

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

This work was performed for the U.S. Environmental Protection Agency (U.S. EPA) under Dynamac Contract No. 68-C-99-256, Task # WA-2-ST-1. The technical work was performed by GeoTrans under Subcontract No. AD02-103.

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.

TABLE OF CONTENTS

NOTICE	i
PREFACE	ii
TABLE OF CONTENTS	iii
1.0 BRIEF SUMMARY OF FORMULATIONS	1
1.1 Variables To Be Optimized	1
1.2 Formulation 1	1
1.3 Formulation 2	2
1.4 Formulation 3	2
2.0 OPTIMIZATION TECHNIQUE	3
3.0 OPTIMIZATION RESULTS	4
3.1 Pre-Optimization Simulations	4
3.1.1 FS Report Simulations	4
3.1.2 Initial Solution Provided By GeoTrans	4
3.2 Formulation 1: Minimize Total Cost	4
3.2.1 Optimal Solution, Formulation 1	4
3.2.2 General Approach to Determining the Optimal Solution, Formulation 1	6
3.3 Formulation 2: Minimize Cost with Diversion of 2400gpm	6
3.3.1 Optimal Solution, Formulation 2.	7
3.3.2 General Approach to Determining the Optimal Solution, Formulation 2	7
3.4 Formulation 3: Minimize Cost, Cleanup Constraint, Reduced Source Term	8
3.4.1 Optimal Solution, Formulation 3	8
3.4.2 General Approach to Determining the Optimal Solution, Formulation 3	9
4.0 ADDITIONAL SIMULATIONS	11
5.0 COMPUTATIONAL PERFORMANCE	12
6.0 SENSITIVITY ANALYSIS (IF PERFORMED)	13
7.0 SUMMARY, SITE-SPECIFIC ITEMS, AND LESSONS LEARNED	14

List of Figures

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.
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

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:

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

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:

Pre-Optimization Objective Values

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

Major Simulations 1-3

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.

Major Simulations 4-11

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.

Major Simulations 12-15

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.

Major Simulation 16-18

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

Major Simulations 19-22 (**optimal solution was Major Simulation 21, Total Simulation 55)

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	\$3,200K
CCT: Capital cost of treatment	\$1,595K
CCD: Capital cost of discharge	\$2,392.5K
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	\$8,025.620K
VCD: Variable cost of discharge	\$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:

$$\text{total cost} = \text{capital cost} + \text{annual cost} \times \text{time}$$

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 its 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.

Additional Simulations “A”

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.

Additional Simulations “B”

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.

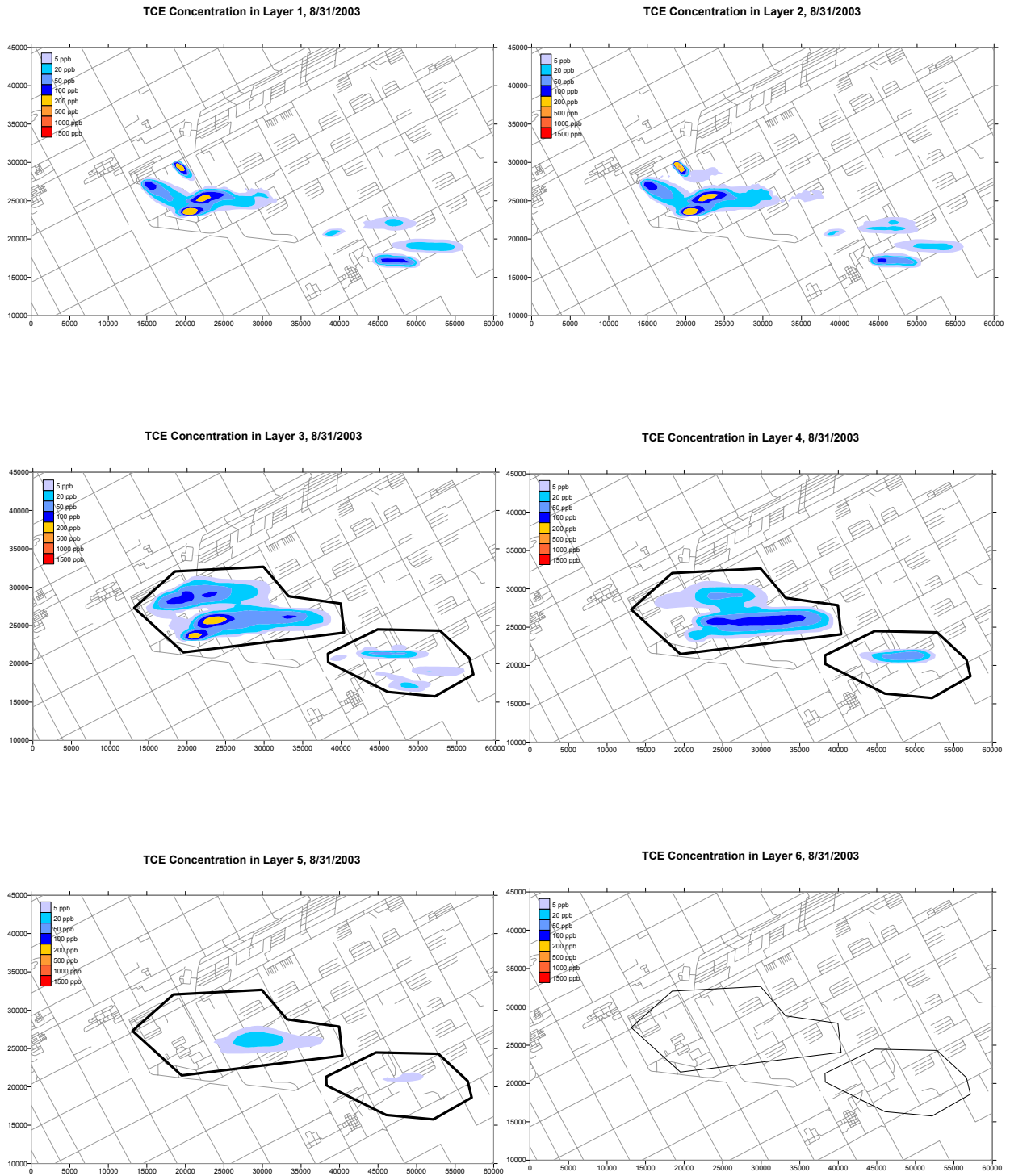


Figure 2. Initial concentrations for TNT at beginning of optimization simulations.

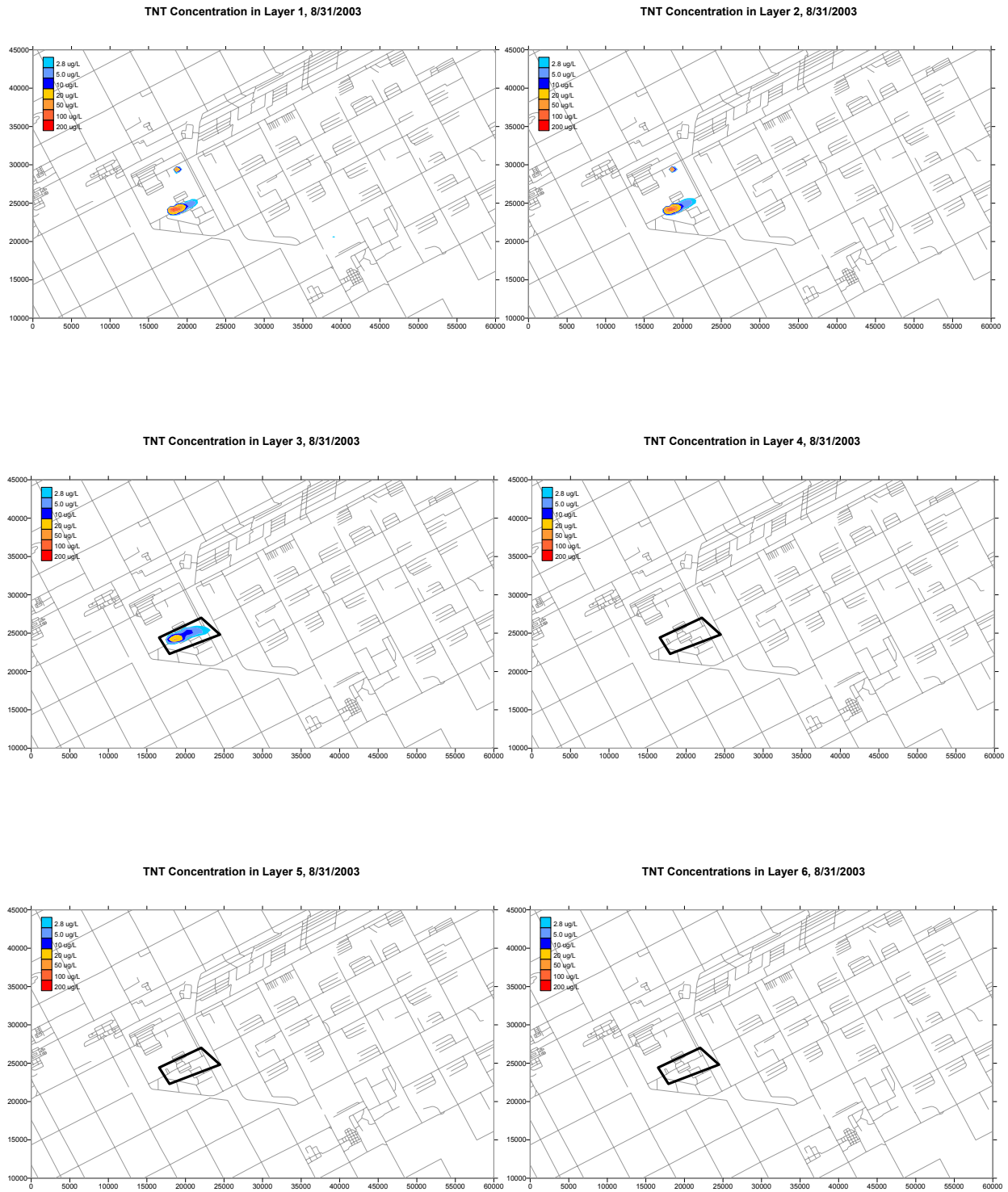


Figure 3. TCE concentrations, layer 3, Formulation 1 optimal solution

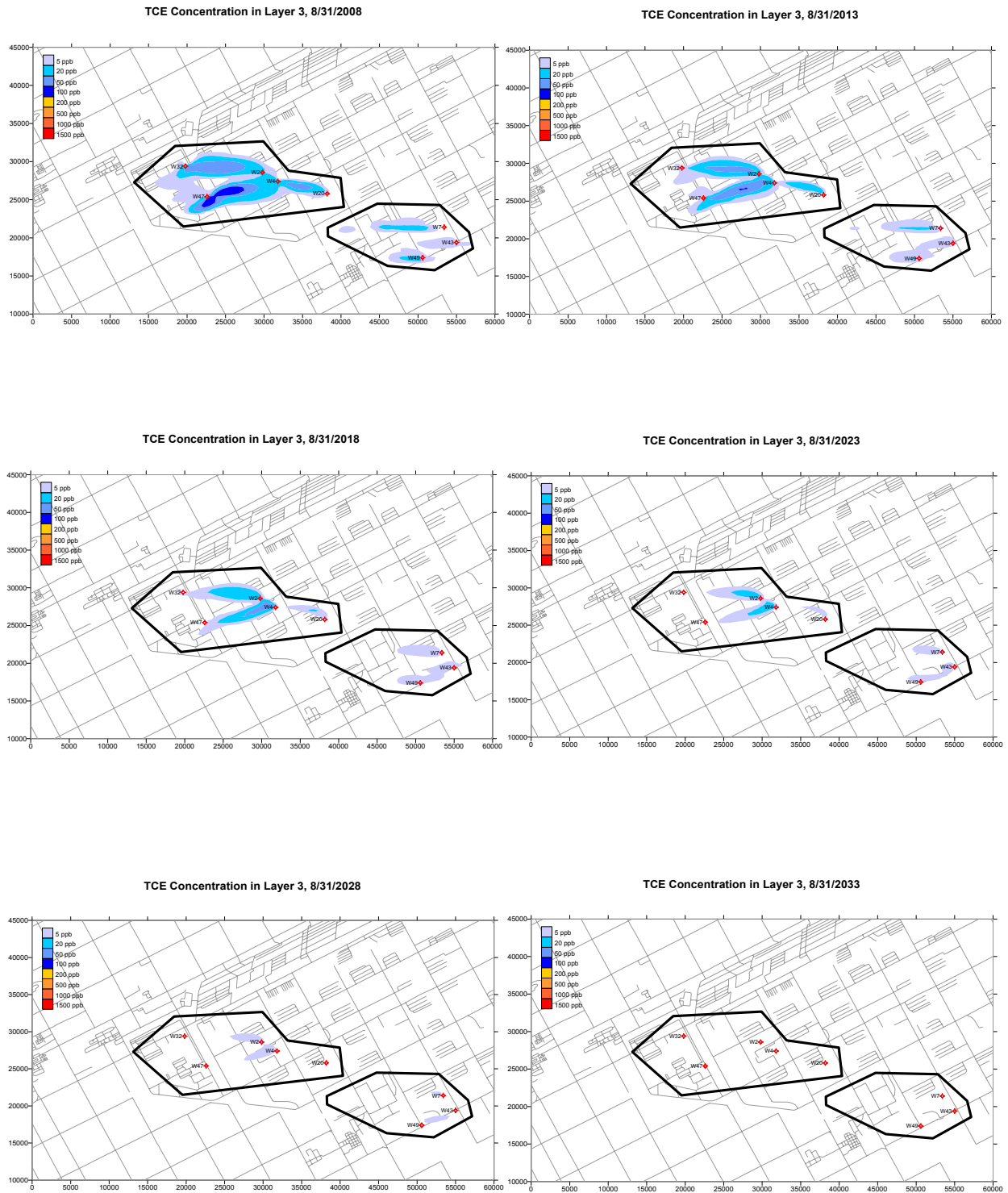


Figure 4. TCE concentrations, layer 4, Formulation 1 optimal solution

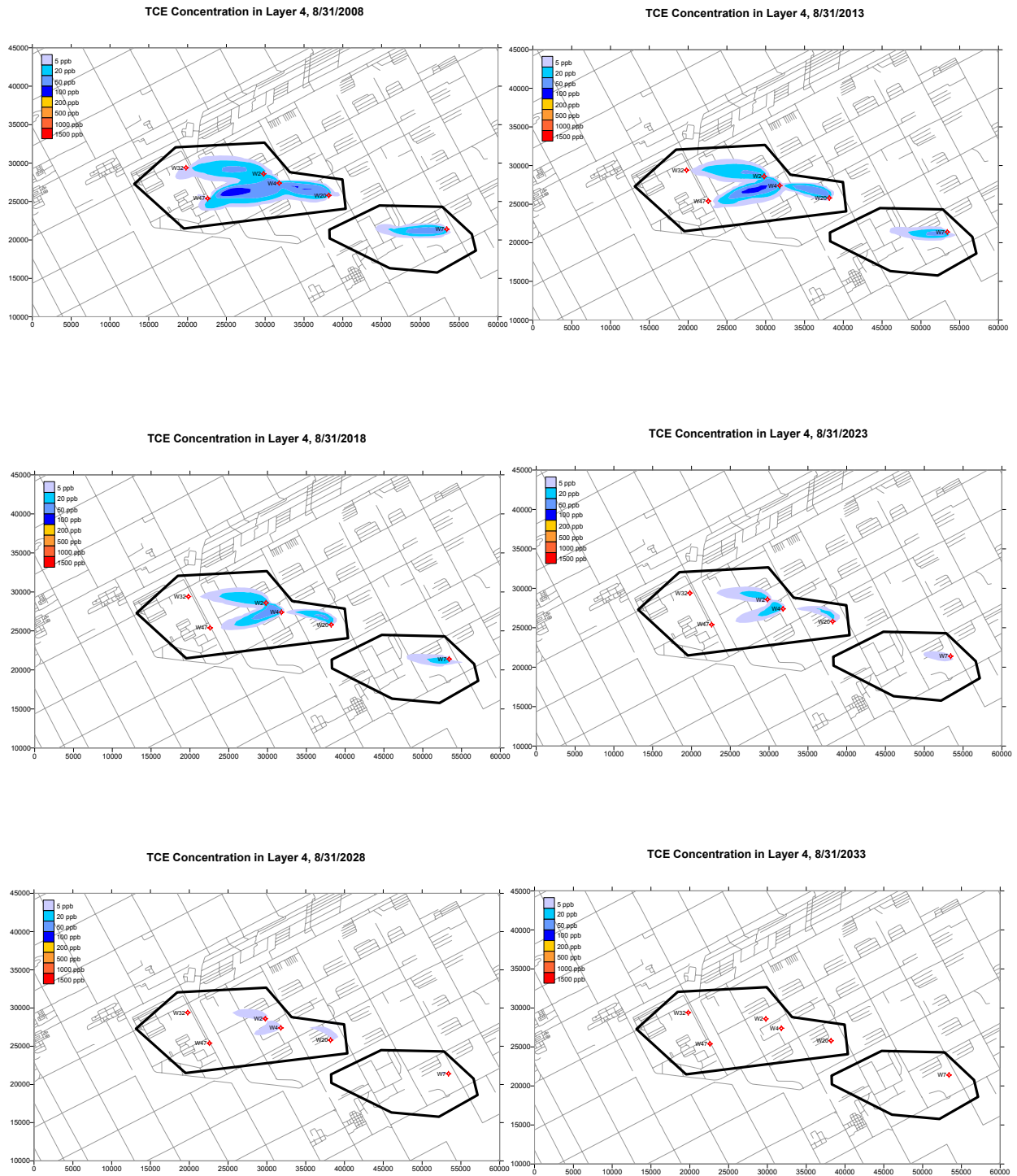


Figure 5. TCE concentrations, layer 5, Formulation 1 optimal solution

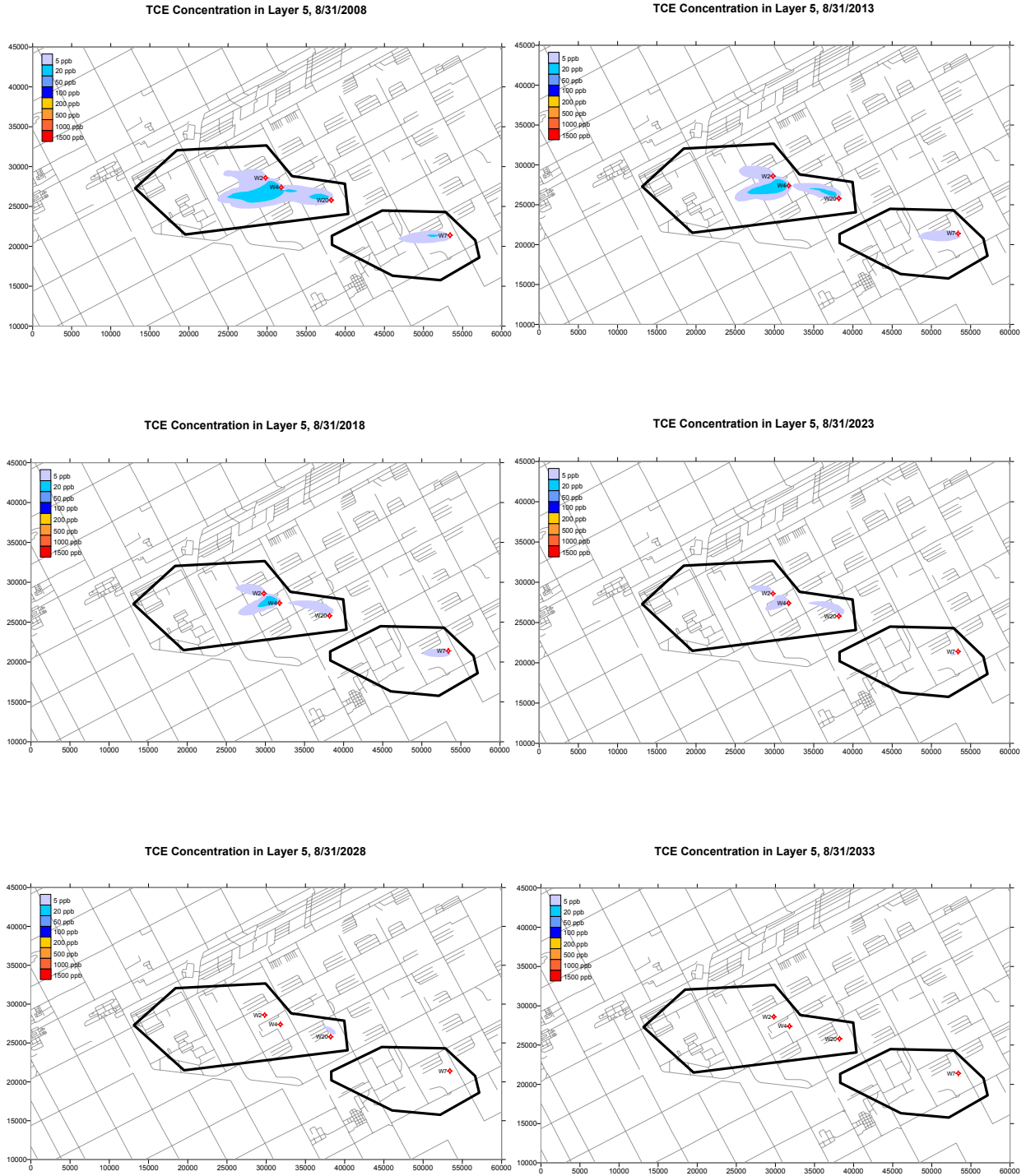


Figure 6. TNT concentrations, layer 3, Formulation 1 optimal solution

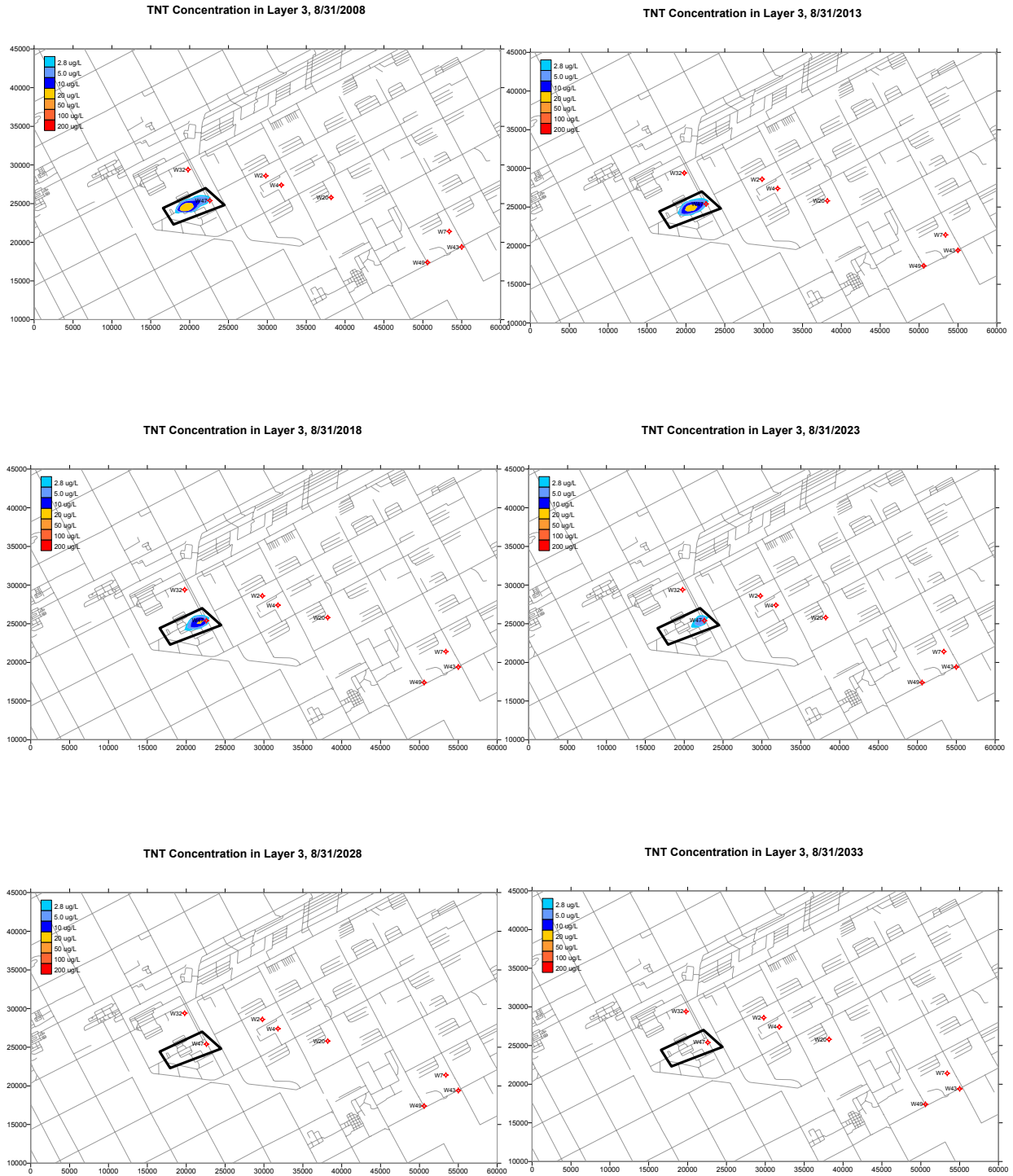


Figure 7. TNT concentrations, layer 4, Formulation 1 optimal solution

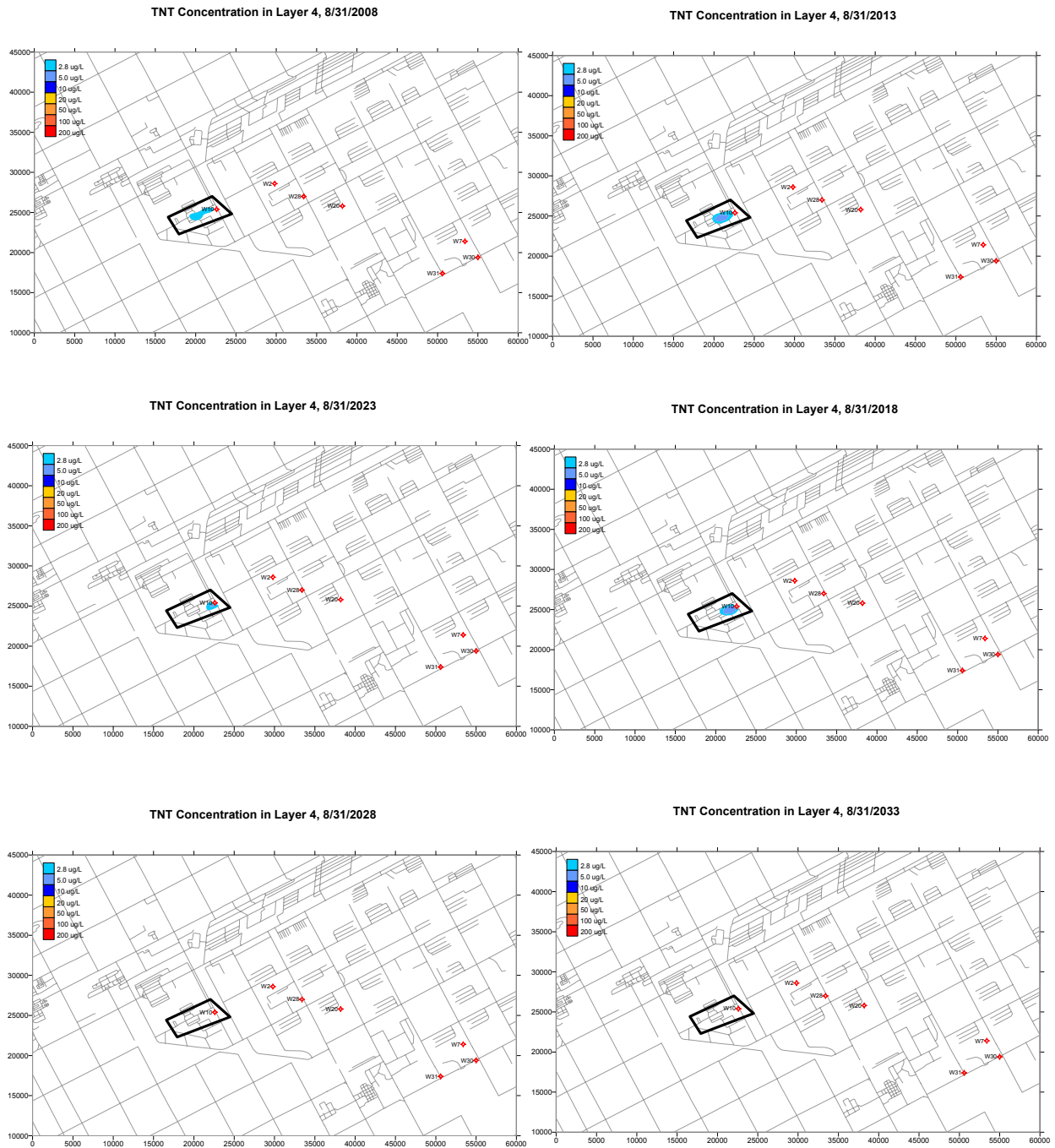


Figure 8. Objective function value by major run, Formulation 1

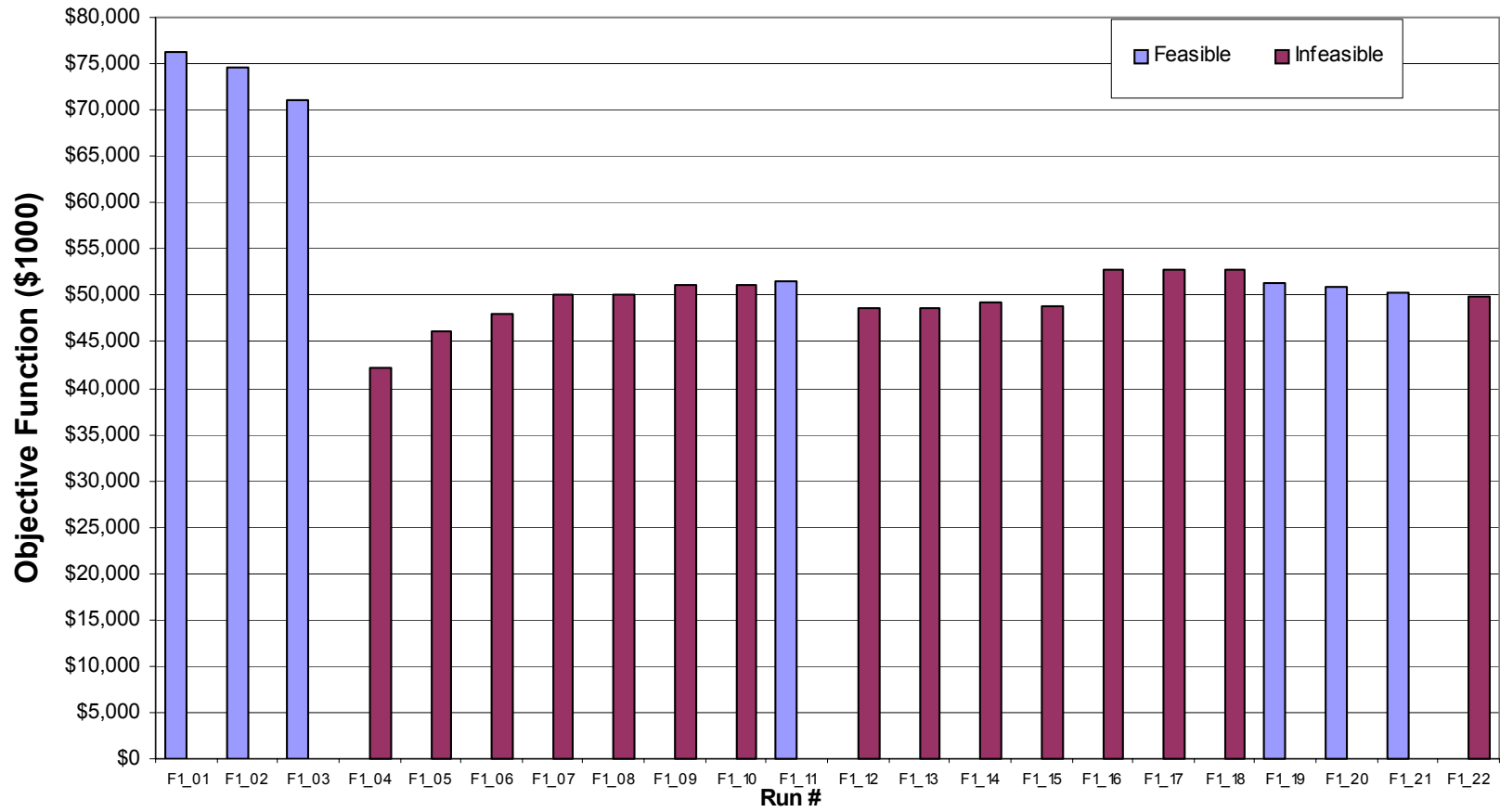


Figure 9. TCE concentrations, layer 3, Formulation 3 optimal solution

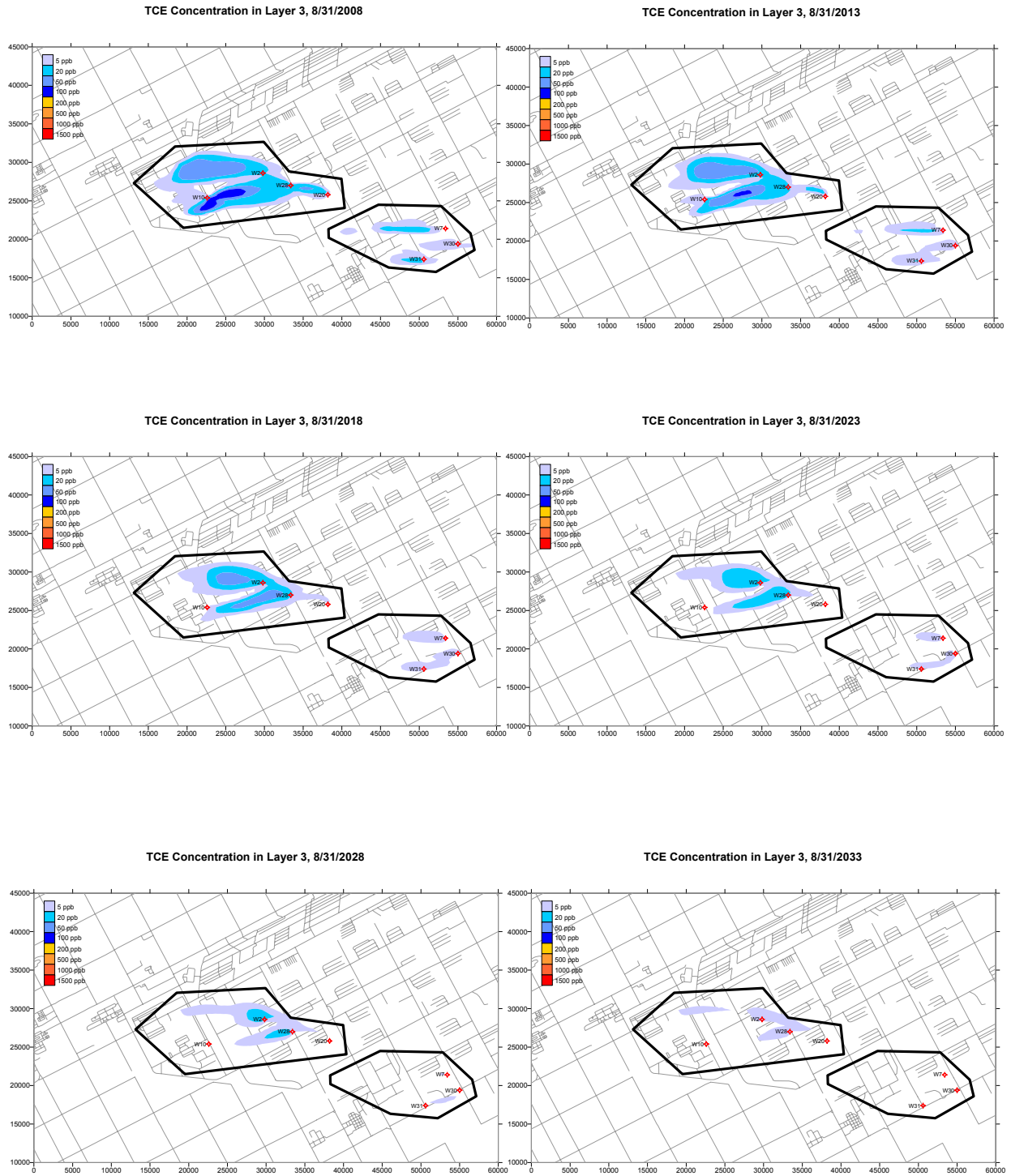


Figure 10. TCE concentrations, layer 4, Formulation 3 optimal solution

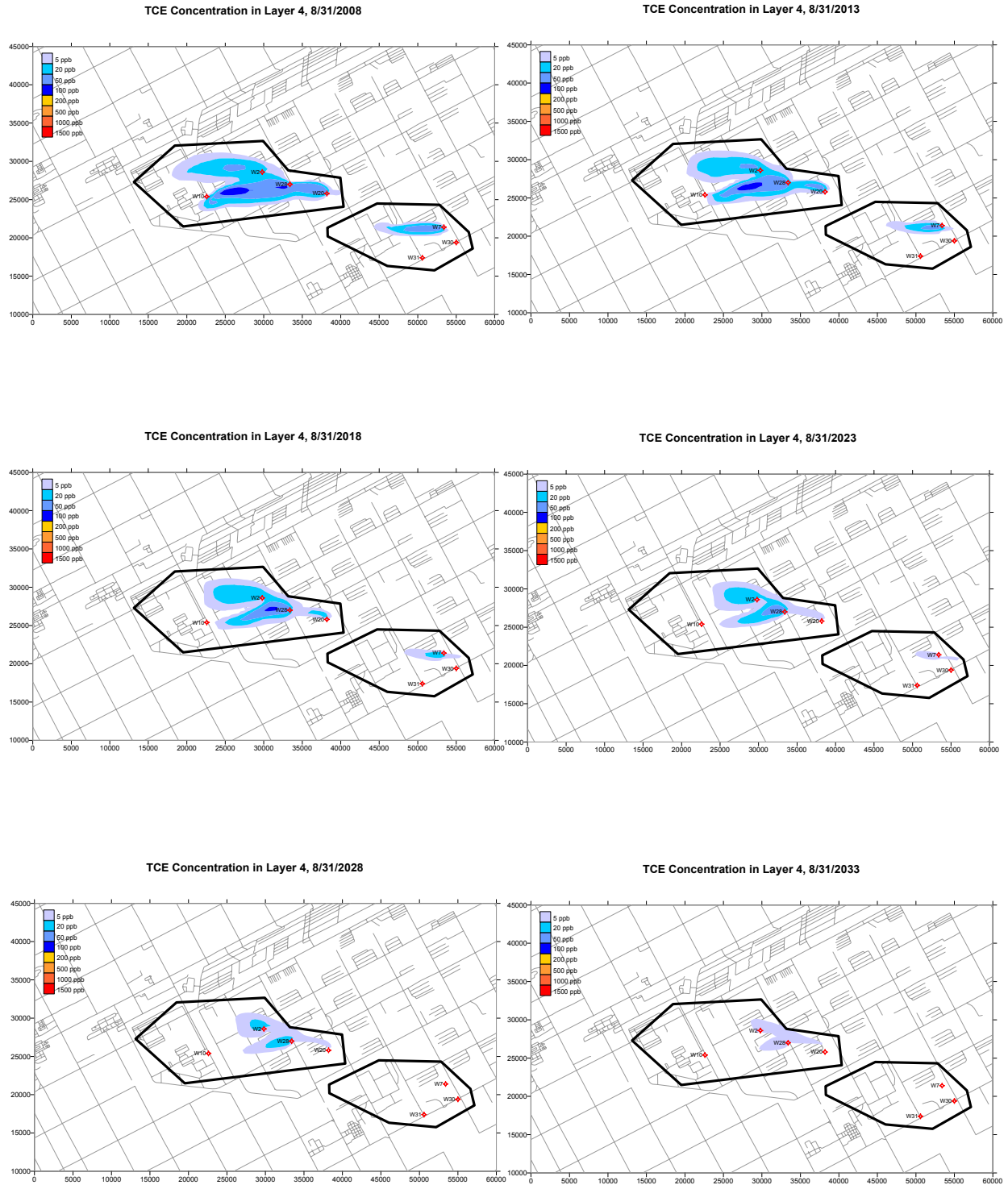


Figure 11. TCE concentrations, layer 5, Formulation 3 optimal solution

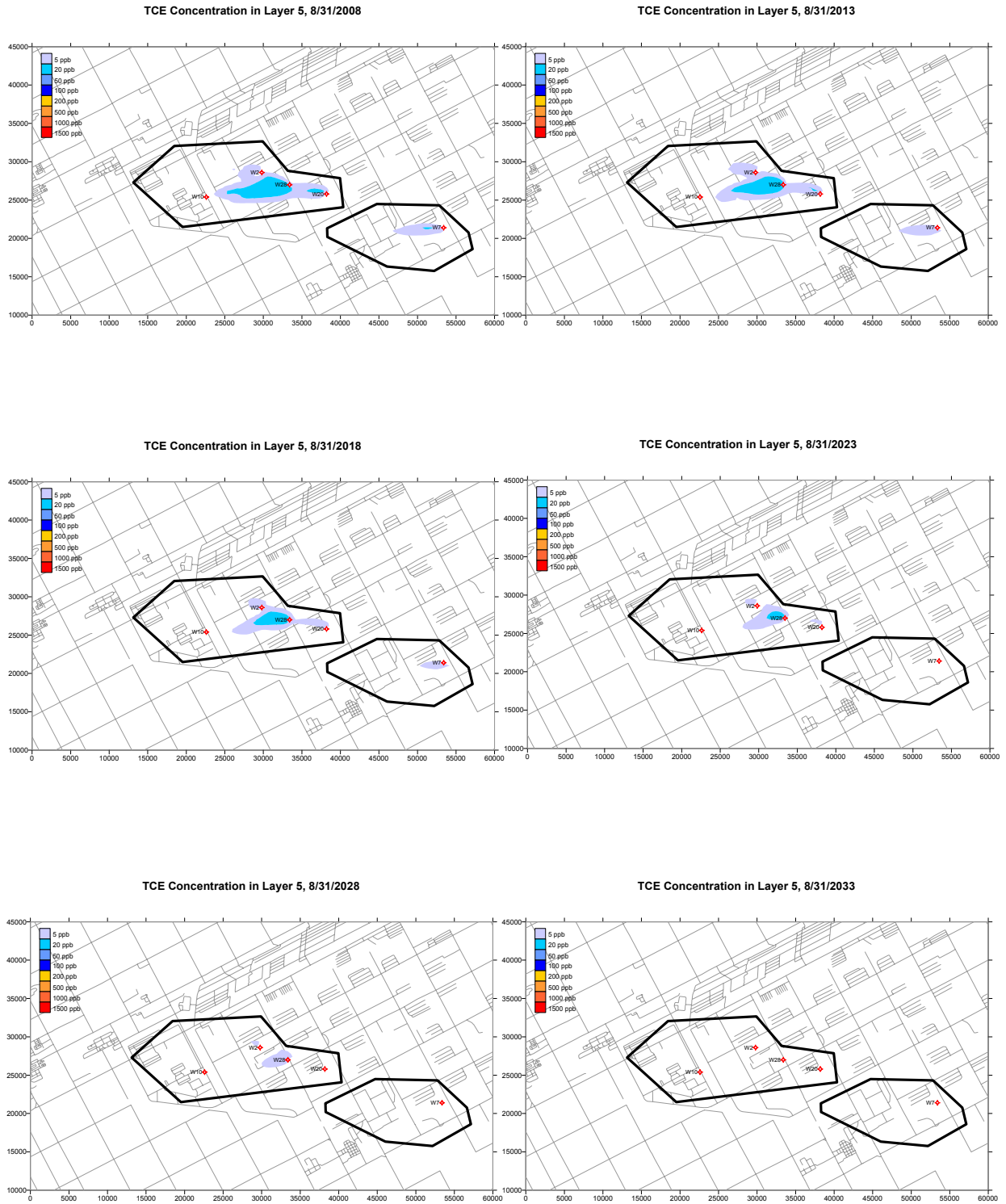


Figure 12. TNT concentrations, layer 3, Formulation 3 optimal solution

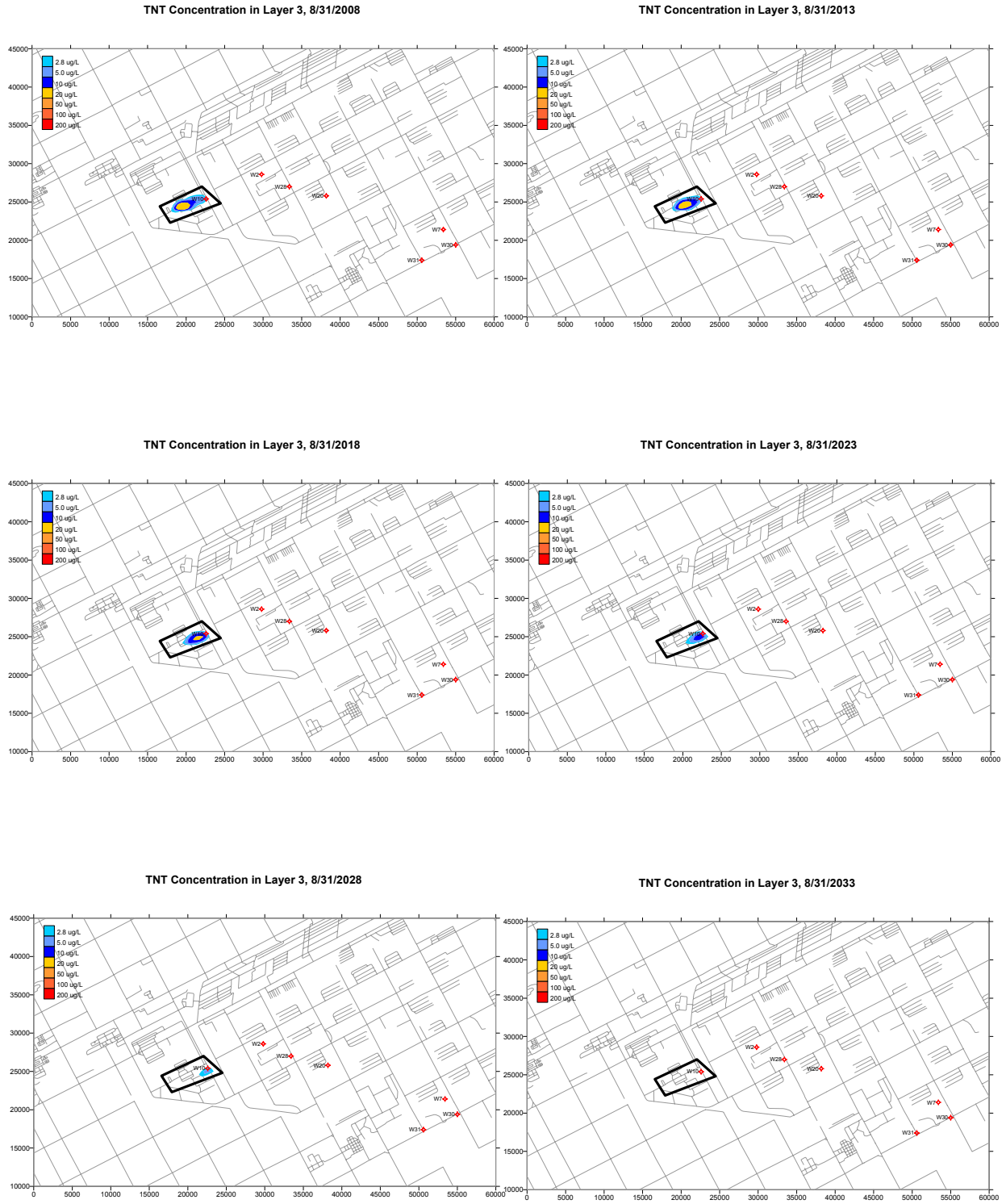


Figure 13. TNT concentrations, layer 4, Formulation 3 optimal solution

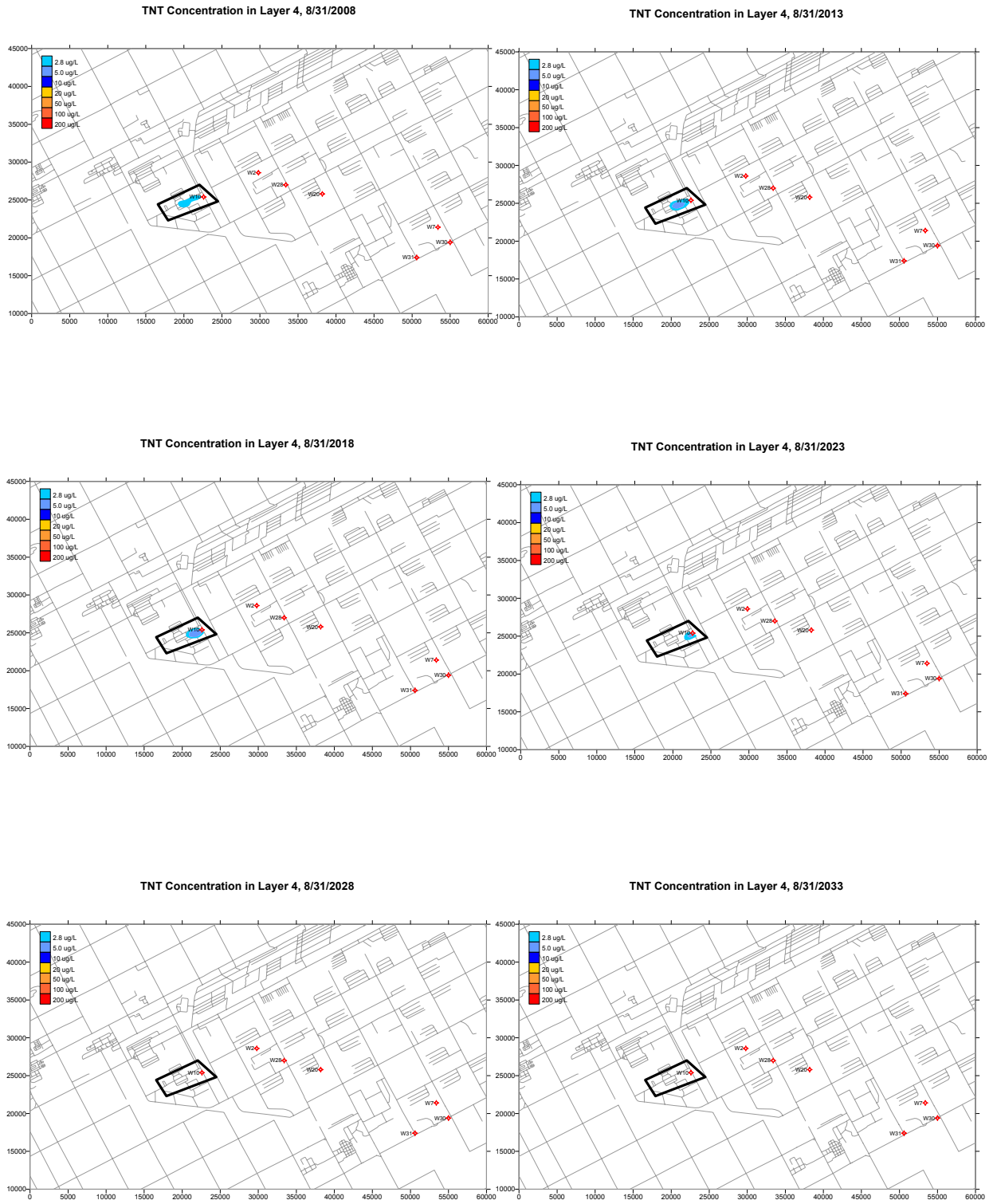


Figure 14. Objective function value by major run, Formulation 3

