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Reducing Long-Term Remedial Costs by Transport Modeling Optimization

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ground water

Reducing Long-Term Remedial Costs by Transport Modeling Optimization

by David Becker[1], Barbara Minsker[2], Robert Greenwald[3], Yan Zhang[3], Karla Harre[4], Kathleen Yager[5], Chunmiao Zheng[6], and Richard Peralta[7]

Abstract

The Department of Defense (DoD) Environmental Security Technology Certification Program and the Environmental Protection Agency sponsored a project to evaluate the benefits and utility of contaminant transport simulation-optimization algorithms against traditional (trial and error) modeling approaches. Three pump-and-treat facilities operated by the DoD were selected for inclusion in the project. Three optimization formulations were developed for each facility and solved independently by three modeling teams (two using simulation-optimization algorithms and one applying trial-and-error methods). The results clearly indicate that simulation-optimization methods are able to search a wider range of well locations and flow rates and identify better solutions than current trial-and-error approaches. The solutions found were 5% to 50% better than those obtained using trial-and-error (measured using optimal objective function values), with an average improvement of ~20%. This translated into potential savings ranging from $600,000 to $10,000,000 for the three sites. In nearly all cases, the cost savings easily outweighed the costs of the optimization. To reduce computational requirements, in some cases the simulation-optimization groups applied multiple mathematical algorithms, solved a series of modified subproblems, and/or fit "meta-models" such as neural networks or regression models to replace time-consuming simulation models in the optimization algorithm. The optimal solutions did not account for the uncertainties inherent in the modeling process. This project illustrates that transport simulation-optimization techniques are practical for real problems. However, applying the techniques in an efficient manner requires expertise and should involve iterative modification to the formulations based on interim results.

Introduction

We document the benefits and lessons learned in the application of coupled optimization and transport simulation models to three pump-and-treat systems. Recent studies completed by the U.S. EPA (2002) and the Navy (Naval Facilities Engineering Command 2003) indicate that the majority of existing pump-and-treat systems are not operating as designed and have not been optimized since installation. Even when the initial pump-and-treat system has been appropriately designed, changes in plume configuration, aquifer conditions, and regulatory climates result in the need for system optimization.

Traditionally, pump-and-treat systems are designed or improved by applying a trial-and-error approach that attempts to identify the "best" well and flow configuration following numerous iterative runs of the flow and transport model. Simulation-optimization models link mathematical optimization techniques with simulations of ground water flow and/or solute transport to determine, in a largely

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automated fashion, the "best" combination of well locations and pumping rates. The optimal solution is defined by an explicit measure, such as life cycle cost or mass remaining, termed the "objective function." The optimal solution must meet site-specific constraints, such as limits on pumping rates, costs, concentrations, or well locations. Together, the objective function and constraints comprise the "formulation," which defines the problem to be solved.

Transport simulation optimization has previously been demonstrated at several U.S. Air Force sites. The two most recent of these were conducted at Wurtsmith Air Force Base, Michigan (Aly and Peralta 1997), and Massachusetts Military Reservation (Peralta et al. 1999a, 1999b; Peralta 2001; Zheng and Wang 2002b). In these cases, aspects of the optimal results were implemented. Peralta (2001) also describes some earlier applications of simulation optimization to Air Force ground water extraction systems.

The U.S. EPA sponsored a demonstration of flow-only simulation optimization at three existing ground water extraction systems using the MODMAN package (U.S. EPA 1999a, 1999b). The MODMAN results indicated a typical potential reduction of 10% to 20% relative to the annual costs of the existing systems. One recommendation of that study was to perform additional demonstrations using transport simulation-optimization tools.

We pursued a demonstration of transport simulation-optimization approaches with financial support from the Department of Defense Environmental Security Technology Certification Program (ESTCP) and the U.S. EPA. The primary objective of this project was to demonstrate the cost benefit, if any, of applying transport simulation-optimization codes to three pump-and-treat systems (two existing and one in the design phase) relative to a traditional trial-and-error modeling approach (a scientific control) used to solve the same formulations. A secondary objective was to provide each installation with alternate pumping strategies that are feasible and cost effective to implement. Three formulations per site were developed in conjunction with the installation staff and their contractors in order to address problems of interest to them. While the installations were encouraged to implement optimization suggestions resulting from the demonstration, they were not required to do so.

Approach

For this demonstration, transport simulation-optimization was performed for three sites: Umatilla Chemical Depot, Hermiston, Oregon; Tooele Army Depot, Tooele, Utah; and the former Blaine Naval Ammunition Depot, Hastings, Nebraska.

The demonstration used existing ground water flow and transport models for each site. A prerequisite of selecting a site for inclusion in the project was the existence of a numerical transport model (MODFLOW 96 [Harbaugh and McDonald 1996]/MT3D [Zheng and Wang 1999]) considered to be up to date and acceptable for design purposes. The three sites and the models are summarized subsequently and in Table 1. To speed the optimization process, the simulation models were modified as necessary to require no more than 2 h of computational time per run and to include no more than two simulated constituents.

Umatilla Chemical Depot

Umatilla is a large military reservation located in northeastern Oregon, established in 1941 as an ordnance depot for storage and handling of munitions. Explosives in wash water from a washout plant migrated into the soil and ground water at the site. The two most common ground water contaminants are RDX (hexahydro-1,3,5-trinitro-1,3,5-triazine) and TNT (2,4,6-trinitrotoluene). Figure 1 illustrates the concentrations and extent of the RDX and TNT plumes prior to start of remediation and the current locations of extraction wells and recharge basins. Table 1 summarizes site conditions, the existing pump-and-treat system, and the models used in the project.

The site overlies an unconsolidated aquifer that includes sands and gravels displaying very high permeabilities deposited during catastrophic glacial lake releases. An underlying silt layer sits upon basalt bedrock. Ground water flow directions are generally to the south and southeast, but flow directions vary due to regional irrigation pumping.

Tooele Army Depot

Tooele Army Depot was established in 1942 largely to provide maintenance and storage of wheeled vehicles and conventional weapons. Trichloroethylene (TCE) is the primary contaminant of concern. Two major plumes, the "main" and northeast, emanate from multiple-source areas. Figure 2 shows the extent of TCE contamination and the current locations of extraction and injection wells. The Northeast Plume extends beyond the property boundary, and the off-site extent is not fully characterized. Concentrations of the main plume are significantly lower in the deeper portions of the aquifer than in shallow portions of the aquifer. Historically, the target containment zone has been defined by the 5 μg/L TCE contour. However, a smaller target containment zone is now being considered.

The aquifer generally consists of coarse but heterogeneous alluvial deposits 120 to 210 m thick; however, there is an uplifted bedrock high at the site where ground water is forced to flow from the alluvial deposits into fractured and weathered rock (bedrock) and then back into alluvial deposits. The uplifted bedrock high and bounding low–hydraulic conductivity materials (possibly fault gouge) are the hydraulically controlling features of the study area due to the steep gradients they cause. Ground water of the main plume generally flows in a northwest direction though flow is diverted to the northeast near the bedrock block. Additional information on the site hydrogeology, pump-and-treat system, and existing models is provided in Table 1.

Former Blaine Naval Ammunition Depot

Blaine consists of 200 km^2 located immediately east of Hastings, Nebraska. Blaine was built during World War II as an active "load, assemble, and pack" ammunition facility. Ground water and soil has been contaminated by explosives residues (primarily RDX, TNT, and degradation

Table 1
Site Background Information

Site Name	Contaminants	Depth to Water	Hydraulic Conductivities	Existing System (start date)	System Flow, Treatment, Annual Cost	Model Dimensions (all models MODFLOW and MT3DMS)	Model Run Time (Pentium III, 1 GHz)
Umatilla Chemical Depot	RDX, TNT	~15 m	Alluvial deposits: 3.5E−4 to 1.8 cm/s; silt/weathered basalt: 3.5E−4 to 2.1E−3 cm/s	Three recharge basins, three extraction wells (1997)	4280 L/min, carbon adsorption, $430,000	125 rows (8–200 m), 132 columns (7–200 m), and 5 layers. Layer 1: alluvial aquifer, layers 2–5: silt + weathered basalt	10 min
Tooele Army Depot	TCE	45–120 m	Alluvial deposits: 0.02–0.14 cm/s; central bedrock block: 1.4E−5 to 3.4E−4 cm/s	16 extraction wells, 13 injection wells (1993)	26,400 L/min, air stripping, >$1M	165 rows, 99 columns, (cells 60 by 60 m), four layers (45, 30, 45, and 90 m thick)	10 min
Former Blaine Naval Ammunition Depot	PCE, TCE, 1,1 DCE, 1,1,1 TCA, RDX, TNT (only TCE and TNT simulated for this project)	30 m	Unconfined aquifer: 3.5E−3 to 2.8E−2 cm/s (saturated thickness = 3 m); confining unit: 7E−7 to 1.8E−4 cm/s (thickness 0–6 m); Semiconfined aquifer: 5.3E−2 to 8.8E−2 cm/s (30–45 m thick)	None, currently in FS phase. Alternatives range from 17 to 34 extraction wells	9500–16,700 L/min, air stripping and carbon adsorption, estimated annual cost >$2M	82 rows, 136 columns (120 by 120 m expanding to 600 by 600 m near model edges), six layers. Layer 1: unconfined aquifer, layer 2: confining unit, layers 3–6: semiconfined aquifer	2 h

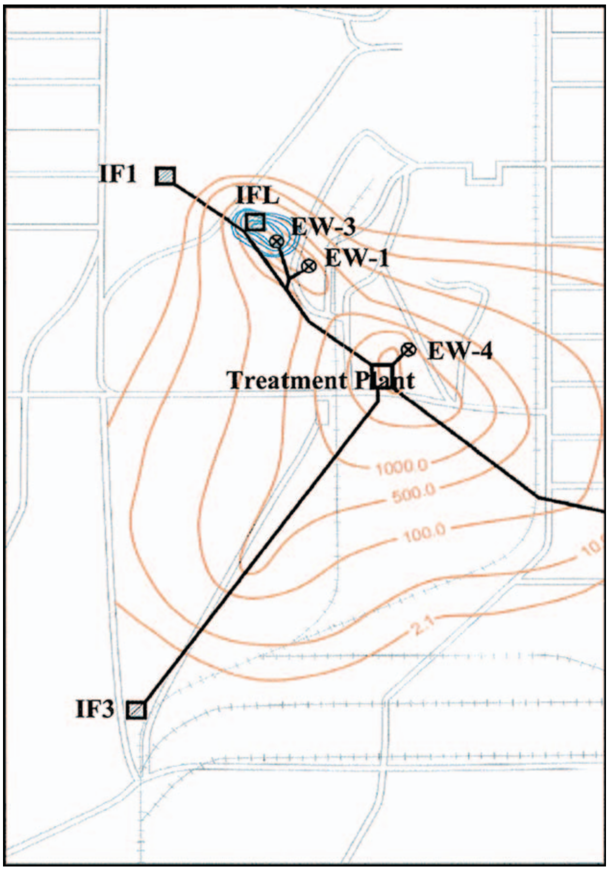

Figure 1. Umatilla Chemical Depot, contaminant plumes and remediation system.

products) and chlorinated solvents (primarily tetrachloroethene, TCE, 1,1-dichloroethene, and 1,1,1-trichloroethanol). Several separate plumes, some nearly 6 km long, have been defined, including some with comingled solvents and explosives residues (Figure 3). These plumes have impacted both shallow and deep water bearing hydrostratigraphic units. The deeper unit is a major water supply aquifer for municipal, industrial, and irrigation needs. The ground water flow direction is predominantly to the east and southeast during non-irrigation seasons, but irrigation pumping dramatically alters the flow direction.

There is no existing ground water extraction remediation system at Blaine. The planned ground water remedy is in the design stage, based on a feasibility study (FS) performed in August 2000. The FS focused on remediation alternatives ranging from containment to aggressive remediation of the ground water with predicted cleanup times of <50 to 60 years. The flow rates used for the alternatives and the model geometry are summarized in Table 1.

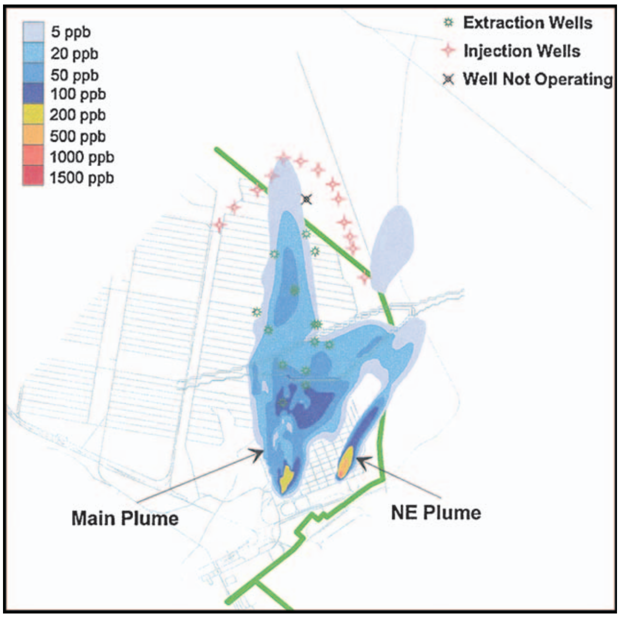

Figure 2. Tooele Army Depot, contaminant plumes and remediation system.

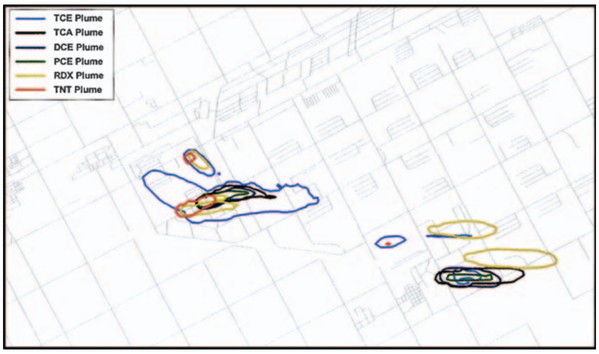

Figure 3. Former Blaine Naval Ammunition Depot, contaminant plumes.

Optimization Packages

The project used two simulation-optimization packages: SOMOS, developed at Utah State University (USU) (Systems Simulation/Optimization Laboratory and Peralta and Associates Inc. 2001; Peralta 2003), and MGO, developed at the University of Alabama (UA) (Zheng and Wang 2002a). The investigators were selected based on the availability of their optimization packages and on the prior field implementation of their optimization packages in a way similar to what was intended for this project.

Both of the packages used in this project implement "heuristic" algorithms, meaning that they are not guaranteed to find the globally optimal solution but have usually been found in practice to identify optimal or near-optimal solutions. The algorithms include genetic algorithms (Holland 1975; Goldberg 1989), simulated annealing (Metropolis et al. 1953), and tabu search (Glover 1986, 1989). These global methods often require intensive computational effort but have become more practical for application on personal computers as computer speeds have increased. They can also handle any form of objective function and constraints and any type of simulation model, along with relatively straightforward linking of simulation models with the optimization algorithm. In addition, the SOMOS code can implement artificial neural networks as an efficient surrogate for the primary simulation model (Rumelhart 1987; Principe et al. 1999).

Trial-and-Error Control

In order to make a rigorous comparison of the benefits of the optimization packages over a more traditional trial-and-error approach to selecting pump-and-treat designs, independent modelers were selected from GeoTrans Inc. to act as a "scientific control" group. These modelers were very experienced in the design and optimization of ground water extraction systems. They used the same MODFLOW and MT3D models and solved the same formulations but did so using professional judgment to select well locations and pumping rates based on the results of previous model runs. Modeling runs were continued until no further improvement in the results (as measured by a predetermined objective function) could be obtained within the available resources.

Summary of Formulations

Three formulations, consisting of an objective function to be minimized and a set of constraints to be satisfied, were developed for each site. Each formulation mathematically represented problems of interest to the installation. Details of the formulations are provided by Minsker et al. (2003). GeoTrans provided a FORTRAN postprocessor for determining the objective function value and status of the constraints for any specific combination of well rates simulated with the transport model.

Umatilla Chemical Depot

Three different transport optimization formulations were developed for Umatilla based on input provided by the installation and the Army Corps of Engineers Seattle District. The installation expressed interest in achieving cleanup for both RDX and TNT at the lowest life cycle cost. The installation also expressed interest in determining the benefit of increasing the capacity of the granular activated carbon (GAC) treatment process above the current capacity of 4900 L/min. The first two formulations address those interests. A third formulation was then constructed with a goal of minimizing mass remaining to see if substantially different solutions would result.

The first formulation involved a cost function to be minimized that combined the capital costs for new wells or recharge basins and the costs for operations and maintenance (O&M) until cleanup for both RDX and TNT is achieved, assuming a discount rate of 5%. Cleanup, for both RDX (<2.1 μg/L) and TNT (<2.8 μg/L), had to be achieved within the modeling period (by the end of year 20). The total modeled pumping rate, when adjusted for the average amount of uptime, could not exceed 4900 L/min, the current maximum treatment capacity of the plant. The site hydrogeology limits the extraction rates at individual extraction wells to 1500 or 3800 L/min, depending on location, adjusted for system downtime. RDX and TNT concentration levels could not exceed their respective cleanup levels in locations beyond a specified area.

For the second formulation, the objective function was the same as for formulation 1, except another cost term was added for new GAC units. Constraints were the same as for formulation 1, except that treatment plant capacity could be increased in steps of 1200 L/min, from the current capacity of 5000 L/min to a maximum capacity of 7400 L/min.

For the third formulation, the objective function was to minimize the total mass remaining (RDX plus TNT) in layer 1 at the end of 20 years. The constraints were the same as for formulation 1, except that the maximum number of new wells could not exceed four and the maximum number of new recharge basins could not exceed three.

Tooele Army Depot

Three different transport optimization formulations were developed for Tooele based on input from the installation and the Army Corps of Engineers Sacramento District. The Northeast Plume was not well defined at the time of the study, and for the purpose of this study (based on a request from the installation), all formulations included a specified well in the Northeast Plume with 5700 L/min (implemented as 5400 L/min in the well package to account for downtime of 5%) to represent a general containment solution in that area.

Several terms were defined for the formulations. The "point of exposure–main plume" (POE-MP) was located along a portion of the property boundary. The "point of compliance–main plume" (POC-MP1) was defined as the southern boundary of the displaced sediments. The POC-MP2 is defined as the boundary along the upstream edge of the low-permeability gouge surrounding the bedrock high.

The first formulation involved a cost function to be minimized that combined up-front costs with the total of annual costs over a 21-year time frame assuming a discount rate of 5%. The total modeled pumping rate, when adjusted for the average amount of uptime, cannot exceed 30,000 L/min, the current maximum treatment capacity of the plant. The TCE concentration had to be <5 μg/L at the POE in each layer at the end of the first 3-year management period and thereafter. The extraction and injection wells could not exceed specific rate limits.

For the second formulation, the objective function was the same, but additional constraints requiring concentration limits were to be met at the POC (i.e., inside the plume). The concentration of TCE at POC-MP1 had to be 50% of the initial concentrations or <20 μg/L at the end of the first management period (year 3) and thereafter. The TCE concentration at POC-MP2 must be 50 μg/L at the end of 3 years, and 20 μg/L at the end of 9 years and thereafter.

The third formulation also included a source term that declined over time due to gradual natural exhaustion of the mass in the vadose zone, unlike the first two formulations (which have continuing sources at constant strength over time). The objective function was the same as formulations 1 and 2. The constraints were the same as formulation 2, with the following additions. Cleanup (defined as TCE < 50 μg/L) for the main plume (except specifically excluded areas) had to be met at the end of 9 years. The maximum number of new extraction and injection wells could not exceed four and four, respectively.

Former Blaine Naval Ammunition Depot

The project had a limit of only two contaminants to be rigorously simulated in the optimization process, but the installation was concerned about six contaminants, so an approach was developed to rigorously simulate TCE and TNT and to incorporate the distribution of the other constituents in those simulations. The distribution of the other volatile organic constituents and RDX were addressed by including them in the modeled TCE concentrations (based on their similar transport behavior), where the concentrations were weighted relative to the cleanup standards for each. Only surface disposal was considered for discharge of treated ground water, as requested by the site managers.

For the first formulation, a cost function to be minimized was developed that combined 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 to 6 assuming a discount rate of 3.5%. Cleanup, for both TCE and TNT, had to be achieved in model layers 3 to 6 within the modeling period (by the end of year 30). TCE and TNT concentration levels could not exceed their respective cleanup levels in locations beyond specified areas. Site managers used specific capacity assumptions to determine the limits on individual extraction well rates. Some restricted areas were defined where no remediation wells were allowed due to current land use. Remediation wells were not allowed in the same model cells with irrigation wells to prevent excessive dewatering in irrigation wells and/or at remediation wells. No wells were allowed in model layer 6.

Formulation 2 was the same as formulation 1, but assumed diversion of 9120 L/min of extracted water to a nearby utility plant (i.e., the project would not incur treatment or discharge costs for up to 9120 L/min of extracted water).

In formulation 3, the objective was to minimize the maximum total remediation pumping rate in any management period over a 30-year simulation. The constraints were the same as for formulation 1, except the constraint requiring cleanup within 30 years was eliminated and a constraint limiting the number of new remediation wells to 25 was added.

In essence, this formulation was 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.

Optimization Period

Optimization for the three formulations for each site was performed over a period of ~4 months, during which time the three modeling groups were not allowed to discuss their progress with each other or with the installation. Each modeling group submitted a report describing the results for each site after the optimization period (available as appendixes to Minsker et al. 2003).

Results

Since both the MGO and SOMO3 packages contain multiple solution algorithms, different algorithms were used for different individual formulations based on modelers' expertise, as summarized subsequently. The results from each of these two groups were compared to each other and to the results of trial-and-error optimization performed by GeoTrans. This project did not include detailed technical comparison of the numerical techniques implemented in the UA and USU codes, and rather focused on the results.

Umatilla Performance Data

For Umatilla, both UA and USU started with formulation 3, which they reported was the easiest of the three formulations to solve. Once formulation 3 was solved, they then applied the knowledge learned from solving formulation 3 when solving formulations 1 and 2. The trial-and-error group started with formulation 1. All three groups used results from formulation 1 as the initial solution for formulation 2. Table 2 shows the results for formulations 1 through 3.

For formulation 1, the USU and UA teams found very similar solutions. To overcome computational limits, both teams applied sequential approaches to optimization, such as using multiple runs where either flow rates or locations were fixed and the other parameter optimized, to explore possible solutions without solving the entire problem simultaneously. The trial-and-error solution was suboptimal by 34%, based on the objective function value.

All three groups reported that their primary approach involved minimizing the cleanup time. The UA and USU teams were able to improve their objective function values primarily by finding solutions with shorter total cleanup time (4 years) relative to the trial-and-error solution (6 years). The optimal solution from all three groups used two existing pumping wells located in the TNT plume, plus two new wells also located within the TNT plume. TNT sorbs strongly to the soil and hence maximum pumping within the TNT plume is essential to ensure that the cleanup is completed as quickly as possible. All three optimal solutions used the two existing recharge basins located in the southern portion of the study area that were designed to flush the RDX toward the extraction wells. The trial-and-error solution by GeoTrans also used a third existing well located in the center of the RDX plume for the first 5 years. The solutions by the UA and USU teams avoided using an existing recharge basin north of the TNT plume because it would hamper the ability of wells extracting water within the TNT plume to draw back the RDX plume to "clean" within 4 years. GeoTrans continued use of the northern infiltration basin to speed TNT cleanup and added a new recharge basin south of the TNT plume after 5 years to further speed the cleanup of the TNT plume.

The strategy of moving all pumping within the TNT plume is successful according to the model because of high hydraulic conductivity zones in layer 1 of the model, which allow the RDX plume to be pulled to wells located in the TNT plume within just a few years. These modeled hydraulic conductivities are quite high and may be subject to uncertainty. The USU team developed many well combinations that yielded the same objective function value. Therefore, the USU team also performed a limited postoptimization sensitivity analysis to help identify strategies that were more robust. The more robust strategies could handle variations in hydraulic conductivity of ~10% to 15%. Greater variations might lead the strategy to fail, but whether the failure would lead to loss of capture or simply a longer remediation period is not clear without further analysis.

For Formulation 2, the major difference in cost between the groups using transport optimization algorithms

Table 2
Umatilla Formulations 1–3 Results

Formulation 1				Formulation 2				Formulation 3			
Minimize Costs Using Existing Treatment Capacity	Transport Optimization Algorithms		Trial and Error	Same as Formulation 1, but Treatment Capacity Can Be Added	Transport Optimization Algorithms		Trial and Error	Minimize Mass in Layer 1 after 20 years	Transport Optimization Algorithms		Trial and Error
	UA	USU	GeoTrans		UA	USU	GeoTrans		UA	USU	GeoTrans
Objective function value (millions $)	1.66	1.66	2.23	Objective function value	1.66	1.66	2.02	Objective function value	1.66	1.66	2.02
No. of new extraction wells	2	2	2	No. of new extraction wells	2	2	2	No. of new extraction wells	2	2	2
No. of new infiltration basins	0	0	1	No. of new infiltration basins	0	0	0	No. of new infiltration basins	0	0	0
No. of existing extraction wells	2	2	3	No. of new GAC units installed	0	0	2	No. of new GAC units installed	0	0	2
No. of existing infiltration basins	2	2	3	No. of existing extraction wells	2	2	3	No. of existing extraction wells	2	2	3
Elapsed years until cleanup for RDX	4	4	6	No. of existing infiltration basins	2	2	3	No. of existing infiltration basins	2	2	3
Elapsed years until cleanup for TNT	4	4	6	Elapsed years until cleanup for RDX	4	4	4	Elapsed years until cleanup for RDX	4	4	4
Algorithms used	TS	GA, then coupled GA + ANN		Elapsed years until cleanup for TNT	4	4	4	Elapsed years until cleanup for TNT	4	4	4
				Algorithms used	TS	GA, then coupled GA + ANN		Algorithms used	TS	GA, then coupled GA + ANN	

GA, genetic algorithm; TS, tabu search; ANN, artificial neural network.

and the group using trial and error is that the trial-and-error solution required additional treatment capacity, with a capital cost of $300K, to achieve cleanup in 4 years (vs. the trial-and-error solution of 6 years for formulation 1). The groups using transport optimization algorithms achieved the 4-year cleanup time without additional capacity (i.e., using the solution to formulation 1). The transport optimization modeling groups discovered that increasing pumping rates and adding a new GAC unit would not reduce the cost below the optimal solution to formulation 1; thus, they concluded that the optimal solution for formulation 1 is also the optimal solution for formulation 2. The trial-and-error solution was suboptimal2 by ~22% relative to the optimal solution determined with an optimization algorithm.

As with the other formulations, the optimal solutions for formulation 3 developed by the UA and USU teams, using optimization algorithms, are nearly identical. The trial-and-error solution was suboptimal by ~50%, based on objective function value, relative to the optimal solutions determined with the optimization algorithms. At first glance, this formulation appears to be less useful than the others because the optimization results of formulations 1 and 2 indicated the potential for cleanup in 4 to 6 years, while this formulation assumes pumping for a full 20 years. Also, because the mass remaining in the latter years is so low, the model predictions are likely to be in error because of the assumed equilibrium adsorption.

Tooele Performance Data

For Tooele, all three groups started with formulation 1 and then solved formulation 2 based on the results from formulation 1. Also, all three groups quickly concluded that no feasible solution could be found for formulation 3 due to the constraint on the number of new wells allowed. Thus, various alternative formulations to formulation 3 were developed and solved by each group. Table 3 shows the results obtained for Tooele formulations 1 and 2.

For formulation 1, all the groups recognized that minimizing the number of wells installed and operating, rather than minimizing the cleanup duration, would minimize cost at this site. All the teams found solutions that use only 2 of the 16 existing extraction wells, indicating that many of the existing extraction wells may not be needed to meet current objectives. The groups using mathematical optimization, UA and USU, found solutions that cost 13% and 3% less, respectively, than the trial-and-error solution from GeoTrans. Approximately $10M of the costs were fixed O&M costs and could not change with the pumping strategy; however, if these costs were removed, the mathematical optimization solutions were from 42% to 11% less expensive than the trial-and-error solutions.

UA determined that feasible solutions could be achieved with much lower cost by replacing new extraction wells with injection wells. Though allowed by the posed set of constraints, the USU team chose not to inject within the plume, but rather to optimize capture of the 5 µg/L at the facility boundary, as did the GeoTrans strategy.

The UA solution for formulation 2 was 11% less expensive than the trial-and-error solution, which becomes a 30% improvement if the fixed O&M costs are removed. The USU team did not submit a design for formulation 2 as posed because they added a constraint to prevent mass migration around the west side of

Table 3
Tooele Formulation Results

Formulation 1				Formulation 2			
Minimize Cost Subject to Cleanup at Point of Exposure in 3 Years	Transport Optimization Algorithms		Trial and Error	Same as Formulation 1, but also Meet Concentration Goal at Point of Compliance	Transport Optimization Algorithms		Trial and Error
	UA	USU[1]	GeoTrans		UA	USU[2]	GeoTrans
Objective function value (millions $)	12.67	14.14	14.63		14.45	**	16.32
No. of new extraction wells	0	3	4	No. of new extraction wells	1	**	5
No. of new injection wells	4	0	0	No. of new injection wells	7	**	3
No. of existing extraction wells used	2	2	2	No. of existing extraction wells used	2	**	2
No. of existing injection wells used	1	11	8	No. of existing injection wells used	2	**	7
Algorithms used	GA	GA		Algorithms used	GA and TS	GA	

[1] USU constrained their solution and did not allow injection within the plume that might spread the plume (>5 µg/L) into previously cleaner aquifer.
[2] **—USU declined to submit a design for the posed problem because the least cost solution to that problem would (according to the simulation model) cause contamination to move to the west, bypassing the POC-MP1 constraint zone.
GA, genetic algorithm; TS, tabu search.

POC-MP1. Because the USU team solved an alternate formulation that was not the same problem solved by the others, it is not included in the comparison in Table 3.

All the groups found that in order to satisfy the POC constraints for formulation 2, one must inject just upgradient of the central and eastern POC zones. It is not clear that these solutions meet the intended benefit of the POC, which is to implicitly meet the POE-MP by achieving the POC constraints, because all the solutions still require continued pumping at the POE-MP for the entire 21-year period.

Formulation 3 required cleanup of the main plume in 9 years while limiting the number of new wells. All three teams reported that formulation 3 was infeasible as stated due to the restriction on the number of new wells that could be installed. To eliminate this infeasibility, all the groups chose to allow more new wells. Also, each group solved a slightly different problem by modifying one or more constraints, so the results from each group are not directly comparable.

The UA team examined two different alternative formulations using genetic algorithms. The first alternative was to identify the smallest number of new wells that would be required to obtain a feasible solution. They found a solution that used four new extraction wells, six new injection wells, and six existing wells, at a cost \$19.3M. The second alternative was to identify the least costly solution that would allow the number of new injection and pumping wells to exceed the original constraint, which had a solution with five new extraction wells, seven new injection wells, and three existing wells, and a cost of \$18.6M. The USU team used genetic algorithms to identify a solution with nine new extraction wells, three new injection wells, and three existing extraction wells, and a cost of \$17.9M. In identifying this solution, the USU team did not allow injection at locations within the plume other than near POC-MP1. As with formulation 2, they also included an additional constraint preventing plume (>5 μg/L) migration around the western edge of POC-MP1. To reduce costs, they relaxed that constraint in the last periods, allowing 12 μg/L TCE to enter one cell at the western end of POC-MP1.

Finally, the trial-and-error team found a solution with nine new extraction wells, four new injection wells, and two existing extraction wells, and a cost of \$18.6M. This solution was obtained by relaxing the constraint on the number of new wells and satisfying all other original constraints. Although each of the three groups solved slightly different problems, the objective function values found were similar. The optimal well locations and strategies were also highly constrained by locations of continuing sources. In fact, many extraction well locations that were selected are near continuing sources.

Blaine Performance Data

Both the UA and USU groups solved formulation 1 first, then formulation 2, and finally formulation 3. The trial-and-error team started with formulation 3 (after a few initial simulations for formulation 1) because it was the easiest problem to find a feasible solution for (no cleanup constraint), and then solved formulation 1 based on knowledge learned from solving formulation 3. The trial-and-error group never performed any actual simulations for formulation 2, concluding based on logic that the optimal solution for formulation 1 would also be optimal for formulation 2. Table 4 shows each team's results for formulations 1 through 3 for the Blaine site.

The goal of formulation 1 was to minimize life cycle cost to achieve cleanup. All three groups found that the least cost solutions came from minimizing pumping in each 5-year management period, not shortening the cleanup duration. Both groups using optimization algorithms found better solutions than the trial-and-error group. The USU team's solution was ~20% improved over the control group, and the UA team's solution was ~10% improved over the control group. Both groups employed an approach with more wells and increasing pumping rates at later times, while the trial-and-error group installed wells at early periods and then lowered the pumping rates at later times.

Formulation 2 was similar to formulation 1 but allowed part of the flow to be diverted for use (and treatment) by a new nearby utility plant. All three groups found that the solution that was optimal for formulation 1 was also optimal for formulation 2. Diverting part of the extracted water reduced treatment costs substantially but did not change the optimal pumping strategy.

With the reduced treatment costs, the optimal strategy from the USU and UA teams were ~33% and 15% less expensive, respectively, than the trial-and-error team's solution. The UA team's solution would allow all the water extracted during the first management period to be diverted, potentially eliminating the need to install a treatment plant for 5 years. This would only be possible if the TNT levels in the water were low enough to allow diversion of all the water, however.

The goal of formulation 3 was to minimize the maximum pumping rate in any management period to achieve containment of the plumes during a 30-year simulation period (cleanup was not a goal). Again, both groups using optimization algorithms achieved better solutions than the trial-and-error group, with the USU team's solution having 26% improvement and the UA team's solution having 5% improvement. All three groups obtained significantly different solutions, with peak pumping rates ranging from 8089 to 10,900 L/min and 7 to 25 pumping wells. Solutions that used more wells had lower peak pumping rates, as would be expected. Finally, it should be noted that the USU solution might not require treatment plant installation if the 9085 L/min diversion proposed in formulation 2 occurred and TNT levels in the water were sufficiently low.

Analysis and Conclusions

In each and every case, the groups applying the optimization algorithms found improved solutions relative to the trial-and-error group. The solutions found were 5% to 50% better than those obtained using trial-and-error (measured using optimal objective function values), with a typical improvement of ~20%. Because multiple sites

Table 4
Blaine Formulations 1–3 Results

Formulation 1				Formulation 2				Formulation 3			
	Transport Optimization Algorithms		Trial and Error	Same as Formulation 1, but Divert 9085 L/min of Extracted Water to Utility	Transport Optimization Algorithms		Trial and Error	Minimize Pumping to Maintain Containment	Transport Optimization Algorithms		Trial and Error
Minimize Costs for Cleanup in 30 Years	UA	USU	GeoTrans		UA	USU	GeoTrans		UA	USU	GeoTrans
Objective function value (millions $)	45.28	40.82	50.34	Objective function value (millions $)	24.04	18.88	28.39	Objective function value (millions $)	10,360	8097	10,900
No. of new extraction wells	15	10	8	No. of new extraction wells	15	10	8	No. of new extraction wells	13	25	7
Pumping rates (L/min) by 5-year management periods	7450 11,750 12,704 14,006 14,195 14,195	9410 9963 10,009 10,417 12,515 12,787	15,123 15,047 15,123 15,123 14,858 11,754	Elapsed years until cleanup for TCE	30	30	30	Elapsed years until cleanup for TCE	>30	>30	>30
Elapsed years until cleanup for TCE	30	30	30	Elapsed years until cleanup for TNT	30	29	25	Elapsed years until cleanup for TNT	30	>30	30
Elapsed years until cleanup for TNT	30	29	25	Algorithms used	TS and GA	GA, SA, GA coupled with ANN		Algorithms used	TS and GA	GA, SA, GA coupled with ANN	
Algorithms used	TS and GA	GA, SA, GA coupled with ANN									

GA, genetic algorithm; TS, tabu search; SA, simulated annealing.

Table 5
Approximate Number of Simulations Performed For Each Formulation

	Transport Optimization Algorithms	Trial-and-Error
	Optimization Teams	**GeoTrans**
Umatilla	Approximately 1000–8000 simulations	~25–40 simulations
Tooele	Approximately up to 8000 simulations	~60–80 simulations
Blaine	Approximately hundreds/thousands simulations	~60 simulations

were evaluated, and multiple formulations for each site were evaluated, there is a high degree of confidence in the conclusion that the application of optimization algorithms provides improved solutions for problems posed in the manner demonstrated in this project.

Both teams applying mathematical optimization obtained similar results for Umatilla, but the pumping strategy results differed considerably for Tooele and Hastings. The differences may be due to one or several of the following factors: (1) changes that individual modelers made in the formulations (primarily additional constraints) to overcome perceived problems in the solutions they obtained; (2) different approaches taken to overcoming the computational barriers of solving these complex problems; or (3) convergence of the heuristic optimization algorithms to suboptimal solutions.

The first factor arose because each team worked in isolation for 4 months without presenting any initial results to the installation (to ensure independence of each team's results). When this technology has been applied at other sites by a single optimization team, initial results are presented to the installation and the formulations (i.e., objective functions and constraints) are modified as needed to overcome any difficulties identified in the initial solutions. Hence, this factor will not be an issue in future use of this technology. The second factor will likely remain in the foreseeable future. The teams employed sequential solution approaches to reduce computational effort, in which some parts of the problem were fixed while others were optimized. These approaches require substantial expertise and professional insight. The last factor is intrinsic to the heuristic algorithms used in this optimization effort. If the optimization parameters were set appropriately, however, convergence to suboptimal solutions should occur rarely. Hence, we expect that most of the differences in the mathematical optimization groups' results are due to the first two factors.

The simulation-optimization methods clearly search a much larger portion of the solution space than the trial-and-error method and produce better solutions than trial-and-error. Table 5 summarizes the approximate number of runs performed by transport optimization teams vs. the trial-and-error team for each of three sites. Generally, "simulations" refers to the number of runs of the ground water model; however, due to the use of substituted functions in place of the numerical model in some formulations, it is impossible to calculate the number of completed ground water model simulations performed for the optimization codes more exactly. An important limitation of the trial-and-error approach is that the objectives and constraints are often not rigorously stated or complied with in all cases. Also, transport optimization is less prone to bias in selecting well rates and well locations because it is more automated than trial-and-error, and therefore is more likely to discover unexpected solutions.

The optimal solutions do not explicitly consider the uncertainties in the flow and transport model input parameters. Since optimal solutions typically just barely meet the constraints, these uncertainties represent risks when translating the "optimal" results to the real world. Exploration of the sensitivity of the optimal solution to changes in input parameters, such as was done to a limited extent by the USU team at Umatilla, can provide some indication of the magnitude of these risks. Alternatively, the constraints can be posed in a way to provide some "factor of safety." More sophisticated optimization schemes can account for uncertainty but were beyond the scope of this project.

Based on the competitive bids evaluated in this project for selecting the transport optimization groups, the estimated costs for applying the simulation-optimization methods are between $40,000 and $120,000, including site visits, report generation, and project management. Considering the costs of the trial-and-error approach, the premium for applying the transport optimization may be as little as zero, or as much as $40,000. The estimated range in costs results from differing site and model complexities. The likely savings would easily exceed the cost of applying the simulation-optimization methods (Zhang et al. 2003).

In summary, transport simulation-optimization techniques were applied to three "real world" sites and compared to traditional trial-and-error methods. Three formulations were developed for each site that reflected the needs and interests of the installations. In all cases, the simulation-optimization methods found better solutions as measured by the objective functions (e.g., cost, mass remaining). The potential savings of hundreds of thousands to millions of dollars over the lives of the projects far exceed the additional costs for applying the simulation-optimization methods over the costs of traditional trial-and-error methods. Computational complexity still poses challenges for transport simulation-optimization, and expertise is required in the posing and solving of the problems. Further information about the project and free versions of the optimization codes available for public use are available at www.frtr.gov/estcp.htm.

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