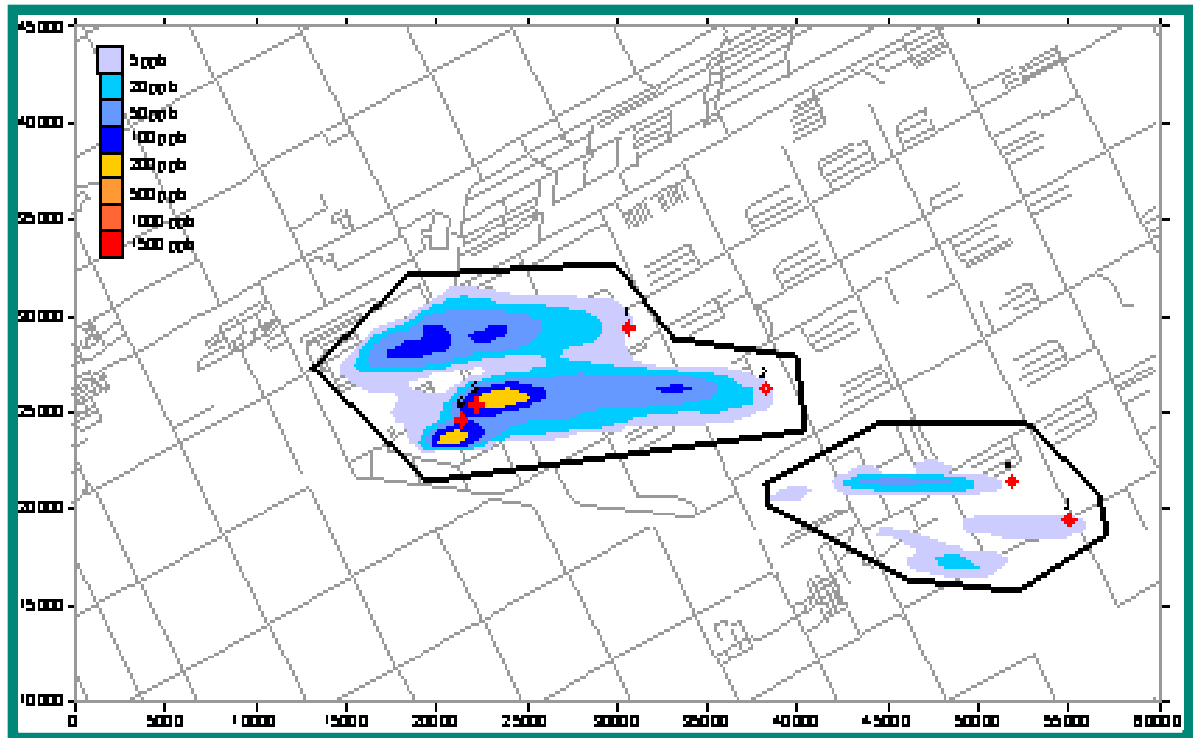# ESTCP
Cost and Performance Report

(CU-0010)

Application of Flow and Transport Optimization Codes to Groundwater Pump-and-Treat Systems

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**ENVIRONMENTAL SECURITY
TECHNOLOGY CERTIFICATION PROGRAM**

U.S. Department of Defense

COST & PERFORMANCE REPORT
ESTCP Project: CU-0010

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ACRONYMS AND ABBREVIATIONS

AFCEE   Air Force Center for Environmental Excellence

CS-10   Chemical Spill-10

DCE   1,2-Dichloroethane
DoD   Department of Defense

ESTCP   Environmental Security Technology Certification Program

GAC   granular activated carbon
gpm   gallons per minute

MODFLOW   modular three-dimensional finite-difference groundwater flow
MT3D   model transport in three dimension

NFESC   Naval Facilities Engineering Service Center

O&M   operating and maintenance

P&T   pump-and-treat
POE   point of exposure
POC   point of compliance
ppb   parts per billion

RDX   royal demolition explosive
RPO   remedial process optimization
RSE   Remediation system evaluation

SVE   soil vapor extraction

TCE   Trichloroethylene
TIO   Technology Innovation Office
TNT   2,4,6-Trinitrotoluene

UA   University of Alabama
USACE   U.S. Army Corps of Engineers
USDA   U.S. Department of Agriculture
USEPA   U.S. Environmental Protection Agency
USU   Utah State University

VOC   volatile organic compounds

ACKNOWLEDGEMENTS

The project team extends thanks to the facility management team and contractors associated with the following three sites for their assistance and support in the execution of this optimization demonstration study at their sites.

$ Umatilla Chemical Depot, Hermiston, Oregon
$ Tooele Army Depot, Tooele, Utah
$ Former Blaine Naval Ammunition Depot, Hastings, Nebraska

Technical material contained in this report has been approved for public release.

1.0   EXECUTIVE SUMMARY

1.1   BACKGROUND

This Environmental Security Technology Certification Program (ESTCP) project evaluated the benefits and utility of applying transport optimization algorithms, operable on desktop computers, versus a traditional trial-and-error approach. The focus was on groundwater pump-and-treat (P&T) systems. The transport optimization algorithms link mathematical optimization techniques with simulations of groundwater flow and contaminant transport to determine the best combination of well locations and pumping rates for a P&T system. These mathematical algorithms can contribute to long-term operating cost reduction and/or improved performance of these systems with respect to compliance objectives (e.g., achieve cleanup standards in less time).

Remediation system evaluation (RSE) or remedial process optimization (RPO) provides a broad assessment of optimization for the remedial systems, including system goals and exit strategy, below-ground performance, above-ground performance, monitoring and reporting, and potential for alternate technology. The pumpage optimization (as demonstrated in this project) is a subset or a component of these more general optimization evaluations for cases where P&T is expected to be a major component moving forward. The pumpage optimization impacts subsurface aspects of the remedy (e.g., cleanup time and containment) and in some cases also impacts above-ground aspects (treatment plant size/flow rate and influent concentrations) and possible monitoring requirements.

A previous project sponsored by the United States Environmental Protection Agency (USEPA, 1999 a and b) demonstrated potential savings of millions of dollars in operating and maintenance (O&M) costs over the projected P&T lifetime at two of three sites through the application of "hydraulic optimization." Hydraulic optimization couples simpler optimization techniques (linear and mixed-integer programming) with simulations of groundwater flow (but not transport). The transport optimization techniques that are the focus of this ESTCP project are potentially more powerful than the hydraulic optimization techniques because they rigorously incorporate predictions of contaminant concentrations, contaminant mass, and/or cleanup duration. However, transport optimization codes are also more complex and difficult to apply than hydraulic optimization codes.

This demonstration project was divided into two phases.

$ Phase 1: Pre-optimization site screening
$ Phase 2: Demonstration of transport optimization codes

For Phase 1, a spreadsheet-based pre-optimization screening methodology was developed and applied at eleven existing Department of Defense (DoD) P&T systems. The objective of Phase 1 was to provide end users with a framework and a simple tool for quickly and inexpensively prioritizing which sites are most likely to benefit from the application of transport optimization codes. For this project, criteria for site selection in addition to those specified in screening methodology included the existence of a flow and transport model considered to be "up-to-date

and acceptable for design purposes" and a willingness to consider implementing changes suggested by the optimization analysis.

For Phase 2, transport optimization was compared with a trial-and-error approach for the following three sites.

$	Umatilla Chemical Depot, Hermiston, Oregon (Umatilla)
$	Tooele Army Depot, Tooele, Utah (Tooele)
$	Former Blaine Naval Ammunition Depot, Hastings, Nebraska (Blaine)

Both the Umatilla and Tooele sites have existing P&T systems in operation, and the Blaine site is a planned P&T system. The pre-optimization screening methodology developed in Phase 1 can be used for both existing and planned systems, and the use of the optimization algorithms in Phase 2 is also applicable to both new and existing P&T systems.

## 1.2	OBJECTIVES OF THE DEMONSTRATION

The primary objective of this project is to demonstrate the cost benefit of applying transport optimization codes to existing P&T systems relative to the traditional trial-and-error approach. At each of the 3 sites, the potential cost savings from applying transport optimization exceeded the expected costs of the technology. Therefore, this objective has been met. A secondary objective was to provide each installation where the demonstration is performed with alternate pumping strategies that would be feasible and cost-effective to implement. Based on the feedback from the respective teams, this objective was partially but not fully met, primarily because the objectives of the installation or the site-specific transport models changed by the time the demonstration was completed. While the installations have been encouraged to implement optimization suggestions resulting from the demonstration, they were not required to do so in order to participate in this project. Several of the installations have indicated an interest in upgrading their current groundwater models for potential future application of optimization codes with the updated models.

It is noted that a numerical groundwater model will never exactly predict groundwater flow and contaminant transport and that any results obtained based on groundwater model predictions must be evaluated in that context. However, those issues pertain equally to any design based on flow and transport modeling, whether obtained using transport optimization algorithms or trial-and-error techniques. This project did not evaluate the impact of the uncertainty associated with simulation model parameters on the optimization solutions. However, this issue could be evaluated in future projects either by examining the impact to optimal solutions from varying model parameter values or by using stochastic optimization methods to identify optimal solutions that are robust despite the uncertainty. Optimal solutions are often at the edge of what is feasible and therefore are not always robust. This project did not evaluate the robustness of the optimal solutions. One way to increase the robustness of the solutions would be to apply a safety factor to the optimization problem (i.e., impose more restrictive constraints than are actually required), which in general will lead to more conservative designs.

1.3   REGULATORY DRIVERS

There are no specific regulations that mandate the use of optimization methods. However, P&T systems that are not showing sufficient hydraulic capture, or where remedial schedules do not seem to be achievable with the existing system design, are prime candidates for regulatory and stakeholder interest and consideration of optimization efforts such as the application of mathematical optimization methods.

Beyond these considerations, there are no technology-specific regulatory issues that need to be directly addressed beyond those that constrain the design and operation of the P&T systems being examined, e.g., such as hydraulic capture boundaries and overall revision of P&T system objectives. Such regulatory issues were represented by the installation and considered during the strategic development of the mathematical formulations that were solved using the transport optimization algorithms. The ESTCP project team encouraged regulatory participation in the process and for each demonstration site offered to help site personnel communicate with their regulatory partners regarding the optimization technology. However, installation personnel were ultimately responsible for keeping regulators involved in the project to the extent desirable and necessary.

1.4   DEMONSTRATION RESULTS

For all three sites, there were two groups applying optimization algorithms and one group applying trial-and-error as a scientific control. For each of the three sites, multiple formulations were solved by each group. In every case, the groups applying the optimization algorithms found improved solutions relative to the trial-and-error group. This project clearly demonstrated that mathematical optimization is capable of identifying substantially improved solutions to real-world problems encountered for optimization of P&T systems. At all three sites, the potential cost savings outweighed the expected costs of applying the technology. The solutions found using transport optimization algorithms were 5% to 50% better than those obtained using trial-and-error (measured using optimal objective function values), with a representative improvement of about 20%.

Please note that optimization results are not compared to the current system. The reason is that the current system was not designed with the current version of the groundwater model, nor was the current system designed to be optimal for any of the formulations solved in this study.

Therefore, it is not fair to compare the current system to the optimal results, and there are no scientific conclusions that can be gained from such a comparison. The focus of this project, by design, is the comparison of solutions obtained with transport optimization algorithms versus trial-and-error approach.

1.5   STAKEHOLDER/END-USER ISSUES

This demonstration was designed to evaluate the potential benefit of transport optimization codes relative to the traditional trial-and-error approach for optimizing pumping strategies for a P&T system. Thus, this effort primarily examined technical and cost related issues, such as the conditions necessary for appropriate or feasible application of the technology, the reasons for

differences in the optimal results between groups, and the factors that influence performance of the technology.

2.0   TECHNOLOGY DESCRIPTION

2.1   TECHNOLOGY DEVELOPMENT AND APPLICATION

Most P&T systems have been designed through the use of numerical flow and/or solute transport simulation models, such as modular three-dimensional finite-difference groundwater flow (MODFLOW) and model transport in three dimension (MT3D). Transport models (e.g., MT3D) allow for prediction of contaminant concentrations, contaminant mass, and cleanup times. The most common decision variables determined with groundwater modeling are well locations, on/off status of particular wells, and the extraction or injection rates. The goal is to identify the best (or optimal) combination of values for the decision variables, which traditionally means that an "objective function" is minimized or maximized, and all "constraints" are satisfied. Potential objective functions include "minimize total cost," "minimize cleanup time," and many others.

Constraints are limits on the extraction/injection rates, the number of wells, well locations, hydraulic heads, concentrations, total capital investment, and many other constraints.

Traditionally, the groundwater simulation model is run repeatedly to simulate different pumping scenarios (trial-and-error). Each pumping scenario is entered manually with respect to locations of wells and the pumping/injection rates.   When the simulation is completed, the modeler determines by inspection if cleanup/containment is achieved and if all other design constraints are satisfied.

This trial-and-error approach relies heavily on the experience and insight of the modeler. With this approach, a limited number of simulations are performed (typically 10 to 50) and a preferred pumping strategy is then selected. A limitation of this approach is that only a small number of pumping strategies can be investigated, and the objective function and constraints are often not rigorously stated (in mathematical terms). Another limitation is that the nonlinear relationship between pumping rates and groundwater concentrations (i.e., concentrations do not change proportionally with pumping rates) makes it difficult to select promising well locations and pumping rates based on earlier choices.

Transport optimization codes (the focus of this demonstration project) couple transport models with nonlinear mathematical optimization to allow a more rigorous evaluation of potential pumping strategies (i.e., using mathematical algorithms instead of manual iteration). Nonlinear optimization algorithms are required because concentration changes and/or cleanup time changes are not linearly related to pumping rate.   The coupled simulation-optimization approach is appealing because it can presumably identify improved pumping strategies for a given objective function and constraint set by more efficiently searching the range of potential combinations of well rates and locations.

The nonlinear optimization problem that results from the transport optimization formulations can be conceptualized as a mountain range with a series of peaks and valleys. The optimal solution is either the highest peak or the lowest valley, depending on the nature of the objective function (maximize or minimize). There are many algorithms for solving these nonlinear problems.

Traditional approaches use derivatives of the objective function and constraints to go "uphill" from the starting point of the search until the peak is found. These approaches find only the highest peak or lowest valley nearest the starting point of the search. They are also difficult to implement with complex transport models, which may not be differentiable.

A newer class of optimization methods, referred to as "heuristic global optimization methods," has emerged in recent years. These methods include simulated annealing, genetic algorithms, outer approximation, and tabu search, and they are designed to search the potential solution space for the highest peak or lowest valley. These methods often require intensive computational effort but have become more practical for application on personal computers as computer speeds have increased. Heuristic techniques 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. The transport optimization codes demonstrated in this project use a variety of heuristic global optimization methods.

This project evaluates the utility of applying transport optimization codes for optimizing extraction/injection rates and extraction/injection locations. Optimization can potentially result in reduced cleanup time and/or reduced life-cycle costs. The objective function associated with each formulation is designed to be a metric for comparing one solution to another within the optimization approach, and therefore is ideally suited for measuring performance of one pumping strategy versus another when all of the constraints are satisfied.

2.2 PROCESS DESCRIPTION

The process of performing transport optimization generally consists of the following steps:

$ *Model development.* Calibrate a groundwater model to the point where it is considered acceptable for design purposes.

$ *Develop optimization formulations.* Define in mathematical terms an objective function to be minimized/maximized and a set of constraints that must all be satisfied.

$ *Solve optimization formulations.* Determine if there are any feasible solutions (i.e., those that satisfy all the constraints), and if so, determine the best or optimal solution.

After an optimization formulation is solved, the solution often reveals additional constraints or changes in the objective function that may better target the solution to meet overall project goals. Hence, it is common to modify one or more aspects of the formulation and then to solve the modified formulation.

To solve the optimization formulations, transport optimization codes that use a variety of mathematical algorithms have been developed (as discussed above). These optimization codes link to the transport model simulation input and output and require one or more input files that specify parameters and options to be used by the optimization code. In some cases, the process of solving the optimization formulation also requires the user to simplify the optimization formulation and/or place limits on the potential range of values for decision variables to avoid excessive computational requirements. This might include limiting the potential well locations,

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only considering specific pumping or injection rates (e.g., increments of 50 gallons per minute [gpm]), not allowing pumping or injection rates to change over time, etc.

2.3   PREVIOUS TESTING OF THE TECHNOLOGY

Since the 1980s, many researchers have coupled groundwater simulation models with mathematical optimization techniques to address groundwater management issues. Several universities have developed transport optimization codes, and some have been tested at actual field sites. Three examples of recent applications of transport optimization are:

$ Utah State University: Wurtsmith Air Force Base
$ University of Alabama (UA): Massachusetts Military Reservation
$ Utah State University (USU): Massachusetts Military Reservation

Each is described below. Peralta (2001) describes other recent real-world design projects using the Utah State University model.

Wurtsmith Air Force Base, Oscada, Michigan: Optimizing Contaminant Mass Removal Using Artificial Neural Network – Utah State University

In this case (Aly, A.H. and R.C. Peralta, 1997), transport optimization was used to develop an optimal strategy for remediating trichloroethylene (TCE) and 1,2-Dichloroethane (DCE) groundwater plumes. Management goals and restrictions were identified and prioritized as follows.

$ Capture the TCE and DCE dissolved phase groundwater plumes.

$ Reduce TCE and DCE concentrations to less than 94 parts per billion (ppb) and less than 230 ppb, respectively, within 6 years.

$ Total extraction of groundwater cannot exceed 400 gpm.

$ No treated water may be injected into the groundwater.

$ Treatment facility effluent cannot exceed 5 ppb of TCE.

An artificial neural network was used to simulate contaminant concentrations in the optimization model. The model considered a total of 24 potential extraction well locations. Six alternative optimal pumping strategies were ultimately evaluated for the final design. After discussions with stakeholders, a final strategy was chosen based on its minimization of total pumping rates, minimization of total time to meet objectives, and overall benefit to the stakeholders.

Chemical Spill-10 (CS-10) site at the Massachusetts Military Reservation – University of Alabama and Utah State University

Two of the three recent study applications of transport optimization were applied for the CS-10 plume at the Massachusetts Military Reservation. A P&T system is operating to remediate and contain a TCE plume approximately 17,000 feet long, 6,000 feet wide, and up to 140 feet thick. Between the fall of 1999 and the spring of 2000, transport optimization codes were utilized to maximize TCE mass removal over a 30-year time horizon, subject to the following constraints: (1) the TCE concentration must be lower than or equal to 5 ppb beyond the base boundary, (2) all extracted water must be reinjected into infiltration trenches, (3) individual wells are subject to pumping capacities, and (4) the total pumping rate should be restricted for cost considerations. The decision variables were the extraction rates and well locations for four perimeter wells that were being considered, and the extraction rates for five in-plume wells that were already constructed.

Results for the two optimization studies are summarized below.

University of Alabama. In this case (Air Force Center for Environmental Excellence [AFCEE], 1999; Zheng and Wang, 2002), the optimal strategy, as determined by the simulation-optimization analyses, suggests using only one perimeter well (rather than four wells) and a maximum pumping rate of 2,700 gpm. The results of the analysis demonstrate that it is possible to remove more TCE mass (approximately 3.5%) under the same amount of pumping assumed in the trial-and-error design, and that it can also lead to substantial cost savings by reducing the number of wells needed and adapting dynamic pumping. Preliminary cost estimates indicated that this strategy would yield life-cycle cost savings of $2.4 million. Some elements of the design were implemented.

Utah State University. In this case (Peralta et al, 1999a, b), the simulation-optimization modeling enhanced mass removal rates and aided in well placement, with an additional constraint of preventing the plume from contaminating clean aquifer between the western and central lobes. Specifically, the modeling identified a configuration that would extract approximately 6% more mass over 30 years, while reducing the extraction rate by 50 gpm and could cost $0.54 million less in construction cost alone. With slight tweaking, this design was constructed and is functioning as expected.

2.4   ADVANTAGES AND LIMITATIONS OF THE TECHNOLOGY

A properly defined optimization problem can be solved through manual trial-and-error adjustment or using a formal optimization technique. While the trial-and-error method is simple and widely used, it is usually limited in practice to a small number of simulations (typically 10-50) because it is labor intensive. The transport optimization codes more efficiently search the potential solution space, such that thousands of simulations are typically performed automatically, and each successive round of new simulations is designed to be more promising than the previous round.

Key advantages of transport optimization codes include the following.

$\quad$ Many more combinations of extraction and injection well rates can be evaluated using search algorithms that are far more efficient than trial-and-error or random search.

$\quad$ The process of mathematically specifying an objective function and a set of constraints is required for transport optimization, and this process (frequently overlooked during trial-and-error modeling) forces competing goals and strategies to be considered and compared.

$\quad$ Because it is more automated than trial-and-error, transport optimization is less prone to bias in selecting well rates and well locations, and is therefore more likely to discover unexpected solutions.

Limitations of transport optimization codes include:

$\quad$ The site must develop a transport model that is considered a reasonable predictor for design purposes (also true for trial-and-error).

$\quad$ The complexity of applying the nonlinear transport algorithms may require specialized expertise for many real-world groundwater modeling problems.

$\quad$ The codes are very computer-intensive for most real-world groundwater modeling problems, potentially requiring simplification of the simulation model and/or dedicated use of one or more computers; these simplifications require specialized expertise.

A limitation that pertains to both trial-and-error and the use of transport optimization algorithms is that the optimal results are based on model predictions, which are subject to uncertainty. A number of approaches exist for considering uncertainty in the optimization process, but these were not evaluated in this project.

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3.0   DEMONSTRATION DESIGN

3.1   PERFORMANCE OBJECTIVES

The objective of the overall project is to demonstrate the cost benefit of applying transport optimization codes by addressing the following questions:

$ 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?

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

Three optimization formulations were developed for each of the three sites, based on interaction with the installation. Two modeling groups used their own independently developed transport optimization software, and the other group used a traditional trial-and-error optimization method. The results from two separate transport optimization software programs can be compared to each other and to the trial-and-error group to assess performance objectives.

Table 1 summarizes performance criteria discussed in the Demonstration Plan, including the expected performance to be achieved. The last column indicates whether or not the performance objectives were met according to project results.

Table 1.   Performance Objectives for Overall Project.

Type of Performance Objectives	Primary Performance Criteria*	Expected Performance* (Metric)	Performance Objective Met?
Qualitative	Reduce annual operating costs	Annual operating costs are reduced	**
	Faster remediation	Increased contaminant removal efficiency	**
	Reduce cost of system life cycle	Reduced annual cost and/or reduced cleanup time	Yes
Quantitative	Reduce annual operating costs	> 20%****	**
	Reduce system life cycle costs	> 20%***	Yes***

*Based on a comparison of results obtained with optimization algorithms versus trial-and-error
**As discussed in Section 4.3, the cases based on cost objectives were formulated in terms of life-cycle costs, which incorporate tradeoffs between annual costs and cleanup time. Therefore, only life-cycle cost reduction was directly evaluated. In some cases, life-cycle cost reductions were due to lower annual costs (e.g., Blaine), and in some cases, life-cycle cost reductions were due to reductions in cleanup time (e.g., Umatilla).
***Metric achieved for multiple formulations, but not for all formulations
**** The criterion of >20% was originally in the Demonstration Plan Part II. It was based on general experience in applying optimization to groundwater modeling problems provided by discussions with GeoTrans, Dr. Peralta, and Dr. Zheng.

3.2   SELECTION OF TEST SITES

In this project, a screening method was developed for site selection (see Appendix G of the Technical Summary Report). The screening analysis is a two-stage procedure. The first stage is intended to quickly remove sites from consideration if they are not likely to benefit from either hydraulic or transport optimization, based on the following simple questions.

$ Are O&M costs > $100,000/year?
$ Is the system flowrate > 50 gpm?
$ Is the estimated cleanup time > 5 years?

If the answers to all three questions are "yes," a potential benefit from hydraulic and/or transport optimization is suggested, and the second stage (i.e., quantitative potential cost saving evaluation) is recommended to classify the sites into tiers regarding potential benefits that might be realized by performing a hydraulic optimization or a transport optimization analysis.

Three sites were ultimately selected for the transport optimization demonstration.

$ Umatilla Chemical Depot, Hermiston, Oregon (Umatilla)
$ Tooele Army Depot, Tooele, Utah (Tooele)
$ Former Blaine Naval Ammunition Depot, Hastings, Nebraska (Blaine)

Umatilla and Tooele have existing P&T systems in operation, and Blaine is in the design stage for a planned P&T system. Table 2 summarizes the results of the screening analysis for these three sites.

Table 2. Selection Criteria of Demonstration Sites.

Selection Criteria	Umatilla	Tooele	Blaine
O&M costs > $100K/yr?	$430K/yr	$1M/yr	$2M/yr
System flowrate > 50 gpm?	1,300 gpm	> 5,000 gpm	4,000 ~ 5,000 gpm
Estimated cleanup time > 5 yrs?	10 ~ 30 years	> 5 years	50 ~ 80 years
Maximum potential cost savings (life-cycle)-hydraulic optimization*	$415,485	$3,379,423	$11,488,043
Maximum potential cost savings (life-cycle)-transport optimization*	$362,986 - $1,298,000	$3,329,423 - $5,683,687	$11,435,543 - $14,359,313

* These are pre-optimization estimates, not actual optimization results.
* For calculations of potential cost savings, it was assumed that the system durations of hydraulic optimization for Umatilla, Tooele, and Blaine were 20 years, 20 years, and 50 years, respectively. For the transport optimization, calculations were based on a 10-30% reduction in cleanup duration.

For the purpose of this demonstration, two other criteria were used for site selection, which were met by all three sites.

$ Up-to-date flow and transport models exist that are considered reasonable to apply for design purposes at the site.

$ Site managers expressed a willingness to consider implementing the recommendations that might arise from the optimization results.

3.3   TEST SITE/FACILITY HISTORY/CHARACTERISTICS

Brief descriptions of the test facilities are provided below. More detail is provided in the Technical Summary Report.

3.3.1 Umatilla Chemical Depot (Umatilla)

Umatilla is in northeastern Oregon, 3 miles south of the Columbia River and 6 miles west of Hermiston, Oregon. From the 1950s until 1965, the depot operated an on-site explosives washout plant. The plant processed munitions to remove and recover explosives using a pressurized hot water system. The wash water from the plant was disposed of in two unlined lagoons, located northwest of the plant, where wash water infiltrated into the soil.

Explosives contained in the wash water migrated into the soil and groundwater at the site. Two of the most common contaminants in groundwater are royal demolition explosive (RDX) and 2,4,6-Trinitrotoluene (TNT). These constituents are used as indicator parameters because they are found at high concentrations relative to other parameters. Remediation of the groundwater is scheduled to continue until the concentration of explosives in the aquifer meets cleanup levels. The cleanup level for RDX is 2.1 micrograms per liter (µg/L) and for TNT is 2.8 µg/L.

The hydrogeology for Umatilla consists of an alluvial aquifer overlying silt and weathered basalt. The RDX plume is much bigger in area than the TNT plume because TNT is more strongly absorbed to the aquifer materials; therefore, its movement is retarded relative to groundwater velocity to a much greater extent than RDX. A groundwater P&T system was implemented in January 1997. Its design was based in part on the results of groundwater modeling studies. The current P&T system has three active extraction wells and three active infiltration basins. The infiltration basins are located around the perimeter of the pre-pumping RDX plume and were intended to augment hydraulic control. An additional infiltration basin (the location of a former industrial lagoon) was used as an infiltration basin in the early stages of the remedy to promote in-situ flushing of the unsaturated zone. However, use of that location for infiltration was terminated due to concerns that it could cause unwanted spreading of the TNT plume. The contaminated groundwater is extracted from the wells and then sent to granular activated carbon (GAC) units, which remove the contaminants. The treated water is discharged to the infiltration basins. The annual O&M cost for the current system is approximately $430,000/year.

3.3.2 Tooele Army Depot (Tooele)

Tooele, located several miles south of the Great Salt Lake in Utah, was established in 1942 to provide storage, maintenance, and demilitarization of troop support equipment, especially wheeled vehicles and conventional weapons. From 1942 to 1966, large quantities of hazardous materials were used and generated from these operations in the industrial area and discharged into ditches and ponds. Ultimately, groundwater was impacted, and the primary contaminant of concern is TCE, which was used as a solvent in the repair operations of military equipment.

The aquifer of concern generally consists of alluvial deposits. However, there is an uplifted bedrock block at the site where groundwater is forced to flow from the alluvial deposits into fractured and weathered rock (bedrock), then back into alluvial deposits. The uplifted bedrock block and adjoining low hydraulic conductivity alluvium are the hydraulically controlling features of the study area due to the steep gradients they cause. Flow through the bedrock block consists of a steep gradient when entering the bedrock, a flatter gradient through the bedrock core, and a steep gradient when exiting the bedrock. The impacts have been divided into a "main plume" and a "northeast plume." This optimization study pertained to the main plume.

Concentrations are significantly lower in the deeper portions of the aquifer than in the shallow portions. Also, the extents of the shallow and deep plumes do not directly align, indicating a complex pattern of contaminant sources and groundwater flow. Continuing sources of dissolved contamination are believed to exist.

A P&T system has been operating since 1993. The system consists of 16 extraction wells (15 operating and one not operating) and 13 injection wells. An air-stripping plant in the center of the plume is capable of treating 8,000 gpm of water (currently treats about 5,000 gpm). Based on the well locations and previous plume delineations, the original design was for cleanup, but subsequently it was determined that the source area extended further to the south. As a result, the current system essentially functions as a containment system (there are no extraction wells in the area of greatest contaminant concentration). Historically, the target containment zone has been defined by the 5 ppb TCE contour. Given the current well locations and continuing sources, a prolonged cleanup time is anticipated. However, a revised (i.e., smaller) target containment zone is now being considered, based on risks to potential receptors. A revised target containment zone might correspond to the 20 ppb or 50 ppb TCE contour. Annual O&M cost is approximately $1 million.

3.3.3   Former Blaine Naval Ammunition Depot (Blaine)

Blaine is located immediately east of Hastings, Nebraska, and was built in the early 1940s as an active "load, assemble, and pack" ammunition facility during World War II and the Korean Conflict.   Waste materials were generated through discharge of wastewater to surface impoundments and natural drainage areas of the facility, and disposal of solid waste and explosives. Beginning in the mid-1960s, large tracts of the former depot were either sold to various individuals, businesses, and municipalities or transferred to other governmental agencies. With sale and transfer of the land to the United States Department of Agriculture (USDA) and area farmers, more than 100 irrigation wells have been installed on the former depot. Groundwater contamination at Blaine was discovered in the mid-1980s.   The remedial investigation and the annual groundwater sampling results identified seven source areas for volatile organic compounds (VOC) with plumes commingling at six of the source areas and one primary source for explosives. Extensive remediation of source areas by soil vapor extraction (SVE) or soil excavation is being implemented or has been completed.

Groundwater is encountered in the study area approximately 100 feet below ground surface. The three saturated hydrogeologic units of primary interest in this study are an unconfined aquifer, a confining layer, and a semiconfined aquifer. During irrigation season, which lasts about 2½ months, heavy pumping from extensive irrigation wells dramatically alters the groundwater flow direction. VOC plumes encompass nearly 6½ square miles. Groundwater contamination from explosives extends over an area of approximately 3 square miles and is commingled with the VOC plumes in several areas.

There is no existing groundwater extraction remediation system at Blaine. This site is in the conceptual design stages, based on a draft Feasibility Study performed in August 2000. The optimization project is restricted to simulation of two parameters. Site managers selected TCE and TNT as the parameters most important to remedial design but indicated that other parameters

should not be ignored. Therefore, an approach was developed to indirectly incorporate the distribution of other constituents of concern.

3.4 PHYSICAL SET-UP AND OPERATION

The traditional trial-and-error method was used by GeoTrans to serve as a scientific control for the transport optimization groups. Two transport optimization modeling groups, Dr. Chunmiao Zheng of the University of Alabama and Dr. Richard Peralta of Utah State University, used their own independently developed simulation-optimization software for this study. These investigators were chosen based on the existence of optimization packages and prior field implementation of their optimization packages similar to this project, although the specific codes and algorithms they would apply for this project were their choice.

Once sites were selected (Phase 1), the following activities were associated with performing the transport optimization for each site (Phase 2).

$ An initial draft of potential optimization formulations was developed by the ESTCP project team, based on a site visit (performed in Phase 1) and subsequent phone conversations and/or e- mails with the installation.

$ Feedback on the initial draft optimization formulations was provided by the installation, including details on cost coefficients and/or constraint values.

$ The simulation models were modified (as necessary) to require no more than 2 hours of computational time and to include no more than two constituents.

$ The formulations were finalized and distributed to each modeling group by GeoTrans, including a feasible solution if one had been determined during the formulation process; a FORTRAN post-processor for determining the objective function value and status of the constraints for any specific combination of well rates simulated with the transport model was also provided by GeoTrans.

$ Optimization of each of the three formulations for the site was performed over a period of approximately 4 months, during which time the three modeling groups were not allowed to discuss their progress with each other or with the installation. (Biweekly progress reports were submitted by each group to the U.S. Navy.)

$ After the optimization period for a specific site, each modeling group submitted a report describing the results for each formulation.

$ The ESTCP project team met to present and interpret results, with a subsequent presentation of results to the installation by a subset of the ESTCP project team.

A summary of these activities for each of the three demonstration sites, including the schedule, is presented in Table 3.

Table 3. Summary of Activities.

Activity	Umatilla	Tooele	Blaine
Site visit (Phase 1)	8/23/00	5/31/01	10/17/01
Develop formulations	10/16/00 – 3/21/01	6/4/01 – 10/31/01	1/15/02 – 5/15/02
Optimization period	3/22/01 – 7/16/01	11/1/01 – 2/28/02	5/17/02 – 9/17/02
Project team meeting to present results	10/18/01	3/20/02	9/19/02
Present results to installation	11/15/01	5/16/02	9/30/02
Follow-up with installation	3/19/02	12/02	12/02

A third-party expert (Dr. Barbara Minsker) was added to the project team during the beginning of Phase 2 to evaluate and interpret the results and their meaning relative to overall project objectives.

Brief descriptions of the setup of the optimization problems/formulations are provided below. More detail is provided in the Technical Summary Report.

Umatilla

A simple description of the formulations is as follows.

Formulation 1. Minimize the life-cycle cost (until cleanup of both RDX and TNT), providing that the current capacity of the treatment plant is held constant and the cleanup of both RDX and TNT is completed within 20 years.

Formulation 2. Same as Formulation 1 but allows the capacity of the treatment plant to increase to a maximum of 1950 gpm.

Formulation 3. Minimize the total mass remaining (RDX plus TNT) in layer 1 within 20 years.

Tooele

A simple description of the formulations is as follows.

Formulation 1. Minimize total cost over 21 years, subject to meeting specific concentration limits at the point of exposure (POE) boundary, located along a portion of the downgradient property boundary.

Formulation 2. Same as formulation 1 but also meet aggressive concentration limits at point of compliance (POC) boundaries, located in the interior portion of the site.

Formulation 3. Same as Formulation 2 but include a declining source term rather than a continuous source term for unremediated sources and add additional cleanup constraints within the plume.

Blaine

A simple description of the formulations is as follows.

Formulation 1. Minimize life-cycle cost (until cleanup) providing that the plumes cannot spread above cleanup levels beyond specified areas and that cleanup of both TCE and TNT is within 30 years in model layers 3-6.

Formulation 2. Same as Formulation 1 but assumes diversion of 2,400 gpm of extracted water to a utility (i.e., that water does not require treatment and subsequent discharge).

Formulation 3. Ensure that the maximum total remediation pumping rate in any management period over a 30-year simulation is such that the plumes not spread above cleanup levels beyond specified areas.

A brief summary of the formulations for each site is provided in Table 4. The detailed formulations are provided in the Appendices of the Technical Summary Report.

Table 4. Formulation Summary (Key Aspects) for the Three Demonstration Sites.

Site Name		Objective Function	Major Constraints
Umatilla	Formulation 1	Minimize life-cycle cost until cleanup	1. Current treatment capacity 2. Cleanup of RDX and TNT < 20 yrs
	Formulation 2	Minimize life-cycle cost until cleanup	1. Increased treatment capacity 2. Cleanup of RDX and TNT < 20 yrs Umatilla
	Formulation 3	Minimize total mass remaining in layer 1 after 20 yrs	1. Cleanup of RDX and TNT 2. Limit on number of new wells and recharge basins
Tooele	Formulation 1	Minimize total cost over 21 years	1. POE concentration limit for TCE at site boundary after 3 yrs
	Formulation 2	Minimize total cost over 21 years	1. POE concentration limit for TCE at site boundary after 3 yrs 2. POC concentration limits for TCE at specific locations/times within site boundary
	Formulation 3	Minimize total cost over 21 years	1. POE/POC concentration limits 2. Declining source term 3. Cleanup (TCE < 50 ppb) at most locations < 9 yrs
Blaine	Formulation 1	Minimize life-cycle cost until cleanup	1. Plume containment 2. Cleanup of TCE and TNT < 30 yrs
	Formulation 2	Minimize life-cycle cost until cleanup w/ 2,400 gpm extracted water diverted	1. Plume containment 2. Cleanup of TCE and TNT < 30 yrs Blaine
	Formulation 3	Minimize maximum total pumping	1. Plume containment 2. Limit on number of new wells

*Note: See Appendices D-F in Technical Summary Report for detailed formulations for each site

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4.0   PERFORMANCE ASSESSMENT

4.1   PERFORMANCE DATA

To assess performance of the transport optimization algorithms relative to the conventional trial-and-error approach, the optimization formulations were solved by the UA team and the USU team using optimization algorithms, and by the GeoTrans team using trial-and-error as a scientific control. The results were then compared. The detailed results comparison and individual modeling group reports are included in the Technical Summary Report. The comparative results are summarized below.

Umatilla Performance Data

Table 5 shows the results for all three formulations. The objective for Formulations 1 and 2 is to minimize the life-cycle cost until cleanup of both RDX and TNT. The objective for Formulation 3 is to minimize mass remaining (RDX plus TNT) in model layer 1 after 20 years. The detailed formulation document is included in the Technical Summary Report.

Table 5.   Umatilla Results Summary.

	Transport Optimization Algorithms		Trial-and-Error	Percentage Improvement*
	UA	USU	GeoTrans	
Formulation 1: Objective function value	$1.66M	$1.66M	$2.23M	23%
Formulation 2: Objective function value	$1.66M	$1.66M	$2.02M	15%
Formulation 3: Objective function value	0.19 kg	0.20 kg	0.38 kg	50%

* Percentage improvement is for transport optimization algorithms compared to trial-and-error.

Tooele Performance Data

Table 6 shows the results for all three formulations. The objective for all three formulations is to minimize the total cost over 21 years. The USU team did not submit a design for Formulation 2 as posed because they added a constraint to prevent potential for mass migration around one concentration constraint boundary defined in the formulation. Therefore, the USU results for Formulation 2 cannot be directly compared to the results from the other groups. All three teams reported that Formulation 3 was infeasible as stated because of the restriction on the number of new wells that could be installed. The detailed formulation document is included in the Technical Summary Report.

Table 6.   Tooele Results Summary.

	Transport Optimization Algorithms		Trial-and-Error	Percentage Improvement*
	UA	**USU**	**GeoTrans**	
Formulation 1: Objective function value	$12.67M	$14.14M	$14.63M	3% - 13% (11% - 42%)**
Formulation 2: Objective function value	$14.45M	***	$16.32M	11% (30%)**
Formulation 3: Objective function value	****	****	****	NA

*Percentage improvement is for transport optimization algorithms compared to trial-and-error.
**Percentage in parentheses is calculated after removing ~ $10M fixed cost that could not change with pumping strategy because of the fixed system duration. The $10M fixed cost includes ~$7M of fixed O&M cost and ~$3M of the sampling cost that cannot be reduced based on feedback from the optimization modelers.
*** The USU team did not submit a design for Formulation 2 as posed because they added a constraint to prevent potential for mass migration around the west side of POC-MP1, so their results cannot be compared directly to the other groups.
****No solutions could be found that satisfied all the constraints.

<u>Blaine Performance Data</u>

Table 7 shows the results for all three formulations. The objective for Formulations 1 and 2 is to minimize the life-cycle cost until the cleanup of both TCE and TNT within 30 years.   The objective for Formulation 3 is to minimize the maximum total remediation pumping rate in any management period over a 30-year simulation. The detailed formulation document is included in the Technical Summary Report.

Table 7.   Blaine Results Summary.

	Transport Optimization Algorithms		Trial-and-Error	
	UA	**USU**	**GeoTrans**	**Percentage Improvement***
Formulation 1: Objective function value	$45.28M	$40.82M	$50.34M	10% - 20%
Formulation 2: Objective function value	$24.04M	$18.88M	$28.39M	15% - 33%
Formulation 3: Objective function value	2,737 gpm	2,139 gpm	2,879 gpm	5% - 26%

* Percentage improvement is for transport optimization algorithms compared to trial-and-error.

4.2   PERFORMANCE CRITERIA

Primary and secondary performance criteria for the optimization analyses are presented in Table 8. These criteria were applied to the results from each of the optimization analyses.

Table 8. Performance Criteria.

Performance Criteria	Description	Primary or Secondary
Reduce annual operating costs	Does demonstration indicate potential for reducing annual operating costs (based on modeling)?	Primary
Faster remediation	Does demonstration indicate potential for a shorter duration of P&T operations to accomplish a comparable level of cleanup (based on modeling)?	Primary
Reduce life-cycle cost of system	Does demonstration indicate potential for reduced life cycle based on capital costs, modified annual costs, and modified operating (based on modeling)?	Primary
Factors affecting technology performance	Extent to which site-specific factors affect technology performance (or prohibit application of the technology), such as reliability of models, confidence in plume delineation, confidence in source area delineation, etc.	Secondary
Ease of use	What is the required skill level and training required to apply the technology at other sites, and can others be expected to apply technology as effectively (and for similar cost) as the project team for this demonstration project?	Secondary

Primary performance criteria were assessed based on values of the objective functions for competing solutions. The secondary performance criteria are qualitative rather than quantitative. Table 9 shows the primary and secondary performance criteria along with expected performance metrics and performance confirmation methods.

Table 9. Expected Performance and Performance Confirmation Methods.

Performance Criteria	Expected Performance Metric	Performance Confirmation Method
Primary Criteria (Quantitative)		
Reduce annual operating costs	> 20%	Objective function and/or constraint set evaluated using available groundwater model
Faster remediation	> 20%	Objective function and/or constraint set evaluated using available groundwater model
Reduce life-cycle cost of system	> 20%	Objective function and/or constraint set evaluated using available groundwater model
Secondary Criteria (Qualitative)		
Factors affecting technology performance	No metrics assumed	Feedback obtained from three demonstration sites
Ease of use	Useful to transport simulation modelers	Experience of the project team from application of codes at three demonstration sites

Postmodeling adjustments are beyond the scope of this study, and installations are not required to implement modifications based on the demonstration project results. Therefore, the performance evaluation in this section relies solely on the most currently available models at the time of the implementation effort and optimization results for this effort, and not data from future-planned or since-completed adjustments to the groundwater model and/or to the P&T system design.

Please note that optimization results are not compared to the current system because the current system was not designed with the current version of the groundwater model, nor was it designed to be optimal for any of the formulations solved in this study. Therefore, it is not fair to compare the current system to the optimal results, and there are no scientific conclusions that can be gained from such a comparison. The focus of this project, by design, is the comparison of solutions obtained with transport optimization algorithms versus trial-and-error.

4.3   DATA ASSESSMENT

In every case, the groups applying the optimization algorithms found improved solutions relative to the trial-and-error group. Because multiple sites 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 (i.e., mathematical formulations with an objective function to be minimized/maximized and a series of constraints). The five performance criteria listed in Section 4.2 are evaluated below.

Reduce Annual Operating Costs (Quantitative)

During the formulation process for each site, minimizing annual O&M costs was discussed but never selected. Minimizing life-cycle costs rather than O&M costs was always preferred because life-cycle costs can be decreased (by reducing the cleanup time) even if annual O&M costs increase. Life-cycle cost evaluation considers the tradeoff between up-front costs, annual O&M costs, and the cleanup time. Therefore, the performance criterion relating to life-cycle costs (as discussed below) was determined to be more applicable. The results indicated that life-cycle cost could be minimized at Umatilla by minimizing the cleanup duration rather than minimizing annual costs, at Tooele by minimizing the number of new extraction and/or injection wells installed (i.e., capital costs) rather than minimizing annual costs/pumping rates, and at Blaine by minimizing the annual O&M costs rather then shortening the cleanup time.

Faster Remediation (Quantitative)

During the formulation process, minimizing cleanup time was discussed for the Umatilla and Blaine sites but never selected. Minimizing life-cycle costs rather than cleanup time was always preferred because life-cycle costs can be decreased (by reducing annual or up-front costs) even if cleanup time increases. The life-cycle cost evaluation considers the tradeoff between up-front costs, annual O&M costs, and the cleanup time. Therefore, the performance criterion relating to life-cycle costs (as discussed below) was determined to be more applicable.

However, minimizing life-cycle costs within Umatilla Formulations 1 and 2 also effectively minimized the cleanup time. For Formulation 1, the transport optimization algorithms identified solutions with cleanup time in 4 years, versus 6 years for trial-and-error (a 33% improvement). For Formulation 2, all three groups obtained the solutions cleanup in 4 years, but the transport optimization algorithms achieved lower life-cycle costs than the trial-and-error group. In Formulation 3 for Umatilla (Table 5), the mass remaining in solutions from transport optimization groups is approximately 50% less than that of the trial-and-error group. This also represents faster remediation. These results indicate the potential for transport optimization to

provide greater than 20% faster remediation (see Table 9). For Blaine, all three groups found that, although reduction in cleanup time was possible, the least cost solutions came from minimizing pumping in each management period rather than further shortening the cleanup duration. This supports the conclusion that reducing life-cycle cost is a more general performance criterion than minimizing annual costs or cleanup time.

Reduce Life-Cycle Cost of System (Quantitative)

In most of the formulations, the objective was to minimize life-cycle costs. As listed in Table 5, Table 6, and Table 7, the transport optimization algorithms frequently determined solutions with more than 20% life-cycle cost reduction relative to trial-and-error (see Table 9), and 20% appears to be a representative value achieved for life-cycle cost reduction relative to trial-and-error for these cases. (The representative savings are somewhat higher than 20% if fixed costs for the Tooele site are excluded from the formulation, as indicated on Table 6.) The differences in the results between the two optimization groups is likely due to one or more of the following factors (detailed in the Technical Summary Report).

$ Different approaches taken to overcoming the computational barriers of solving these complex problems.

$ Simplifications that individual modelers made in the formulations (primarily additional constraints) to overcome perceived problems in the solutions they obtained.

The project team considers it less likely that the differences are due to convergence of the heuristic optimization algorithms to suboptimal solutions

Factors Affecting Performance (Qualitative)

After obtaining the optimization results from this demonstration project, the site managers of all three sites chose to improve the underlying flow and transport model and/or further delineate the plumes or source areas before implementing optimization solutions. This highlights the fact that, like trial-and-error optimization, these algorithms are only as good as the underlying model. In all cases, there were simplifications made in the formulation process. For instance, the cost of a new well was approximated without location-specific details such as exact well depth or piping costs included. Since simplifications are required in formulating the optimization problems, many different alternative formulations can be developed (e.g., with different simplifications, different cost coefficients, etc.). Also, the demonstration project required the modeling groups to perform the optimization over a fixed period of time, with no contact with the installations. In many cases, questions arose from the initial solutions developed with the optimization algorithms, and the modelers stated that they would have preferred to iterate to an improved formulation based on contact with the installation. Therefore, the project demonstrates the value of such iterations.

Ease of Use (Qualitative)

This project demonstrated that applying the transport optimization algorithms to these complex, real-world sites was more than just "hitting the go button" but required expertise to limit the potential solution space to be searched. The transport optimization teams employed sequential solution approaches to reduce computational effort, which fixed some parts of the problem and optimized others. In some cases, problems were solved one management period at a time, determining well locations by first assuming steady-state pumping rates, then optimizing well rates over time for those predetermined well locations. These approaches require substantial expertise and professional insight.

4.4   TECHNOLOGY COMPARISON

The results clearly indicate that mathematical optimization methods are able to identify solutions that are better than those obtained using traditional trial-and-error approaches. The solutions found were 3% to 50% better than those obtained using trial-and-error (measured using optimal objective function values), with a representative improvement of about 20%. Given the computational limits, it is not practical for the optimization algorithms to search the entire solution space so there is always a chance that global optimal solution will be missed. For the problems solved in this project, better solutions were consistently found by the transport optimization algorithms than with trial-and-error.

This project did not specifically address optimization results versus the current system because the current systems were not designed with the current groundwater model and/or were not designed based on the same optimization formulations considered in this demonstration project (i.e., different objective functions and constraints). For example, the P&T systems may have been installed to achieve hydraulic capture of plume migration whereas the demonstration project may have focused on cleanup. The optimization results would not be directly comparable to the existing design for plume containment. Therefore emphasis on such comparisons is not appropriate. If such comparisons were to be made by calculating the objective function value (using the optimization formulations for the demonstration project) based on the current systems (e.g., existing well rates and well locations), improved objective values for the optimization results would be evident. For instance, for Umatilla Formulation #1, the objective function value for the current system (e.g., existing well rates and well locations) would be $3.8 million, versus $1.66 million from the optimization results. This is due largely to the improved cleanup time (17 years for the current system versus 4 years for the optimization results). However, the trial-and-error group achieved a solution of 6 years for cleanup time, with life-cycle cost of $2.23 million, indicating that much of the improvement associated with the optimization results relative to the current system is not attributed solely to the optimization algorithms. In this example, the benefit of the optimization algorithm (versus trial-and-error) was to lower the simulated cleanup time from 6 years to 4 years, thereby lowering life-cycle costs from $2.23 million to $1.66 million.

The challenges in applying optimization algorithms increased with the complexity of the site hydrogeological features and contamination. The greatest challenge the optimization modeling teams faced was the computational requirements of the optimization algorithms and underlying simulation models. If a single optimization run were set up to solve the entire problem as

formulated, with all possible pumping rates and well locations in all potential management periods, the number of decision variables would be much larger, and the computational times associated with the optimization algorithms would be prohibitive on today's computers. Instead, the teams limited potential well locations and/or 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.

A limitation of the trial-and-error approach is that the objectives and constraints are often not rigorously stated. Another limitation is that the possible number of combinations for well locations and well rates is infinite, but the trial-and-error method is practically limited to only a small number of numerical simulations (typically 10-50). The transport optimization codes more efficiently evaluate the potential solution space, such that many more combinations (i.e., thousands) of extraction and injection well rates and locations can be evaluated. 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 more likely to discover unexpected solutions. This project did not evaluate the impact of uncertainty in model parameter values on the results of the optimization solutions. However, this issue could be evaluated in future projects either by examining the impact to optimal solutions from varying model parameter values or by using stochastic optimization methods to identify optimal solutions that are robust despite the uncertainty.

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5.0   COST ASSESSMENT

5.1   COST REPORTING

This project demonstrated the cost benefit of applying computer-based transport optimization codes, a method that differs from other ESTCP cleanup category technology demonstration projects. Some typical cost tracking categories do not apply, while there are other costs unique to a modeling optimization demonstration effort. Most of the costs related to this demonstration were labor costs of the modelers. There are no capital costs associated with this demonstration since the optimization codes and existing models run on standard PCs. The project cost is summarized in Table 10.

Table 10.   Project Cost Summary for Contractors.

Costs Associated with Three Demonstration Sites					
		Umatilla	Tooele	Blaine	Subtotal
Pre-Optimization Tasks					
1) Site visit and/or transfer information	GeoTrans	$3,500	$3,400	$3,800	$10,700
	UA	$13,796	$14,526	$14,526	$48,848
	USU	$9,141	$9,664	$9.664	$28,469
2) Model modifications*		$7,730	$7,000	$7,000	$21,730
3) Develop three optimization formulations		$16,000	$14,000	$12,000	$42,000
Optimization Reporting					
4) Solve optimization formulations	GeoTrans	$32,000	$30,000	$31,500	$93,500
	UA	$75,996	$60,345	$60,345	$196,686
	USU	$56,152	$52,467	$53,427	$162,046
Reporting					
5) Prepare report and/or present results	GeoTrans	$10,000	$10,500	$9,000	$29,500
	UA	$24,602	$24,602	$24,602	$73,806
	USU	$9,426	$9,756	$9,756	$28,938

*Model modifications were performed by the UA group to for the demonstration purpose of this project.

These contractor costs form the basis for determining what future applications of the technology might cost (Section 5.2). To execute this project, additional costs were incurred for project management and support, including the following activities.

$ Preparation of Technology Demonstration Plans for Phase 1 and Phase 2

$ Site selection activities and the development of the site screening methodology referred to as Phase 1 of the project

$ Site visits to candidate sites that were ultimately not selected (George, Cornhusker, and Shaw)

$ Meetings with installations to present the optimization results

$ Project management and oversight, including contracting, project meetings, and conference calls

$ Preparation of ESTCP Technical Report and Cost-Performance Reporting

$ Briefings to ESTCP

$ Technology transfer activities

The project management costs for executing the entire project are summarized in Table 11.

Table 11.   Cost for Project Management, Entire Project.

Agencies	Costs
Navy – Naval Facilities Engineering Service Center (NFESC)	$170,000*
EPA – Technology Innovation Office (TIO)	$27,000
U.S. Army Corps of Engineers (USACE) – HTRW-CX	(by 8/31/03) $39,500
USACE – WES	$45,000
GeoTrans, Inc.	$129,300**
Dr. Minsker	$40,000
USACE site-specific project team's estimate	$17,500

* Cost includes NFESC labor, travel, other direct costs, and contract administration charges (estimated through completion of project). As of 8/31/03, the amount was $142,000, with an additional $28,000 estimated for completion.
** As of 8/31/03, the total GeoTrans cost was $257,000, estimating with an additional $48,000 estimated for project completion for a total of $305,000. Removing the items from Table 10 ($175,700), the GeoTrans costs related to project management are estimated at $129,300.

5.2   COST ANALYSIS

The major driver for the transport optimization modeling is the model execution time of one flow and transport simulation for the underlying model, which includes model computational time for simulating a chemical constituent and the number of chemical constituents that must be simulated to adequately address the plume management issues at the site. Table 12 lists the chemical constituents simulated, computational time for each flow, transport simulation for each site (not including computational time for optimization), and approximate number of optimization simulations performed for each formulation. Generally "simulations" refers to the number of iterations of the groundwater model. However, due to the use of substituted functions for the numerical model in some formulations, it is impossible to calculate exactly the number of completed groundwater model simulations performed for the optimization codes.

Table 12. Computational Time and Approximate Number of Simulations.

	Constituents Simulated	Computational Time for Each Flow and Transport Simulation	Number of Simulations Performed for Each Formulation	
			Transport Optimization Algorithms UA and USU Teams	Trial-and-Error GeoTrans
Umatilla	2 (RDX & TNT)	~ 10 minutes	~ 1000 – 8000 simulations	~ 25 – 40 simulations
Tooele	1 (TCE)	~ 10 minutes	Up to 8000 simulations	~ 60 – 80 simulations
Blaine	2 (TCE & TNT)	~ 2 hours	~ Hundreds/thousands simulations*	~ 60 simulations

*UA group used less accurate but much faster solvers in MT3DMS in the early stage so that many model simulations were much shorter than 2 hours.

As illustrated in Table 12, several thousand flow and transport simulations are usually performed using the transport optimization algorithms to achieve optimal or near-optimal solutions. Therefore, the computational time for performing one flow and transport simulation is critical during transport optimization modeling. Based on this project, it is recommended that the underlying flow and transport model be modified to the extent possible prior to optimization to shorten the computational time without losing model accuracy.

Based on the competitive bids evaluated in this project for selecting the transport optimization groups, plus the costs associated with GeoTrans' participation in the project, the expected costs (and time duration) of applying this technology at a future site is approximated in Table 13. The estimated range in costs results from differing site and model complexities. The costs to conduct transport optimization in Table 13 are primarily governed by the simulation time and not any specific aspect of site's hydrogeologic complexity.

Table 13. Approximate Cost to Apply Transport Optimization Algorithms at a Site.

Costs Associated With Basic Items*				
	Low Cost	Typical Cost	High Cost	Expected Duration
A1) Site visit and/or transfer information	$2,500	$5,000	$10,000	1-2 months
A2) Develop three optimization formulations	$5,000	$10,000	$15,000	1-2 months
A3) Solve optimization formulations	$25,000	$40,000	$60,000	2-4 months
A4) Prepare report and/or present results	$5,000	$15,000	$25,000	1 month
A5) Project management and/or administration	$2,500	$5,000	$10,000	NA
Total	$40,000	$75,000	$120,000	5-9 months
Costs Associated with Optional Items				
	Low Cost	Typical Cost	High Cost	Expected Duration
B1) Update and improve models	0	$20,000	$50,000	Add 1-3 months
B2) Up to three additional formulations	$15,000	$25,000	$40,000	Add 2-3 months
B3) Additional contaminant	$10,000	$20,000	$30,000	Add 1-2 months
B4) Transport simulation of 3 hrs each (i.e., 1 hr longer)	$10,000	$20,000	$30,000	Add 1-2 months

* assumes 1 or 2 constituents, and simulation time of 2 hours or less.

Note that the actual cost spent by the two transport optimization groups solving three formulations in the demonstration project (Item 4 in Table 10) was generally $50,000 to $60,000 (and in one case more than $75,000), which is at the high estimated cost for solving three optimization formulations (Item A3 in Table 13). This is likely to be attributable to the fact that some cost was incurred by the optimization groups to improve their transport optimization codes while solving the optimization problems during the demonstration project, and also because of the competitive nature of the demonstration project, which probably led to more effort trying to achieve a global optimum than would normally be expended.

With respect to potential cost savings to the government, assume 700 P&T systems at Superfund sites (USEPA, 2003), with an estimated annual O&M cost of $570,000/yr (USEPA, 2003), yielding a total O&M cost of $400 million/yr (700 systems x $570,000/system). If the typical site has a remediation timeframe of 20 years, that represents life-cycle costs of approximately $8 billion, nondiscounted ($400 million/yr x 20 yrs). If it is assumed that 10% of systems have transport optimization potential, and if it is further assumed that transport optimization might save 20% of the life-cycle costs at those sites, then the potential life-cycle cost savings to the government can be estimated to be $160 million, nondiscounted (i.e., $8 billion x 0.1 x 0.2). The costs of implementing this type of effort, as outlined in Table 5 through Table 7, are not included within these cost savings projections.

5.3   COST COMPARISON

The appropriate way to compare the costs of applying transport optimization algorithms with conventional trial-and-error in this demonstration project is to compare the cost associated with Item A3 in Table 10, which is "solving optimization formulations" or searching for the optimum solution based on mathematically stated formulations (objective functions and constraints). The cost comparison associated with solving optimization formulations and the percentage improvement in objective functions for demonstration sites are listed in Table 14. Two teams using transport optimization algorithms spent from $50,000 to $76,000, approximately, to solve three optimization formulations, which is compared to the actual costs of approximately $32,000 for the trial-and-error effort for each of the three sites examined on this project. (Approximately the same amount was budgeted for trial-and-error at each site, so, for more complex models such as Blaine, fewer trial-and-error simulations were performed.)

Table 14.   Cost Comparison Versus Percentage Improvement for Demonstration Sites.

	Costs Associated with Solving Optimization Formulations		Percentage Improvement in Objective Functions Transport Optimization Algorithms Versus Trial-and-Error
	Trial-and-Error	Transport Optimization Algorithms	
Umatilla	$32,000	$ 75,996 (UA) $ 56,152 (USU)	23%, 15%, 50% (UA) 23%, 15%, 47% (USU)
Tooele	$30,000	$ 60,345 (UA) $ 52,467 (USU)	13%, 11%, – /(42%, 30%, –)* (UA) 3%, –, – /(11%, –, –)* (USU)
Blaine	$31,500	$ 60,345 (UA) $ 53,427 (USU)	10%, 15%, 5% (UA) 19%, 33%, 26% (USU)

**Percentage in parentheses is calculated after removing ~ $10M fixed cost that could not change with pumping strategy due to the fixed system duration. The $10M fixed cost includes ~$7M of fixed O&M cost and ~$3M of the sampling cost that cannot be reduced based on feedback from the optimization modelers.

The university team costs in Table 14 likely included some code development that would not typically be a part of an optimization application. Hence, the project team expects that a comparison of expected costs to benefits, shown in Table 13, is more appropriate for estimating future costs and benefits of the technology.

An issue is the extent to which application of transport optimization algorithms cost more than the application of trial-and-error, and to compare that with the anticipated benefits that might be afforded by the application of transport optimization algorithms versus the use of trial-and-error.

As shown in Table 13, the estimated cost of applying transport optimization algorithm (Item A3) for problems like those formulated for this project is approximately $25,000 to $60,000 (i.e., up to two constituents, simulations up to 2 hrs long, up to three formulations). The cost for the trial-and-error group for Item A3 for this project was approximately $30,000 per site, although that group reported for each site that it would have performed fewer simulations if not done within the context of this demonstration project. Thus, it is assumed that for comparable projects (i.e., up to two constituents, simulations up to 2 hrs long, up to three formulations) trial-and-error may cost approximately $20,000 to $25,000. Therefore, the premium for applying the transport optimization may be as little as zero, or as much as $40,000.

The improvements in objective function values achieved in this demonstration project with transport optimization algorithms (versus trial-and-error methodology) range from 3% to 50% with the fixed cost associated with the Tooele site included, which cannot change with the pumping strategy, due to the fixed system duration, and range (for all three sites) from 5% to 50% with that fixed cost removed from the calculation, with a typical value of 20% to 30%. Assuming the objective function is in terms of cost, the potential life-cycle cost savings associated with the application of transport optimization algorithms will almost certainly exceed the premium of up to $40,000 for applying the technology at most sites that satisfy the simple site-screening criteria (more than $100,000/year in annual O&M and expected duration of 5 years or more). For sites with high costs and/or high durations, such as a yet-to-be constructed P&T system where fewer cost and design parameters are fixed, the potential life-cycle cost savings may be even more significant. For example, in the Blaine demonstration, potential cost savings of approximately $10 million were identified relative to the trial-and-error solutions.

For cases where the objective function is not in terms of life-cycle cost, the cost-benefit evaluation is less straightforward (e.g., almost 50% less mass remaining in layer 1 for Umatilla using optimization algorithms versus trial-and-error). It is hard to quantify the extent to which benefits from reduction in mass remaining, or an increase in contaminant removed, can be compared to the additional cost associated with application of transport optimization. However, as discussed earlier, the premium of applying transport optimization algorithms (up to $40,000) instead of a trial-and-error method is not so high that it would be prohibitive for most sites to consider the transport optimization approach, and, qualitatively, it appears that use of transport optimization should be encouraged. Additional investment may be required for uncertainty analysis of the underlying simulation model on the optimal solutions, but such analyses would be performed for the trial-and-error method as well.

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6.0 IMPLEMENTATION ISSUES

6.1 COST OBSERVATIONS

The computational time for performing one flow and transport simulation is critical during transport optimization modeling. Based on this project, it is recommended that the underlying flow and transport model be modified to the extent possible prior to optimization to shorten the computational time without losing model accuracy.

The two transport optimization groups were from universities. It is possible that the costs incurred by universities might differ from those associated with consultants. However, when the optimization groups were selected, a bid was also received from a consulting group, and the bid costs were similar, so this does not appear to be significant issue.

The cost associated with the formulation process is also a major component. The formulation process is inevitable and time consuming whether the trial-and-error approach or the transport optimization algorithms are selected. It is important that the cost associated with the formulation process be considered. In addition, the costs and schedule for making any model modifications in advance of any optimization should also be considered.

6.2 PERFORMANCE OBSERVATIONS

One issue in evaluating performance with respect to this project's performance criteria was "moving targets." The objectives of the installation or the site-specific transport models changed by the time the demonstration was completed, making the results less relevant to the installations. This was largely due to the requirements for this demonstration project that a specific version of the model be selected and then used for the duration of the demonstration, and that the optimization modelers work independently from the installation for an extended period of time. This issue points to the benefit of closer collaboration between an optimization team and an installation during the optimization period.

Minimizing the life-cycle costs was always selected when formulating the problems instead of minimizing annual O&M costs or minimizing cleanup time. This is because life-cycle costs can be reduced even if annual O&M costs increase or cleanup time increases. Therefore, minimizing life-cycle cost appears to represent the more comprehensive approach. For this project, the life-cycle costs were calculated based on the system duration. For two of the cases (Umatilla and Blaine), system duration was a variable that was part of the optimization problem, defined as the time when all concentration criteria are satisfied in the model. In reality, there may be other criteria that need to be satisfied (e.g., a certain period of time where criteria remain satisfied) before a system can be terminated. Long-term monitoring costs following pumping shut-off were also not considered in the life-cycle cost evaluations.

6.3 OTHER SIGNIFICANT OBSERVATIONS

The competitive nature of this project, in which each team worked in isolation from the installation and each other during the entire modeling period, does not necessarily lead to the best results in terms of implementation feasibility. For example, initial results at the Umatilla

site revealed that the mass remaining after 20 years (according to the model) would be extremely low, so that solutions to the third formulation, minimizing mass remaining over 20 years, would require extended pumping for little or no benefit. Had interaction with the installation been possible, this formulation would most likely have been modified to reduce the pumping period. These types of issues reinforce the need for substantial interaction between the optimization team and the installation during application of this technology.

Another factor to be considered during implementation is that the optimization codes required substantial expertise to achieve successful implementation at the types of complex, real-world sites considered in this project (which are the types of sites where this technology is most needed). This factor points to a need for technology transfer to train interested parties for successful future implementation.

6.4   LESSONS LEARNED

The development of mathematical formulations of the optimization problems was a difficult and time-consuming process. However, this formulation process results in a concise and quantifiable statement of project objectives and constraints necessary for transport optimization algorithms and useful for trial-and-error method as well. The formulation process is worthwhile whether or not mathematical optimization algorithms (or even P&T) are ultimately applied.

Some modifications to the existing flow and transport model were necessary prior to optimization. These modifications included changes to model time discretization to correspond with management periods in the optimization formulations, simulating the model under current conditions into the future to provide initial conditions for the optimization simulations, and modifying the model solution package parameters to shorten computational time because the model run time is the limiting factor for transport optimization algorithms to investigate a greater number of potential solutions.

Due to the specific needs of this demonstration project, the optimization formulations were fixed at the beginning of the simulation period, and simulation period length was defined. However, the optimization modeler would normally interact with the installation to develop revised formulations and to adjust to new knowledge as optimization proceeds. This project demonstrates that such iterations should be a useful component of real-world applications.

This project also demonstrated that applying the transport optimization algorithms was more than just "hitting the go button." It required expertise to limit the potential solution space to be searched. If a single optimization run were set up to solve the entire problem as formulated, with all possible pumping rates and well locations in all potential management periods, the number of decision variables would be much larger, and the computational times associated with the optimization algorithms would be prohibitive on today's computers. Instead, the transport optimization teams employed sequential solution approaches to reduce computational effort, in which some parts of the problem were fixed while others were optimized. In some cases, problems were solved one management period at a time, and/or determining well locations first assuming steady-state pumping rates followed by optimizing well rates for those predetermined well locations. At some sites, surrogate functions to the simulation model, such as artificial neural networks, were also used to reduce computational effort. The surrogate functions, which

can be evaluated much more quickly than the original simulation model, are then used in place of the simulation model for optimization. All of these approaches require expertise and professional insight to be used appropriately without introducing significant error.

6.5 END-USER ISSUES

The project teams for the Tooele, Umatilla, and Blaine systems were involved in the demonstration project from the screening phase through the presentation of optimization results. These project teams included the installation managers (for Umatilla and Tooele), the U.S. Army Corps of Engineers (USACE) project managers and technical staff, and, in the case of the Blaine team, contractors responsible for the feasibility study. For the Umatilla project, the Seattle District USACE Innovative Technology Advocate was also involved. The relationships between the ESTCP team and the project teams were extremely constructive. The project teams provided important input on the formulations and were interested in the results. In future applications of the technology, closer contact with base environmental managers throughout the optimization period would also be essential to obtaining results that are as relevant and as up-to-date as possible with the installation's needs.

Currently, both the Umatilla and Blaine teams plan on using the results of the ESTCP demonstration project as a basis for future operational changes. The Umatilla project team has ceased use of one infiltration basin based on the recommendation of the optimization teams and is in the process of seeking funds to update the groundwater flow and transport models to reflect new site characterization data before revisiting the optimization further. The Blaine project team is considering the optimization recommendations as they proceed with preparation of a Proposed Plan and Record of Decision and are planning to update their model based on recent minor site characterization efforts. The Tooele project team has been directed to investigate the temporary (2-year) termination of the operation of the P&T system to evaluate various processes affecting contaminant fate. The implementation of any of the optimization recommendations will be postponed pending this evaluation. Overall, the installations were open to the recommendations and are implementing the recommendations to the extent possible given other constraints.

This project did not address uncertainties in the underlying groundwater transport models. With respect to end users, it is important to remind the end user that the optimization results are determined using model simulations and are subject to uncertainties associated with such predictions. The use of optimization algorithms does not increase or decrease such uncertainties relative to use of trial-and-error.

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APPENDIX A

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