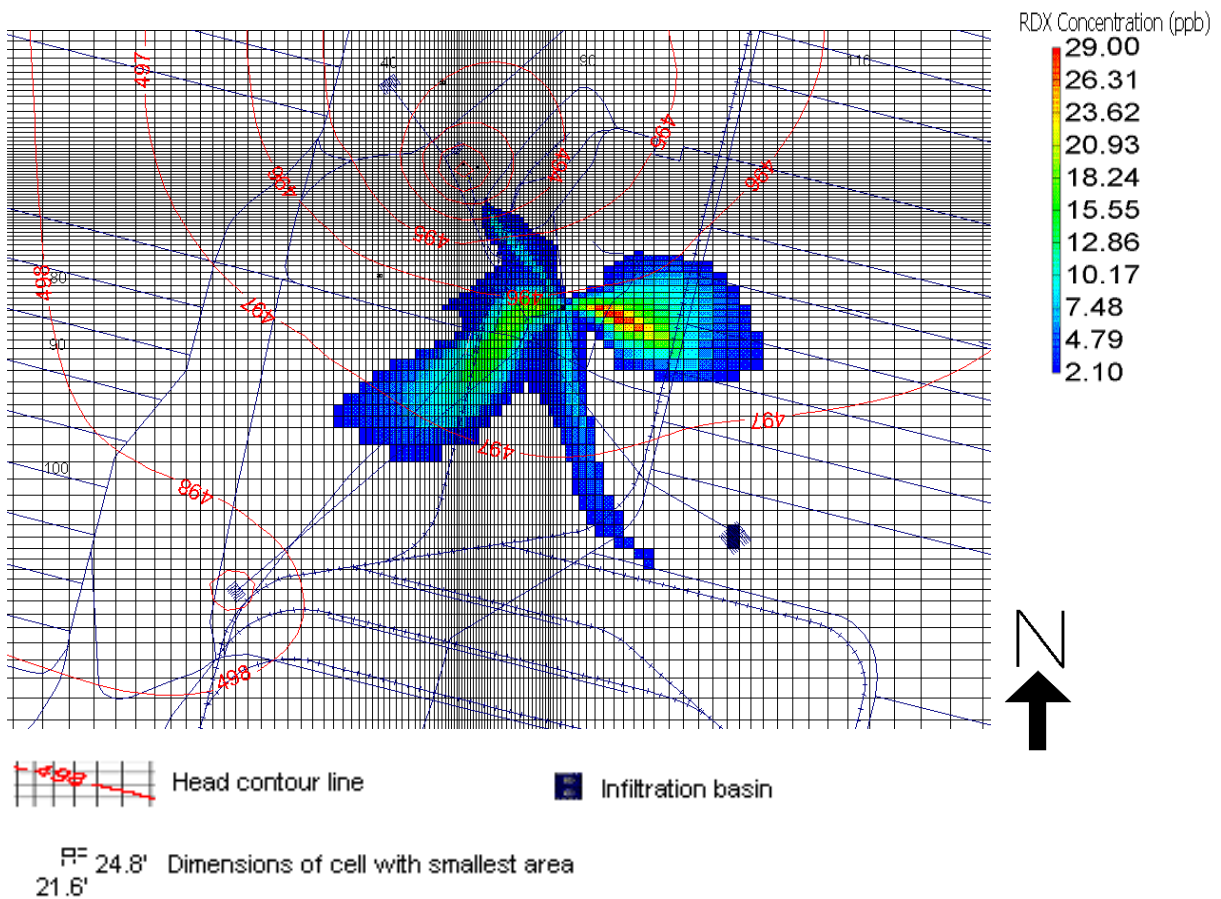


Fig. 19. Strategy USU3: time series of mass remaining.

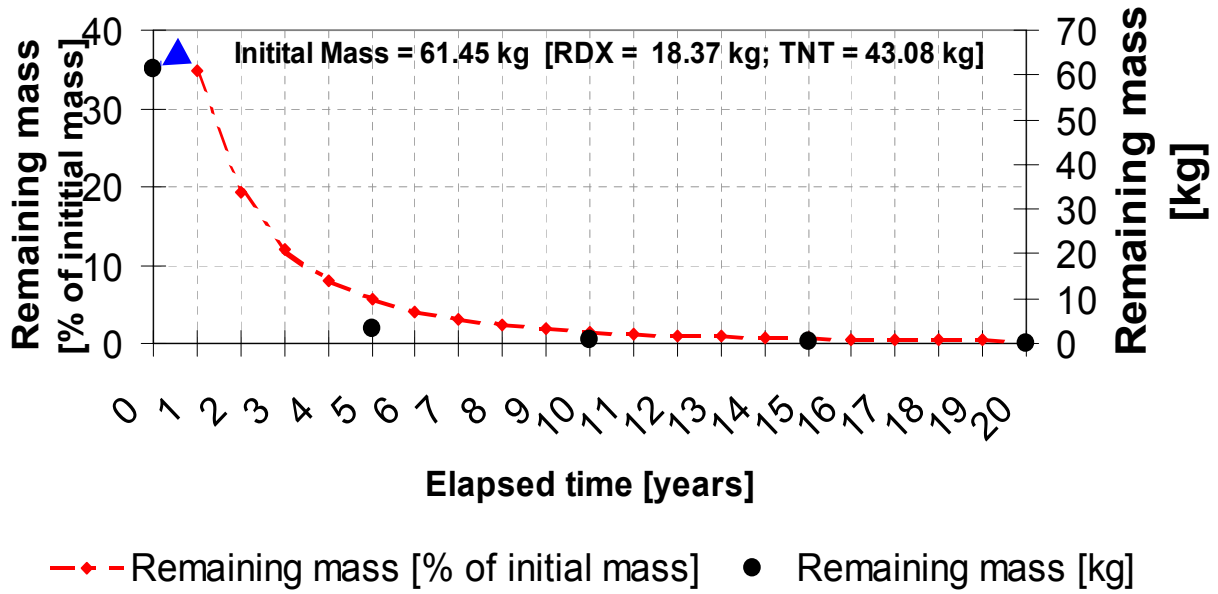


Fig. 20. Formulation 4 optimization problem (minimize cost to reach CL and continued pumping to minimize mass remaining).

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.

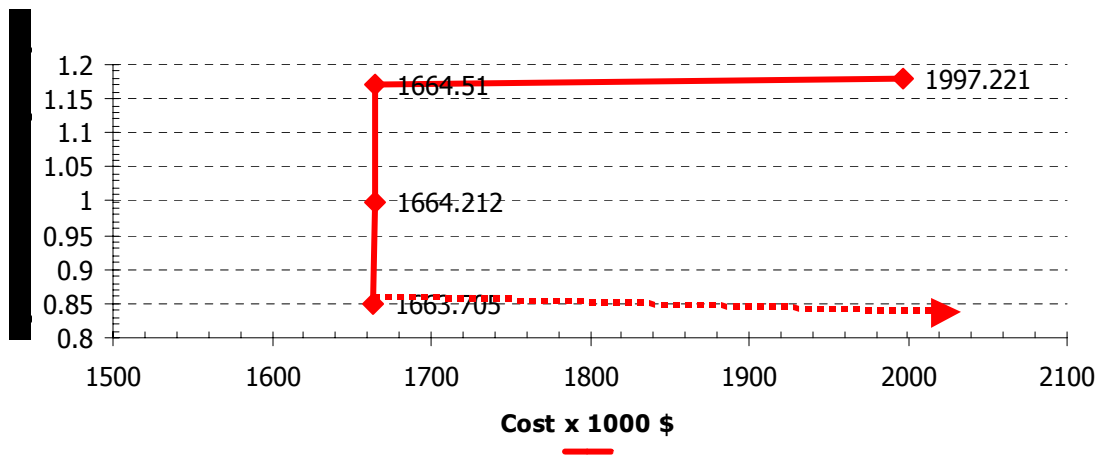


Fig. 22. Layer 1 bottom elevation and wells U-1, EW-3, and EW-1.

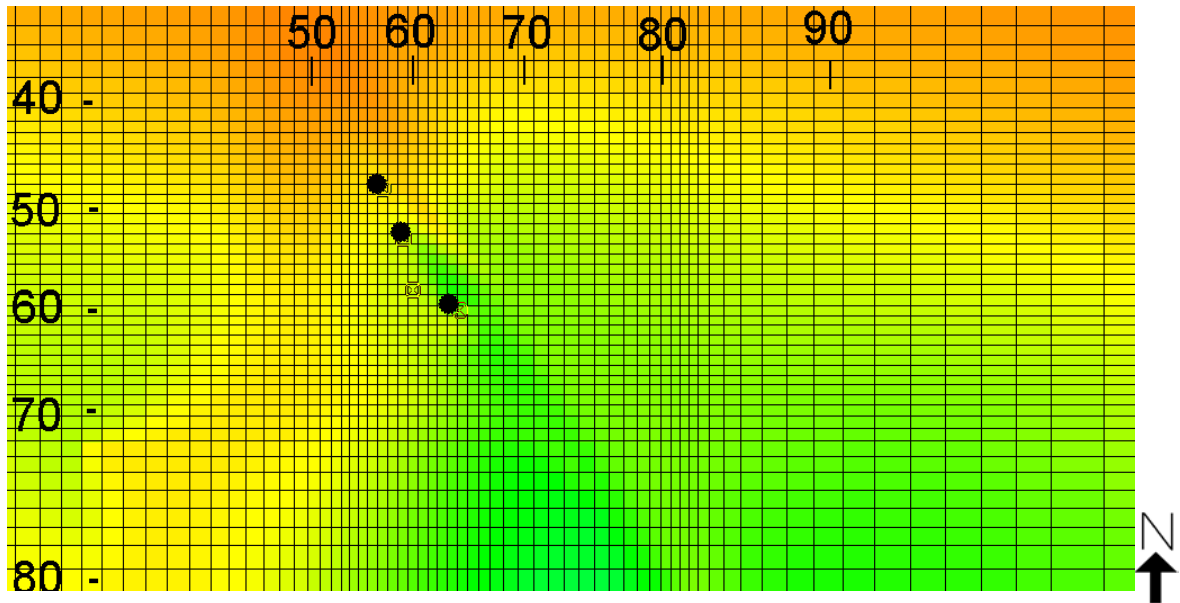


Fig. 23. Row 48, Layers 1-5 bottom elevations (ft MSL).

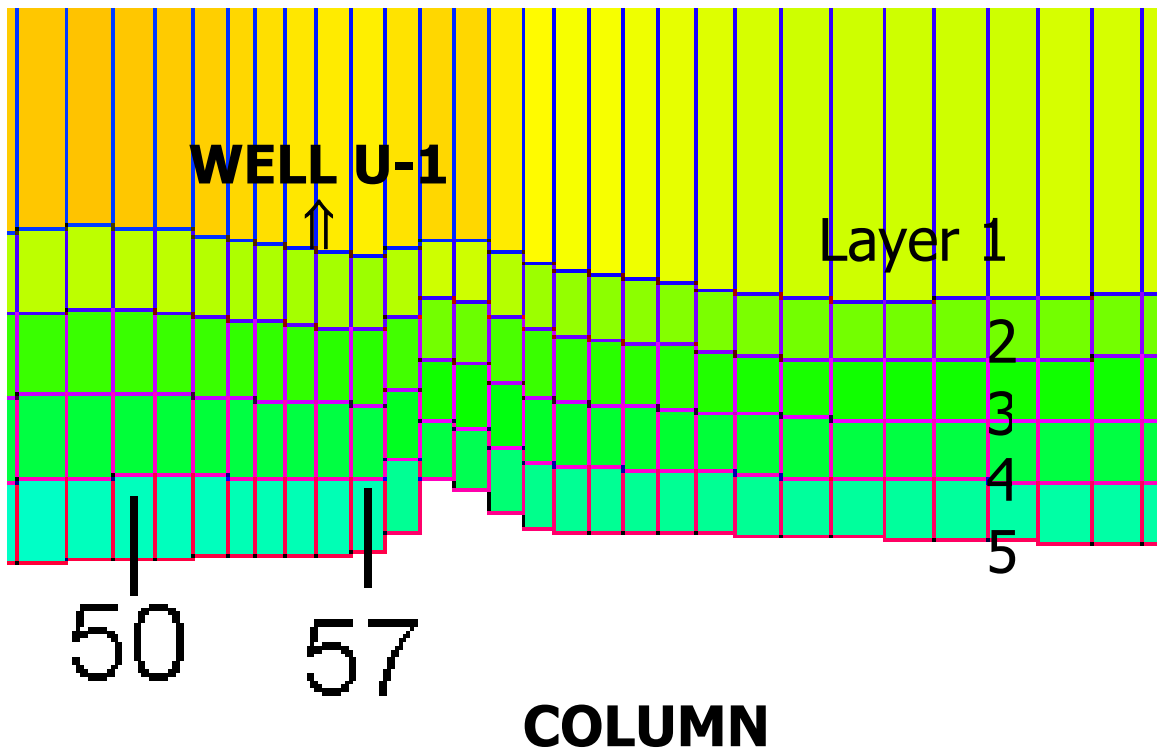
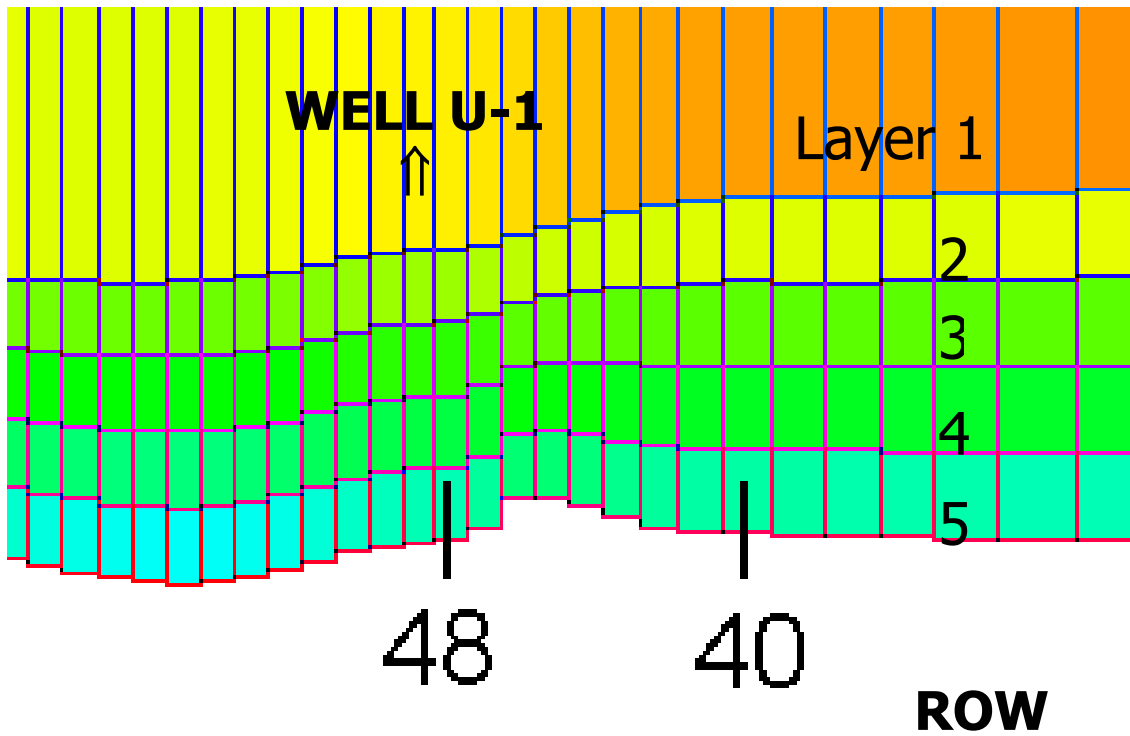


Fig. 24. Column 57, Layers 1-5, bottom elevations (ft MSL).



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 #

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 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

--- 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