OPTIMIZATION RESULTS: GEOTRANS

ESTCP TRANSPORT OPTIMIZATION PROJECT
SITE #2: TOOELE ARMY DEPOT

Prepared By:

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

NOTICE

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PREFACE

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

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

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

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

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

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

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1.0 OPTIMIZATION TECHNIQUE

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

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

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

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, modified pumping/recharge strategies were selected for one or more subsequent simulations, to better address areas of relatively high concentrations and/or areas where cleanup was not progressing fast enough.

2.0 OPTIMIZATION RESULTS

2.1 Current System

2.1.1 Layout of Wells for Current System

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

Well Rates, Current System

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

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

2.1.2 Constraint Evaluations for Current System

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

2.1.3 Costs for Current System

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

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

where

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

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

2.2 Formulation 1: Minimize Cost, POE Constraint

2.2.1 Objective Function and Constraints

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

- The modeling period consists of seven 3-year management periods (21 years total) beginning January 2003;
- Modifications to the system may only occur at the beginning of each management period;

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

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

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

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

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

2.2.2 Optimal Solution

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

Results, Formulation 1

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

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

Optimal Rates, Formulation 1

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

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

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

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

2.2.3 General Approach to Determining the Optimal Solution

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

<u>Major Simulation 1</u>

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

Major Simulation 2

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

Major Simulations 3-4

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

Major Simulation 5

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

Major Simulations 6-11

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

Major Simulations 12-14

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

Major Simulations 15-17

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

Major Simulation 18

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

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

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

2.3 Formulation 2: Minimize Cost, POE and POC Constraints

2.3.1 Objective Function and Constraints

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

- POC-MP1 must be 50% of the initial concentrations or < 20 ug/l at the end of 1st management period (year 3) and thereafter; and
- POC-MP2 must be 50ppb at the end of the 1st management period (3 yrs), and 20ppb at the end of 3rd management period (9 yrs) and thereafter.

2.3.2 Optimal Solution

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

Results, Formulation 2

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

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

Optimal Rates, Formulation 2

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

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

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

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

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

2.3.3 General Approach to Determining the Optimal Solution

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

Major Simulations 1-2

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

Major Simulations 3-8

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

Major Simulations 9-12

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

Major Simulations 13-15

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

Major Simulations 16-26, 39-40

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

Major Simulation 41

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

Major Simulations 27-38, 42

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

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

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

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

2.4.1 Objective Function and Constraints

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

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

2.4.2 Optimal Solution

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

Results, Formulation 3

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

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

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

Optimal Rates, Formulation 3

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

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

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

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

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

2.4.3 General Approach to Determining the Optimal Solution

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

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

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

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

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

Major Simulation 10

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

Major Simulations 11-19

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

Major Simulation 20

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

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

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

3.0 ADDITIONAL SIMULATIONS

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

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

The three major classes of additional simulations were:

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

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

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

The results of these additional simulations are discussed below.

3.1 Additional Simulations A: Attempt Cleanup Beyond Bedrock Block

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

The best solution found is summarized below:

Results, Additional Simulations A

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

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

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

Well Rates, Additional Simulations A

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

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

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

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

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

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

The best solution found is summarized below:

Results, Additional Simulations B

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

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

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

Well Rates, Additional Simulations B

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

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

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

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

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

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

The best solution found is summarized below:

Results, Additional Simulations C

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

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

Well Rates, Additional Simulations C

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

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

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

4.0 COMPUTATIONAL PERFORMANCE

Preliminary Items

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

Solution of the Three Formulations

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

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

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

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

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

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

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

5.0 SENSITIVITY ANALYSIS (IF PERFORMED)

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

6.0 SUMMARY, SITE-SPECIFIC ITEMS, AND LESSONS LEARNED

Formulations Fixed at the Beginning of the Simulation Period

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

Costs of Optimal Solutions Versus Current System

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

Preferred Management Strategy

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

Impact of Extraction Wells and Injection Wells

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

Containment and Cleanup

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

Mass Transfer to Northeast

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

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

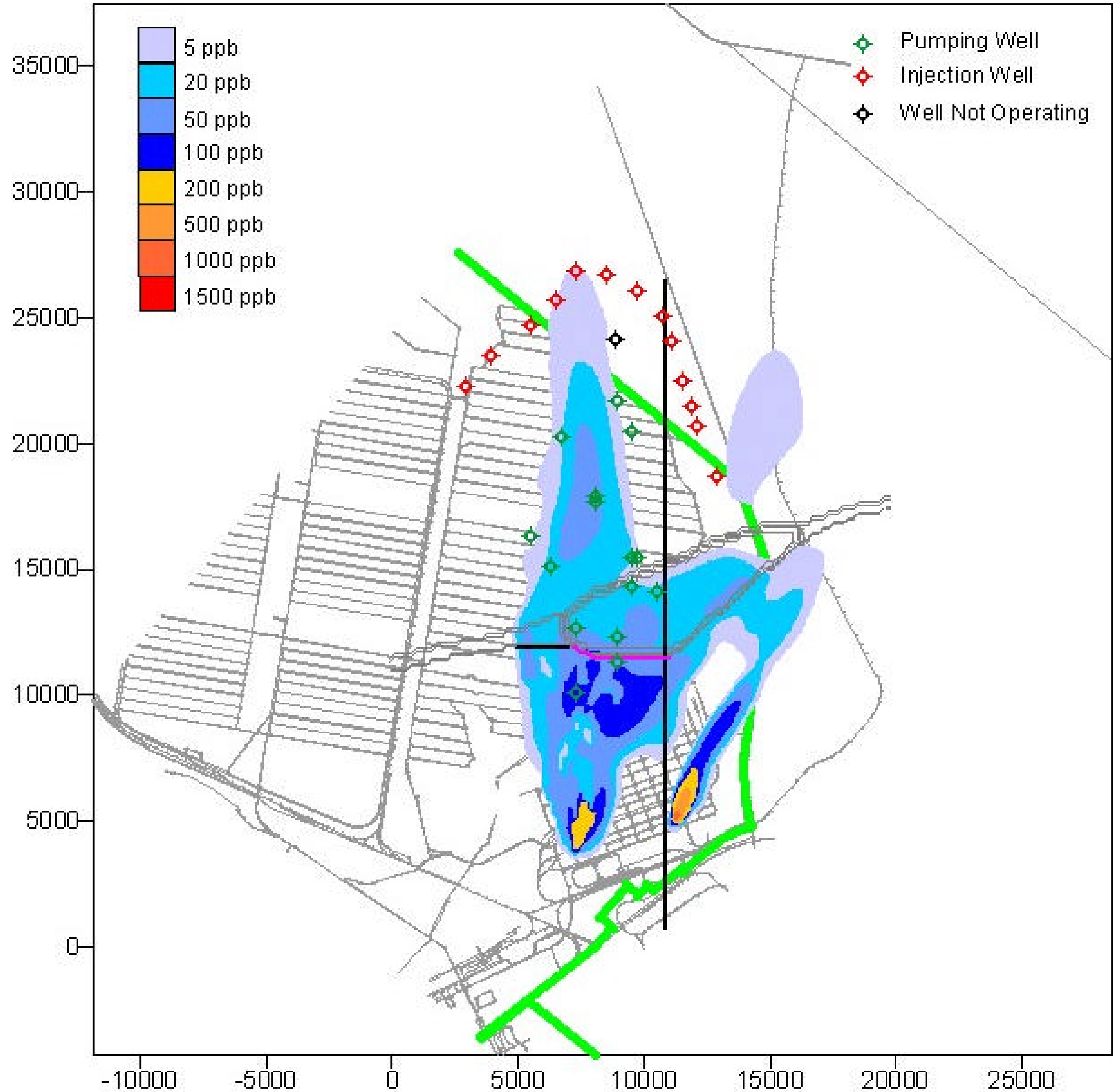

Figure 2-2 Locations of Wells in Optimal Solution, Formulation 1

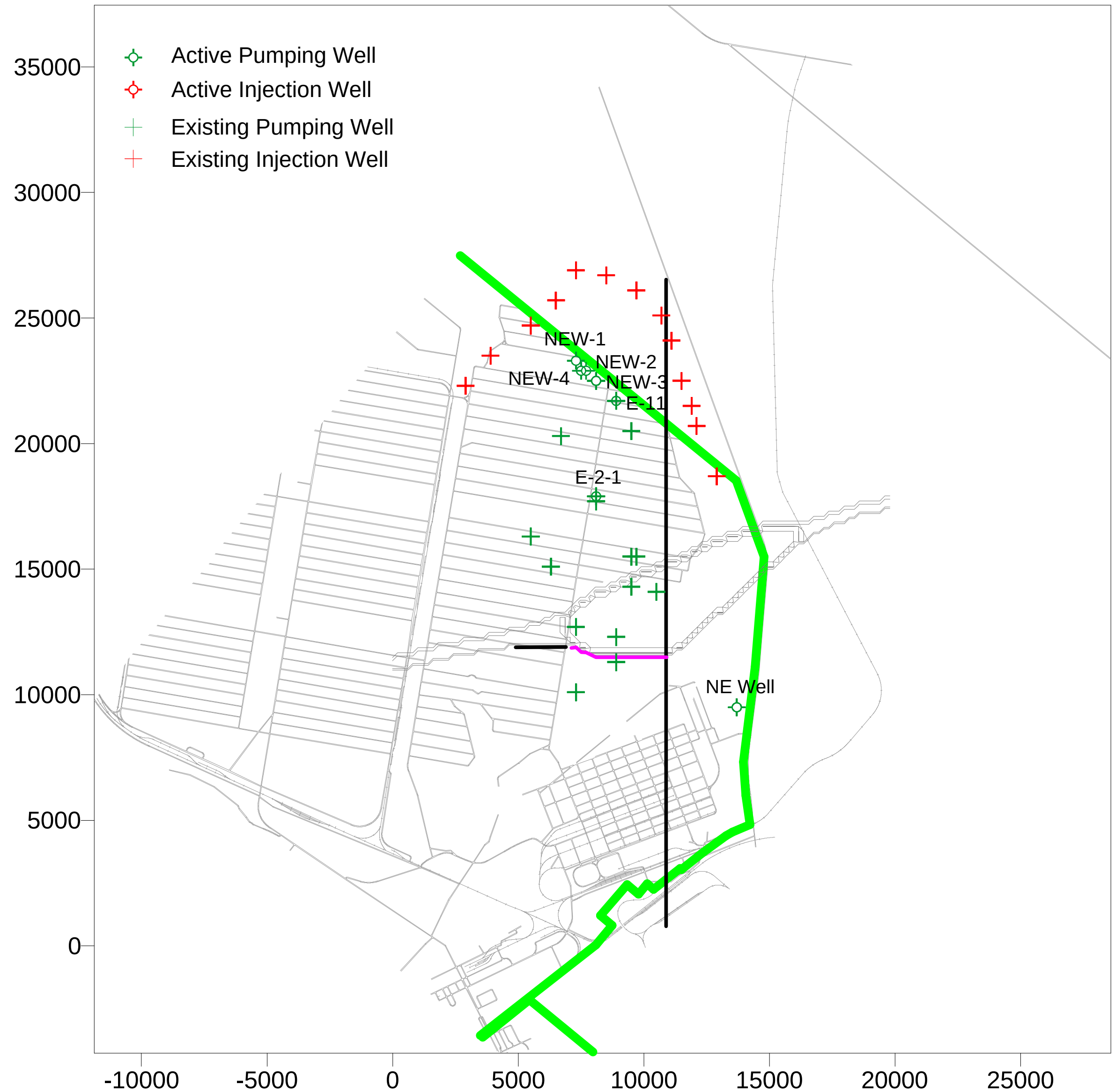

Figure 2-3 Objective Function Value by Major Runs, Formulation 1

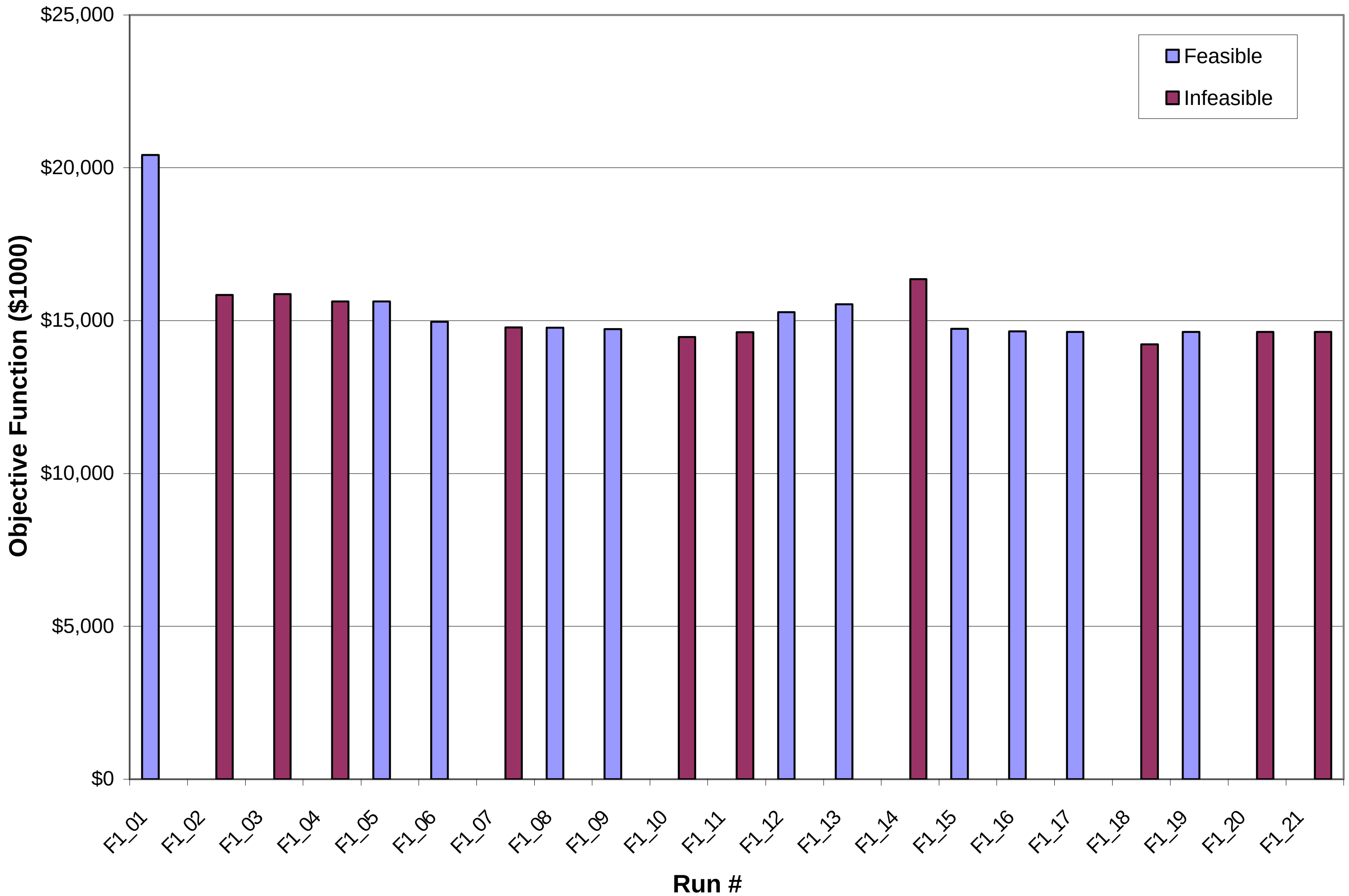

Figure 2-4   Mass Remaining After Each Year, Formulation 1

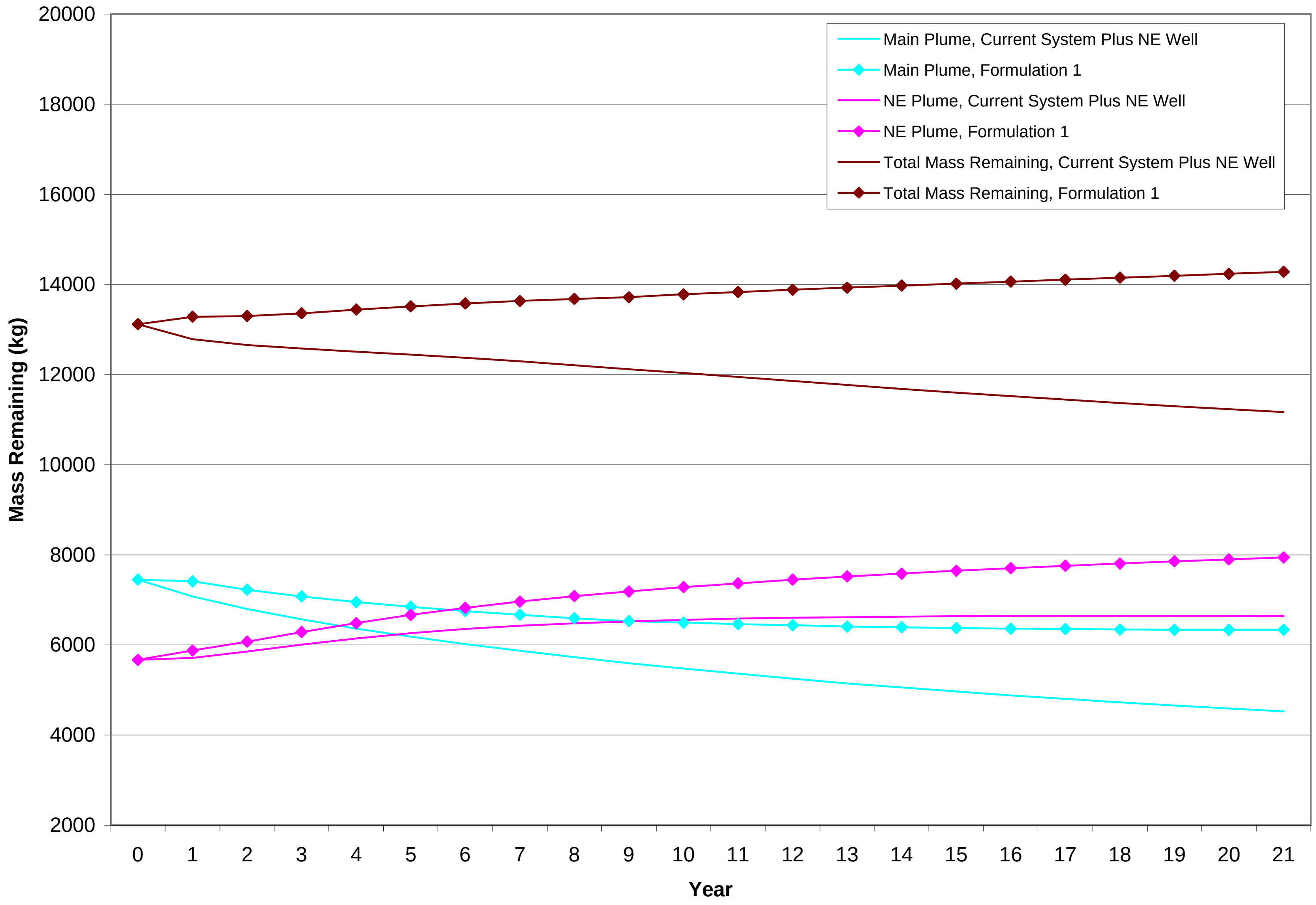

Figure 2-5 Location of Wells in Optimal Solution, Formulation 2

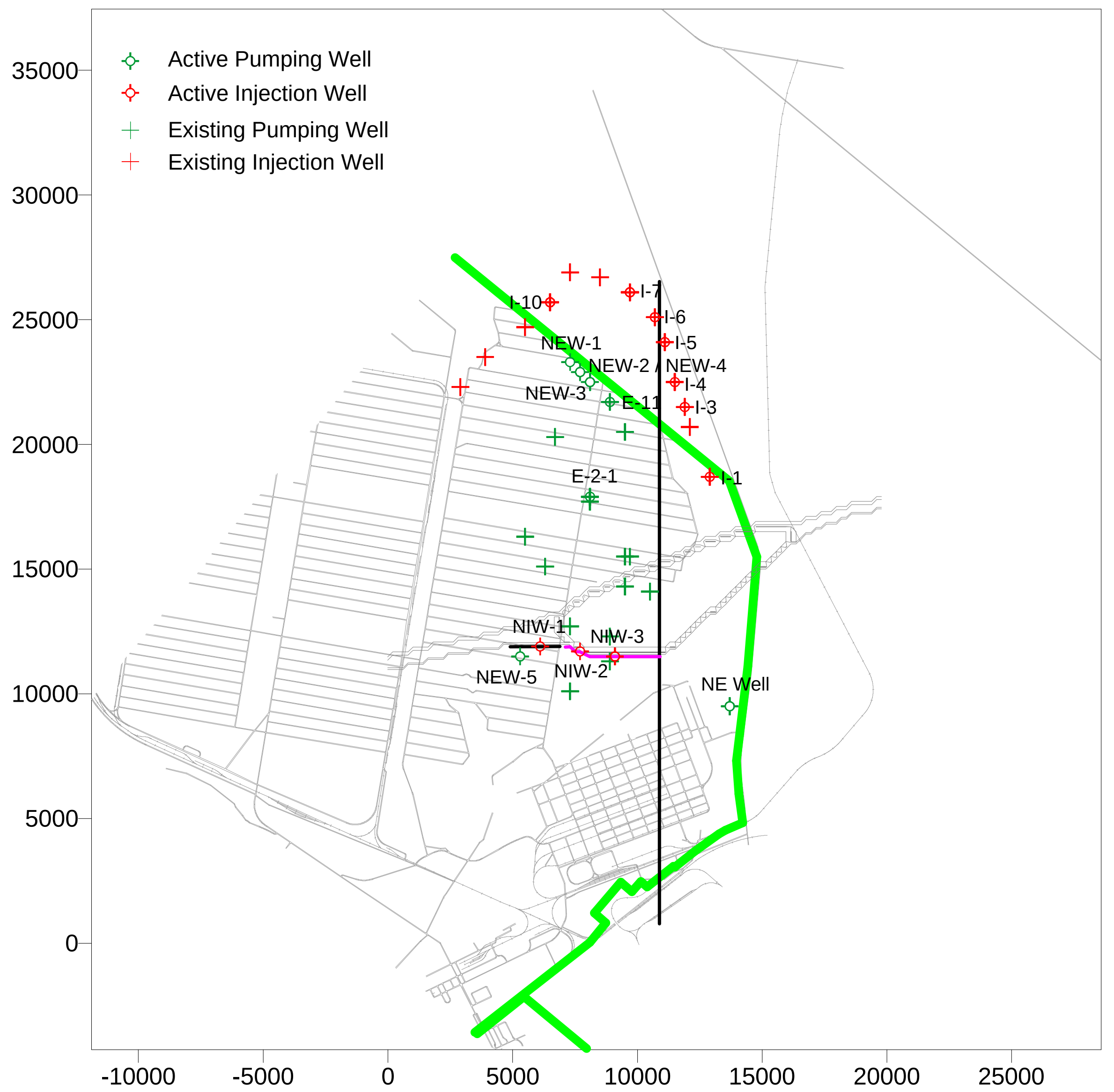

Figure 2-6 Objective Function Value by Major Runs, Formulation 2

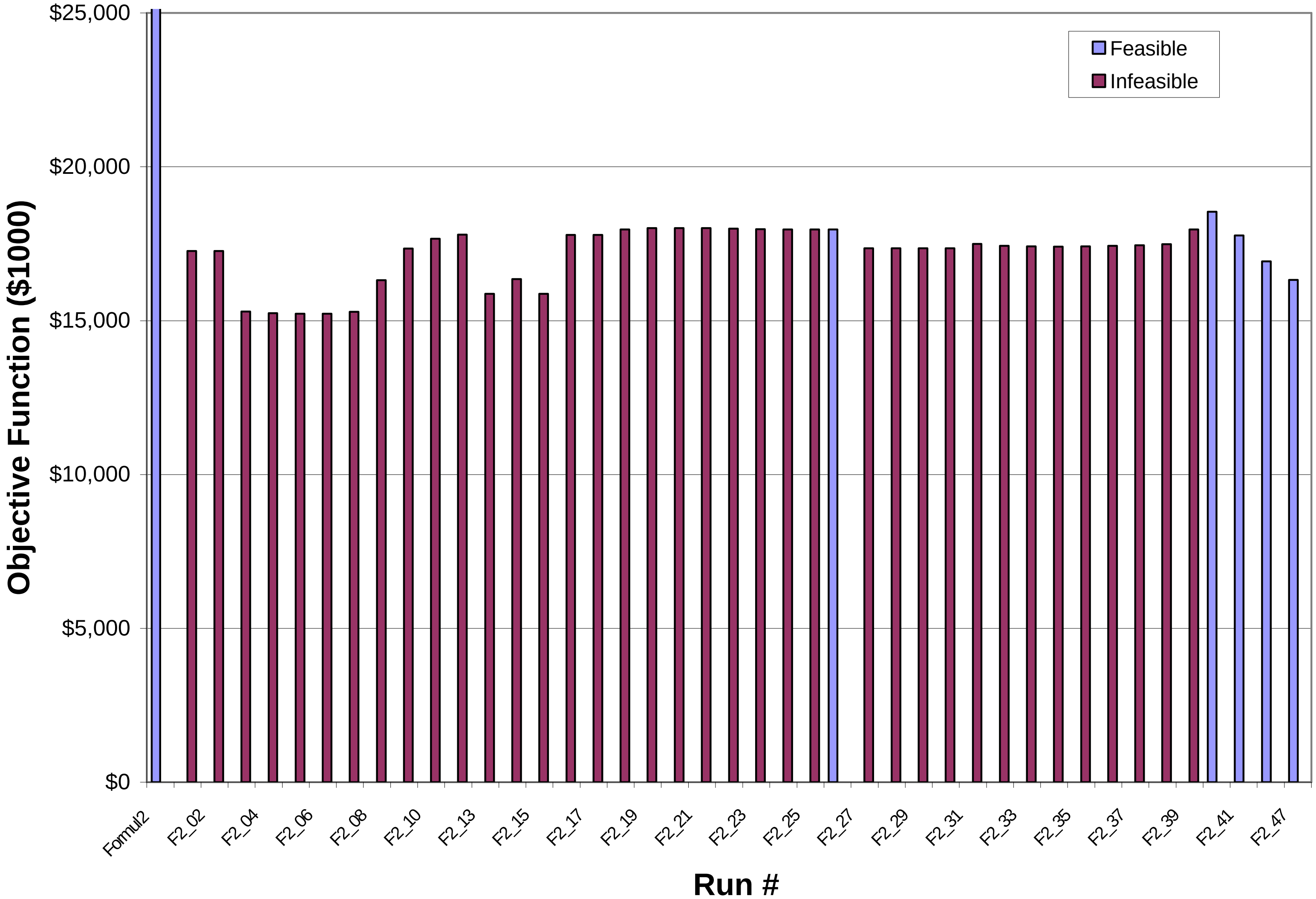

Figure 2-7 Mass Remaining After Each Year, Formulation 2

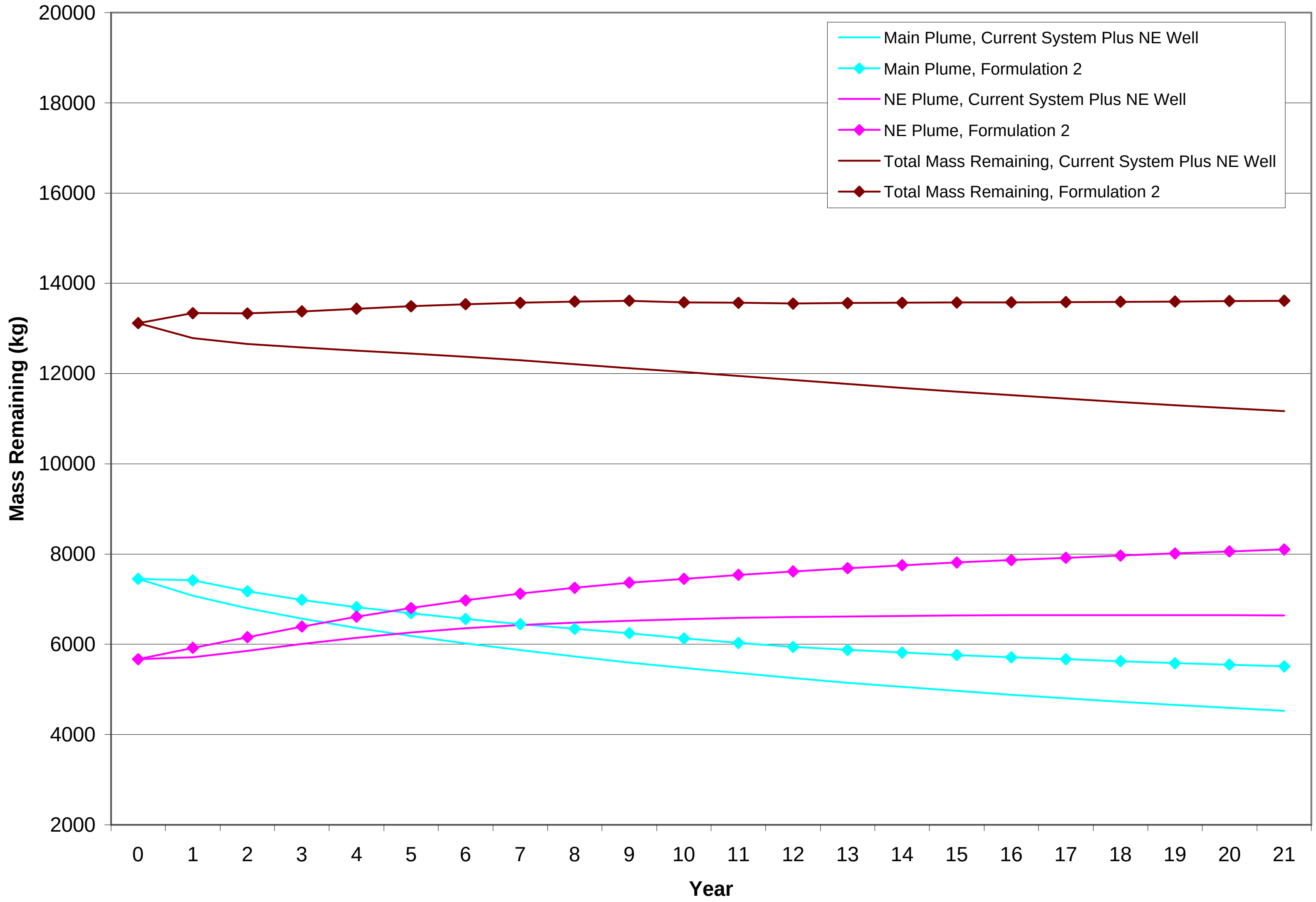

Figure 2-8 Locations of Wells in Optimal Solution, Formulation 3

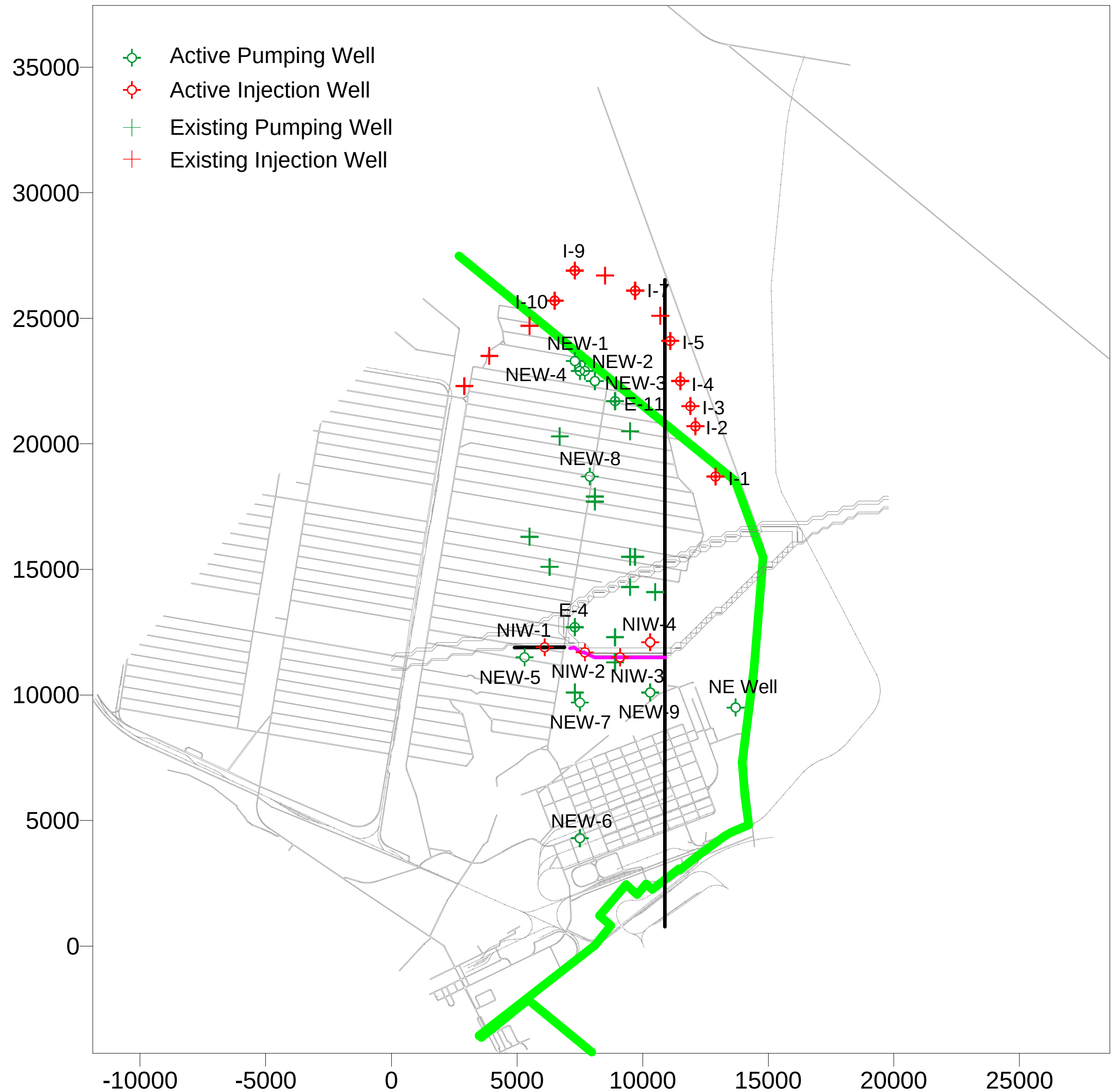

Figure 2-9 Objective Function Value by Major Runs, Formulation 3

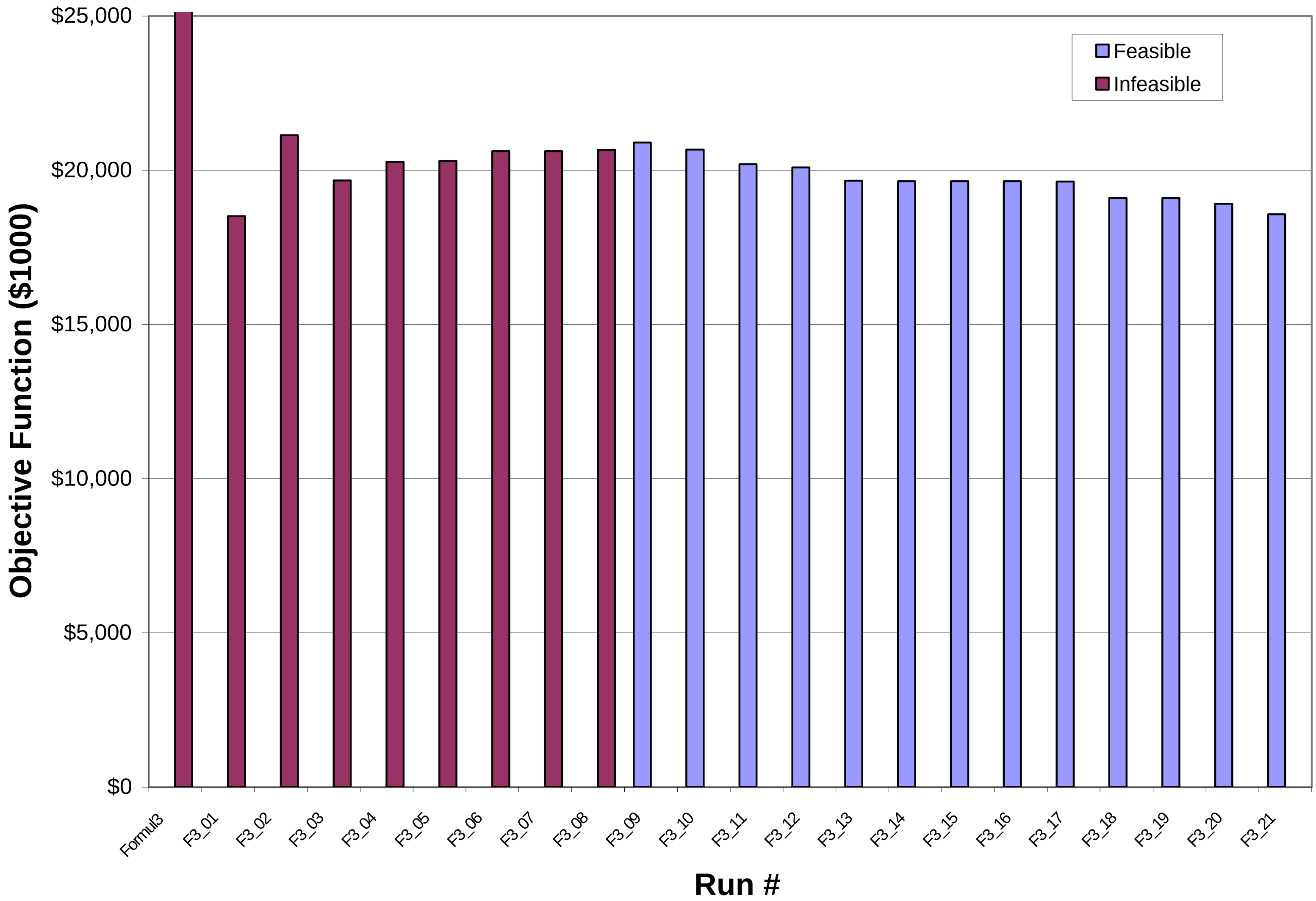

Figure 2-10 Mass Remaining After Each Year, Formulation 3

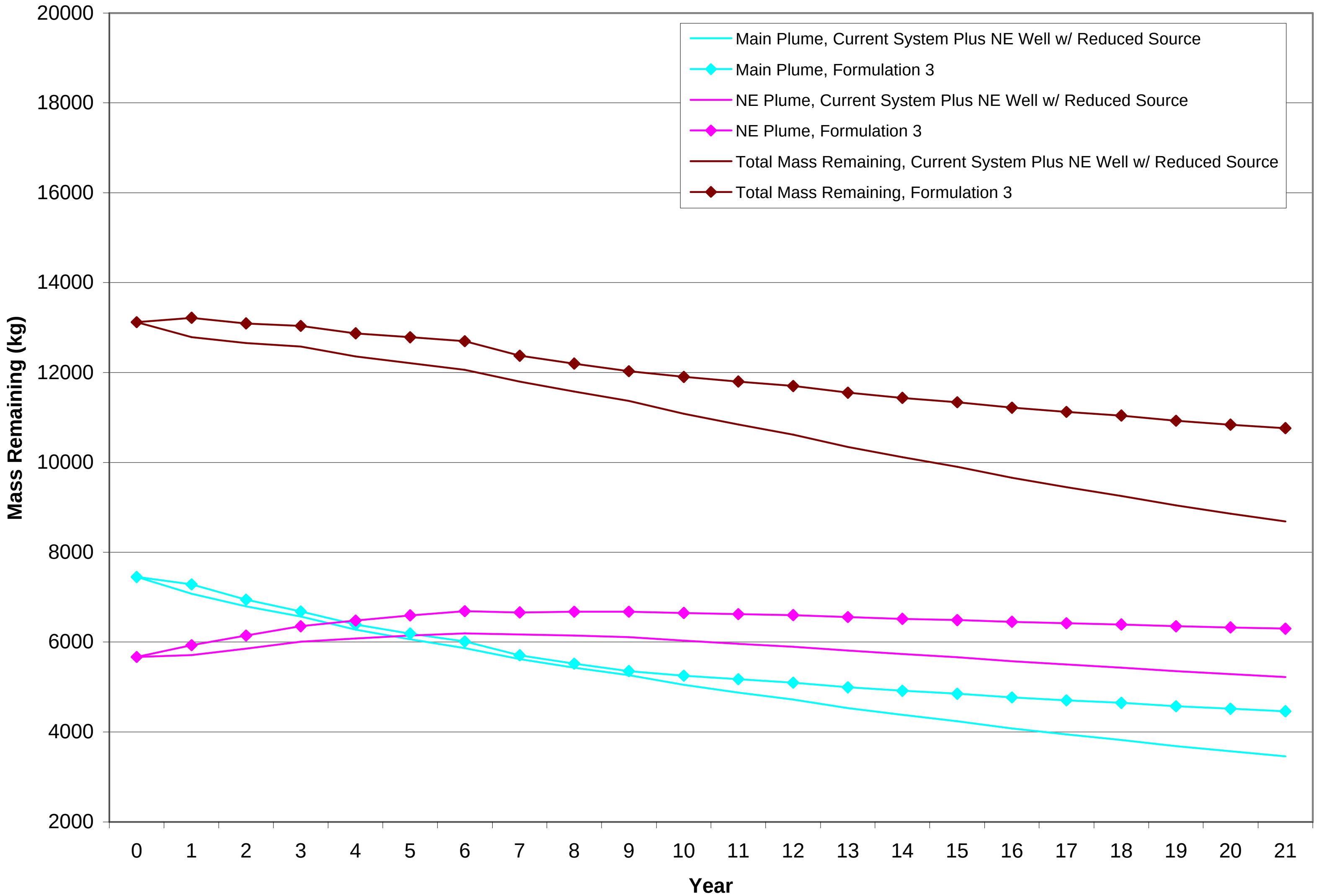

Figure 2-11 TCE Distributions After 21 Years, Model Layers 1 and 2, Additional Simulations A

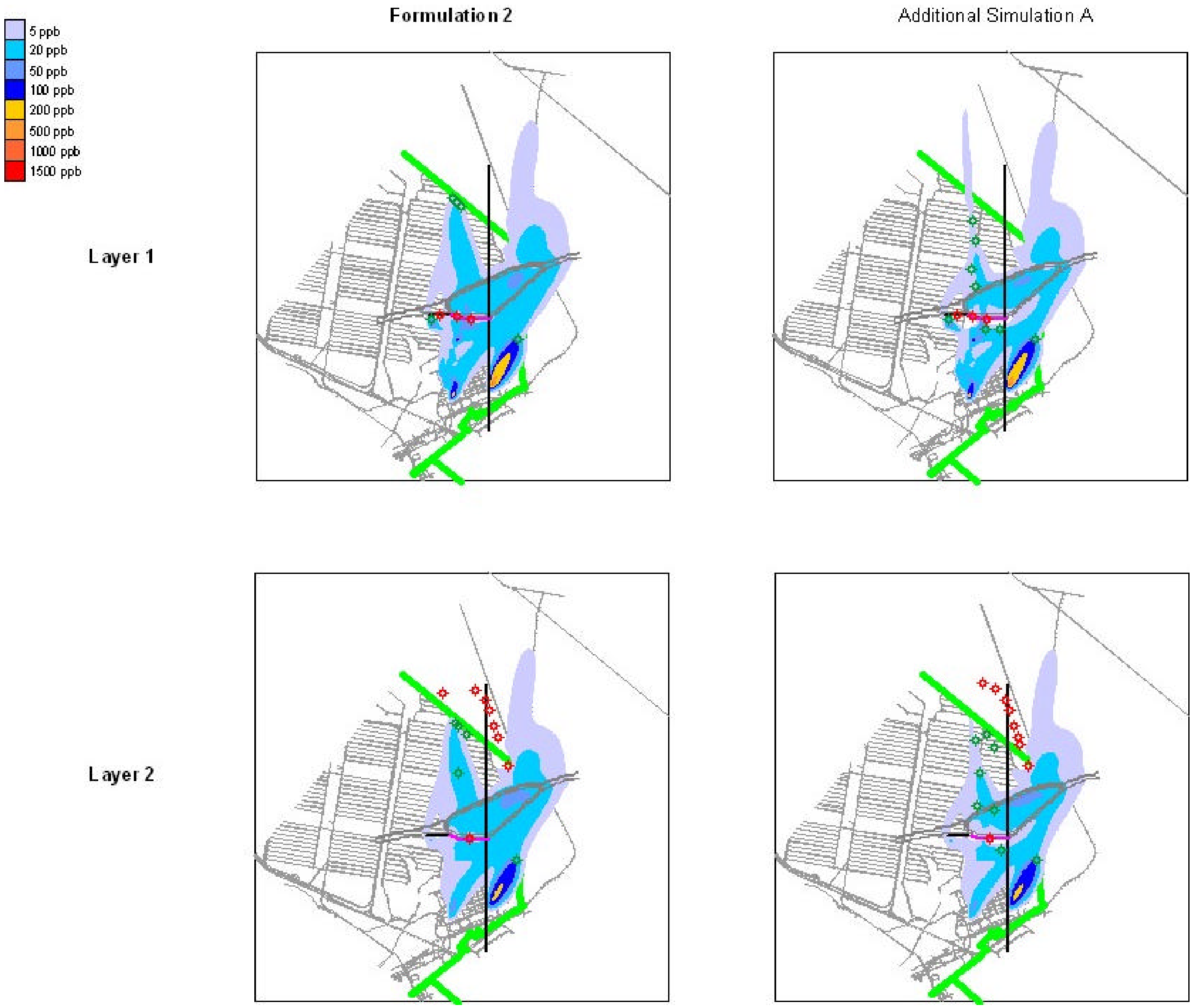

Figure 2-12   Mass Remaining After Each Year, Additional Simulations A

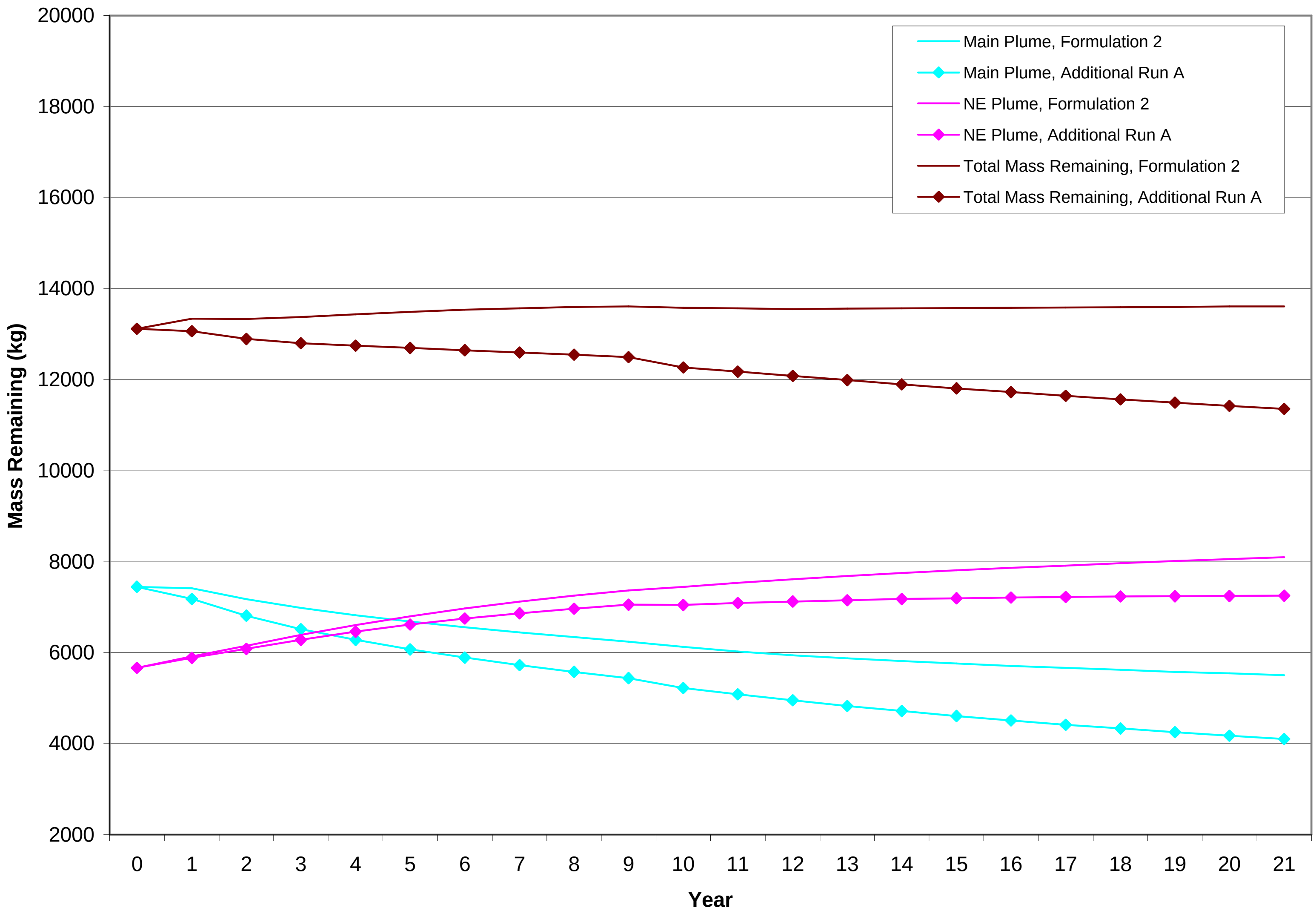

Figure 2-13   TCE Distributions After 21 Years, Model Layers 1 and 2, Additional Simulations B

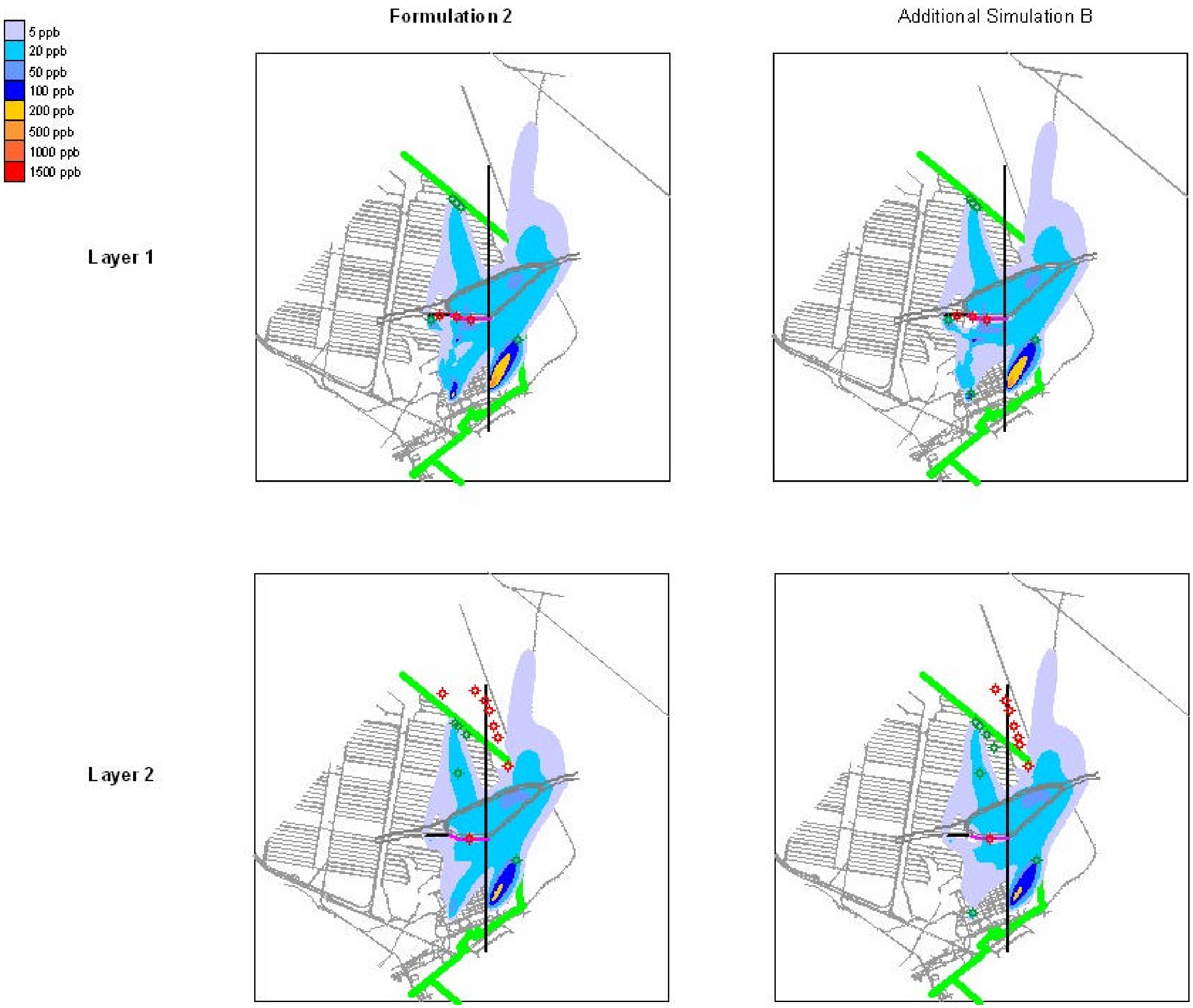

Figure 2-14   Mass Remaining After Each Year, Additional Simulations B

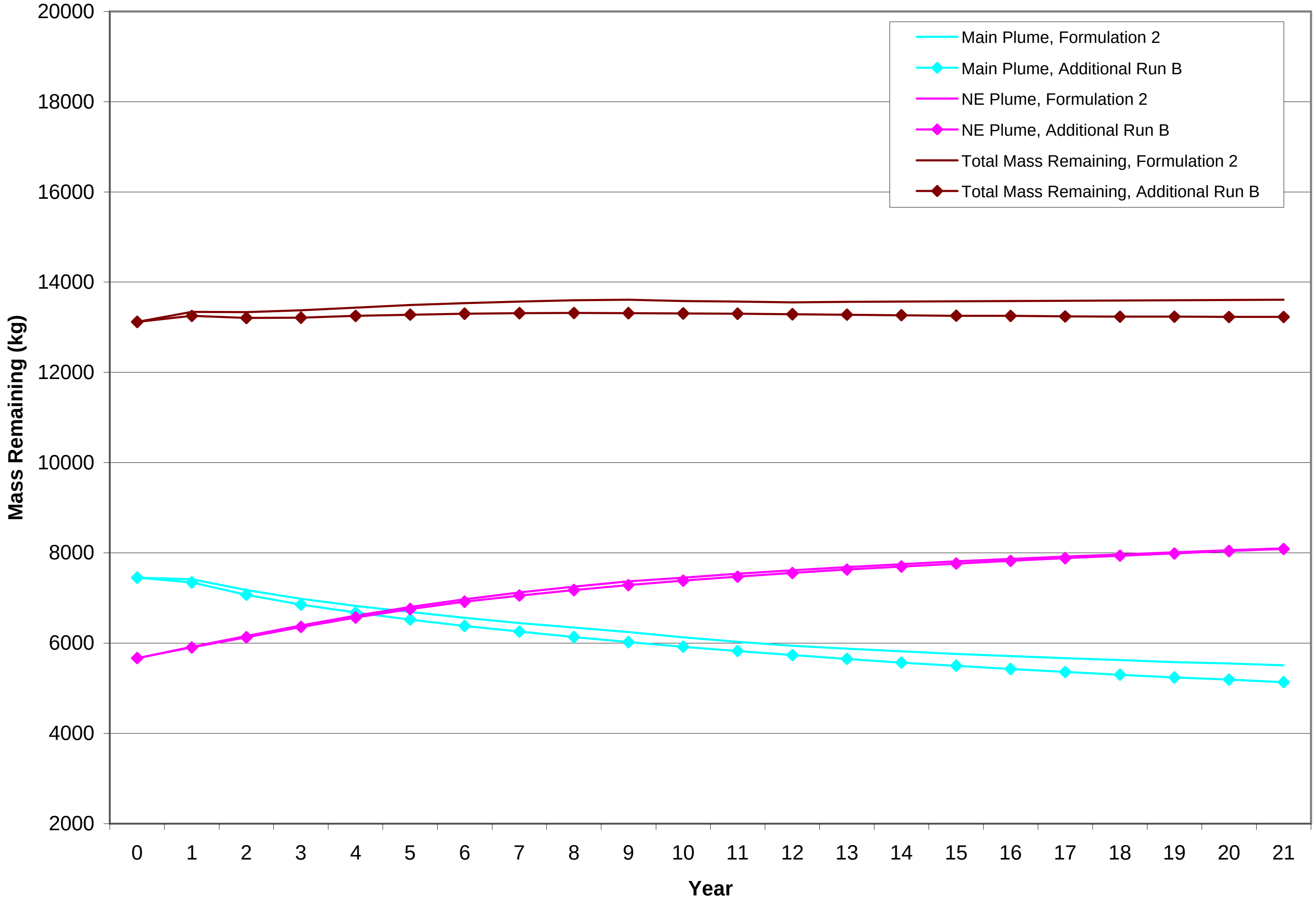

Figure 2-15 TCE Distributions After 21 Years, Model Layers 1 and 2, Additional Simulations C

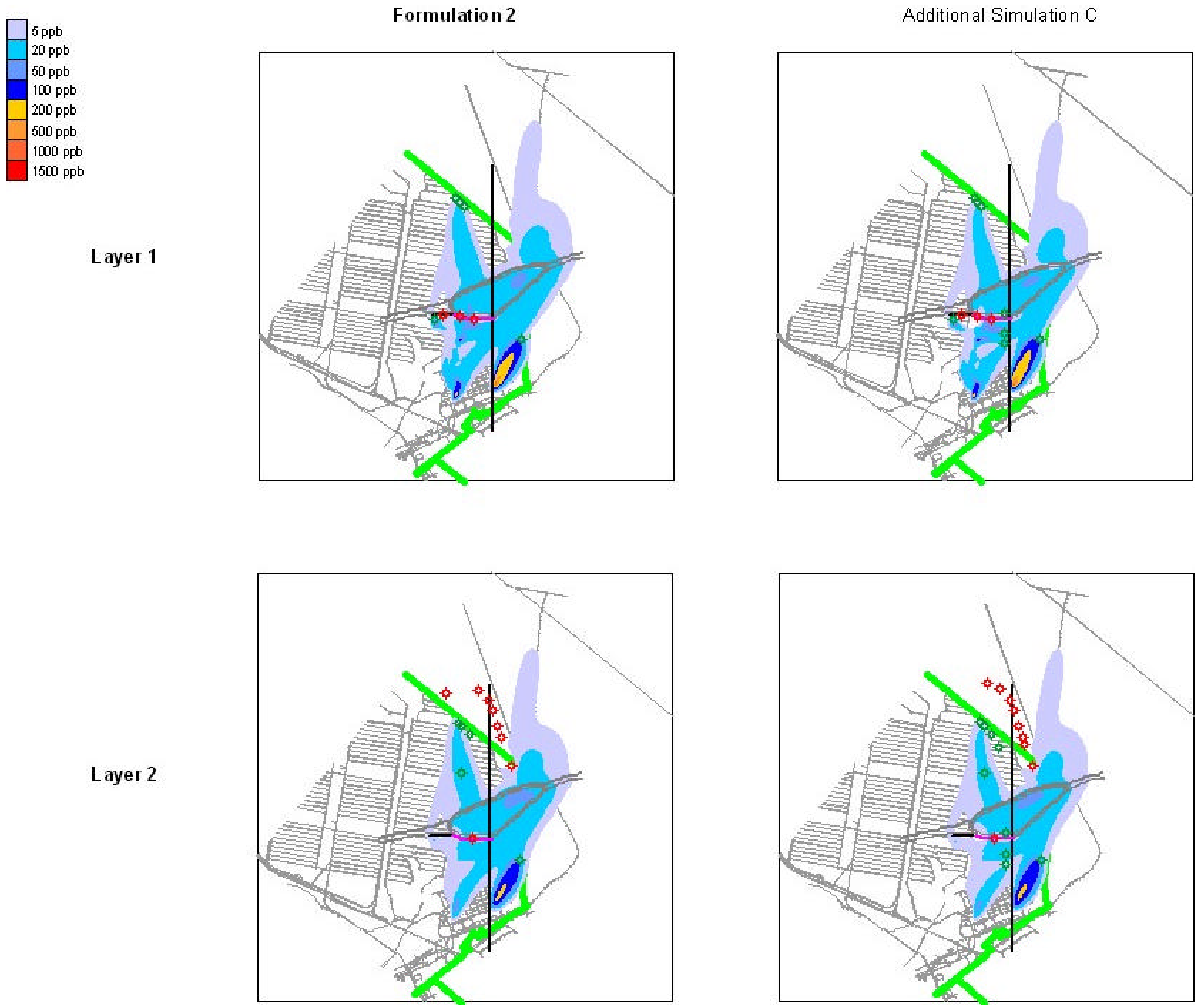

Figure 2-16 Mass Remaining After Each Year, Additional Simulations C