WHICH GROUNDWATER REMEDIATION OBJECTIVE IS BETTER, A REALISTIC ONE OR A SIMPLE ONE?

BY

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ABSTRACT

Numerous coupled optimization and simulation models have been developed to improve groundwater remediation designs. One of the first steps in developing an optimal groundwater remediation design problem is creating appropriate objective functions, which represent the primary goals of the design. This paper explores two issues that can arise in creating objective functions and interpreting multi-objective results: cost function complexity and visualization of high-order multi-objective problems (those with more than 2 objectives). Selecting appropriate objective functions can be challenging. A more realistic objective function, with detailed cost terms for all aspects of the remediation, may yield more accurate results but will require more time and effort to develop an appropriate function for each particular application. This research seeks to identify what situations encountered in remediation design would make the development of a realistic objective function necessary. Once the cost function is defined, solution of high-order multiobjective problems can identify a complex nondominated surface of solutions that can be difficult to visualize. We explore several visualization approaches for identifying tradeoffs among three objectives (total cost, risk, and total cleanup time) for a hypothetical case study. Many existing popular visualization techniques are not suitable for this case study in which all of the objectives are important and the numbers of solutions are large. A new approach is presented that can clearly visualize all of the optimal solutions and all of the relationships among three objectives to improve decision making. With this approach, the results show that if the required risk level is high, a short term remediation is preferred, while for a low risk level, a long term remediation is more cost effective. We then further explore cost function complexity using both a hypothetical case study and a field-scale application at Umatilla Army Depot in Oregon. The results show that realistic cost functions tend to find better solutions than the simplified cost functions, as well as identifying more optimal solutions on the Pareto frontier than the other functions. For both the hypothetical case and the Umatilla case, the realistic cost functions achieved up to 14% improvement in total cost although the degree of loss in accuracy varies substantially for the two case studies considered in this work and for different parameter settings within each case study (such as cleanup length, risk level, or mass remaining).

To Father and Mother

ACKNOWLEDGEMENTS

I have a lot of people to thank. Without them, this thesis wouldn’t be possible. Many thanks to my advisor Dr. Barbara S. Minsker, who has been a great guide and mentor. Thanks to all my research group members: Abhishek Singh, Dara Farrell, Eva Sinha, Felipe Espinoza, Matt Zavislak, Meghna Babbar and Shengquan Yan for their support and help. At last, I would also like to acknowledge the U. S. Army Research Office under grant number DAAD19-001-1-0025 for funding this research.

TABLE OF CONTENTS

LIST OF FIGURES

LIST OF TABLES

1. INTRODUCTION

Many different coupled optimization and simulation models have been developed for improving groundwater remediation designs [e.g. Lee and Kitanidis (1991), Tiedeman and Gorelick (1993), Chan (1994), Ritzel et al (1994), Sawyer et al (1995), Karatzas and Pinder (1996), McKinney and Lin (1996), Rizzo and Dougherty (1996), Sun et al (1996), Zhen and Uber (1996), Culver and Shoemaker (1997), Misirli and Yazicigil (1997), Minsker and Shoemaker (1998), Smalley et al (2000), Hsiao and Chang (2002), Maskey et al (2002), and Gopalakrishnan et al (2003)] One of the first steps involved in developing an optimization model is creating appropriate objective functions, which represent the primary goals of the design. The most commonly used objective for remediation design is to minimize the cost associated with the remediation process. In early work, fixed costs were frequently neglected in groundwater remediation designs and only operation and maintenance costs were considered [e.g. Gorelick et al (1984), Wagner and Gorelick (1987), Andricevic and Kitanidis (1990), and Culver and Shoemaker (1992)]. McKinney and Lin (1995) demonstrated that the omission of fixed capital costs tends to find designs that have a large number of wells pumping at low rates over a long time period. In recent years, the cost function without capital cost has been used primarily for some special purposes, such as uncertainty analysis (Sawyer and Lin (1998)) and comparison of the performance of optimization methods for groundwater remediation (Yoon and Shoemaker 1999). However, the most common cost function used in groundwater remediation problems today is a cost function with fixed capital cost, [e.g. Lee and Kitanidis (1991), Marryott et al (1993), McKinney and Lin (1996), Rizzo and Dougherty (1996), Culver and Shoemaker (1997), Culver and Shenk (1998), Kwanyuan and Fontane (1998), Aly and Peralta (1999), Johnson and Roger (2000), and Medina, Jr. (2002)]. Most of these cost functions are still simplifications of the real costs, considering only the fixed well installation costs and pumping costs. A few researchers have used more complex and realistic cost functions, including fixed and variable capital costs and operational costs in an effort to find more accurate results, e.g. Huang and Mayer (1997), Smalley and Minsker (2000), and Gopalakrishnan et al (2003). In a recently completed demonstration of transport optimization at three field sites (Minsker et al. 2003), detailed cost functions were developed for each individual field site, considering all aspects of the remediation from monitoring to well installation.

A more realistic objective function may yield more accurate results but at the same time it will require more time and effort to develop the appropriate function for a particular application. The ESTCP demonstration project required weeks of negotiations with the field installation personnel at each site to finalize the cost functions. On the other hand, a simple function will save setup time but may sacrifice the accuracy of the results. The purpose of this thesis is to investigate how the choice of cost function affects the optimal solutions found and in which situations the simplified cost function can be substituted for the realistic cost function and still ensure the accuracy of results.

Section 2 provides a brief overview of the multi-objective optimization methodology used in this study. In Section 3, a detailed, realistic cost function is first developed and implemented within a three-objective hypothetical case study. Different methods for visualizing tradeoffs among three objectives are compared and a new visualization method is presented. The realistic function is then compared with simpler cost functions that have been used in the past to assess for the need for more complex functions. In Section 4, we test the cost function complexity findings from the hypothetical case study on a two-objective field-scale application at Umatilla Army Depot in Oregon, which was the first site examined in the ESTCP transport optimization project. Conclusions from the research are then given in Section 5.

2. MULTI-OBJECTIVE OPTIMIZATION METHODOLOGY

The multi-objective optimization approach used in this paper has several components: an optimization formulation, a simulation model to predict the effects of candidate remediation designs, and a multi-objective genetic algorithm called NSGA II (Non-dominated Sorting Genetic Algorithm-II) to search for improved designs. A flow chart of this approach is shown in Fig. 1. The GA first randomly initializes a set of candidate designs and then evaluates each design using the simulation models to obtain the hydraulic heads and the concentrations of the contaminants (and, in the case of the hypothetical case study, the associated human health risk). This information feeds to the objective function and constraints to evaluate fitness of the designs. The GA then creates another set of designs. This process is repeated until the optimal tradeoffs among the objectives are identified. The operations of the NSGA-II are overviewed below; the other components will be introduced subsequently with the case studies, since they vary for each case.

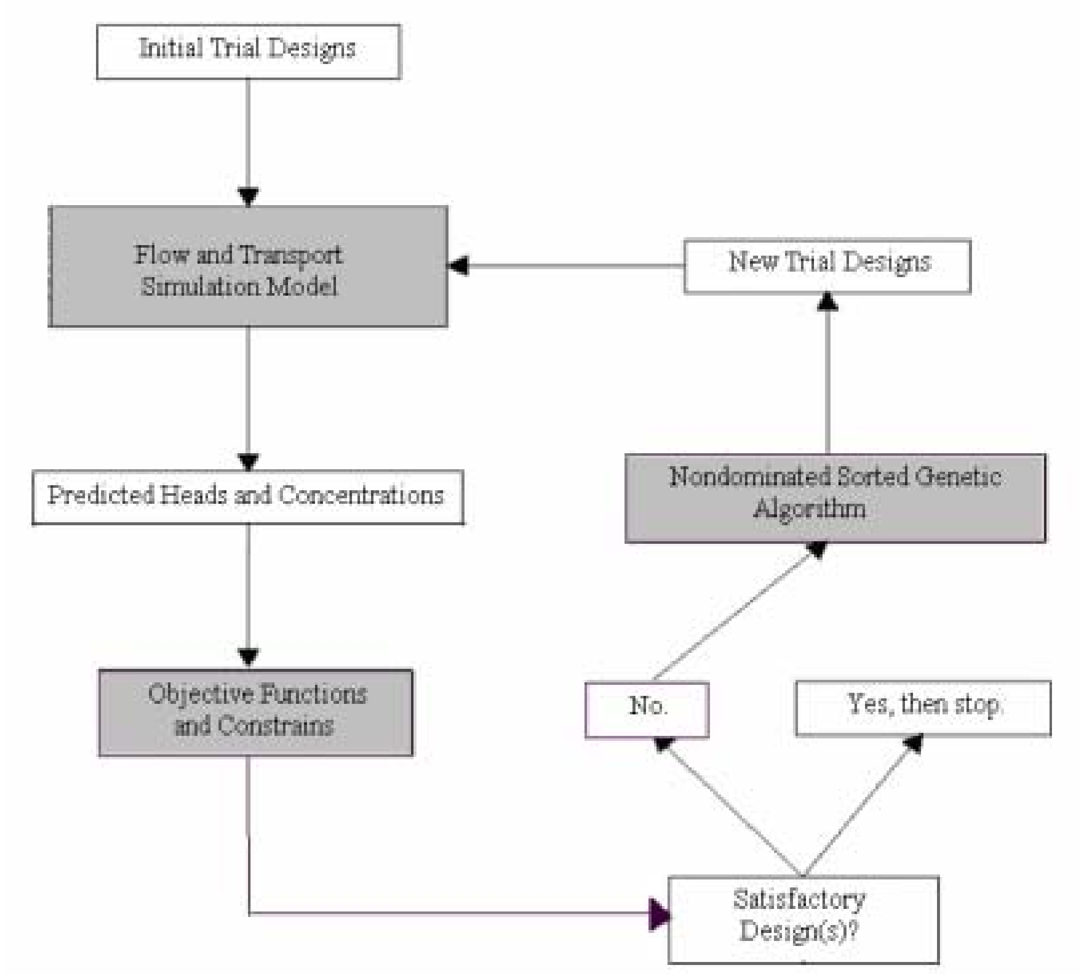


Fig. 1. Flow chart of the model

Genetic algorithms (GAs) are search and optimization techniques based on mechanics analogous to natural selection and genetics. The decision variables, which in this case are the remediation designs for which the GA searches, are coded as a string of binary digits called a "chromosome". Each chromosome represents a trial design. GAs start from a group of chromosomes called a "population" and then use three operators (selection, crossover and mutation) to create a new "generation." The selection process favors the designs that have high fitness, where the fitness is defined by the objective functions, which drives the algorithm to find better solutions until it converges to the optimal or near optimal solutions.

NSGA-II (Non-Dominated Sorting Genetic Algorithm) is an evolutionary multiobjective GA developed by Deb et al (2000) for solving multi-objective optimization problems. NSGA-II evaluates sampling designs in terms of vectors of objectives and the concepts of *Pareto dominance* and *crowding* are used to assign fitness values to the designs. A design is Pareto dominated by another design if it has better or equal performance in all objectives. All current designs that are nondominated are assigned the same nondomination rank and create the first “front” of solutions. These solutions are then removed from the population and the next front is identified, again based on nondominance. Fitness is then defined either in terms of nondomination ranks or crowding distances (Deb et al. (2000)). Crowding distance is the distance from each individual to the nearest individual on the same Pareto front. The individual with lower rank (dominated by fewer solutions) or with the same rank but larger crowding distance (adds more diversity to the population) is then preferred to generate the next population. NSGA-II has been shown to perform as well as or better than other second generation multiobjective genetic algorithms on difficult, high order problems (problems with more than two objectives) (Deb et al. 2001).

3. HYPOTHETICAL CASE STUDY

To test the importance of objective function complexity, we use the multi-objective methodology outlined above to solve two case studies. The first case study is a hypothetical case to find cost-effective pumping strategies for treating a contaminated aquifer using a pump-and-treat system. A summary of the optimization formulation is given in Section 3.1, followed by a description of the simulation models used for this case in Section 3.2. Section 3.3 then addresses visualization issues that arise in such three-objective cases. Finally, Section 3.4 examines the importance of objective function complexity for this case.

3.1 Optimization Formulations

Most groundwater remediation optimization efforts consider only a single objective, usually minimizing the total cost, with other objectives considered only as fixed constraints. A few have considered two objectives. Ritzel et al (1994) minimized the total clean up cost and maximized the reliability of the well system in solving a groundwater pollution containment problem. Cieniawski et al (1995) explored the tradeoffs between maximizing a groundwater monitoring problem's reliability in detecting contaminants and minimizing the contaminated area at the time of first detection. Reed et al (2001) tested an elitist non-dominated sorted genetic algorithm on a long-term groundwater monitoring problem with two objectives: minimizing the sampling cost and minimizing relative interpolation error. More recently, Reed et al (2003 in press) considered tradeoffs among long-term monitoring costs and three other objectives, all of which were different types of interpolation error. Beckford and Chan Hilton (2002) used two objectives, minimizing the total cost and maximizing reliability, to identify cost-effective remediation designs by a multiobjective robust genetic algorith (MRGA). Erickson et al (2002) applied the niched Pareto genetic algorithm (NPGA) to design a groundwater remediation system with two objectives (minimizing the remedial design cost and contaminant mass remaining at the end of the remediation horizon).

In this hypothetical case study, tradeoffs are considered among three objectives: cost of the pump-and-treat design, human health risk, and total clean-up time. To our knowledge, this is the first study to consider groundwater remediation design with more than two objectives. The objectives are shown mathematically below:

$$\text{Min } C_{TOT} = C_{REM} + C_{MON} + C_{SYST} \quad (1)$$

$$\text{Min } (\underset{t,k}{Max}\ Risk_{t,k}^{TOTAL} = Risk_{t,k}^{w} + Risk_{t,k}^{shw} + Risk_{t,k}^{nc}, \forall t, \forall k) \quad (2)$$

$$\text{Min } t_{total} \quad (3)$$

where

C_{TOT} : Total cost ($)

C_{REM} : Capital and operation costs for remediation wells ($)

C_{MON} : Costs for site monitoring ($)

C_{SYST} : Capital and operation costs for the remediation system, including the capital and operation costs for both treatment and discharge ($)

$Risk_{t,k}^{TOTAL}$: Total individual lifetime cancer risk at time t and exposure location k

$Risk_{t,k}^{w}$: Risk from ingestion of contaminated drinking water

$Risk_{t,k}^{shw}$: Risk from inhalation of due to showering

$Risk_{t,k}^{nc}$: Risk from inhalation of volatiles from contaminated water due to other non-consumptive use

t_{total} : The total clean-up time (years)

For detailed functions of C_{REM} , C_{MON} and $Risk_{t,k}^{TOTAL}$, please refer to Smalley et al *(2000).*

The detailed equation for the remediation system, based on Vieux (1999), is

$$C_{SYST} = C_{j,k}^{cap} X_i + C^{cap,POTW} X_i + (C_{j,k}^{op} + C^{ana} g + C^{op,POTW}) * (P \mid A, i, t_{total}) \quad (4)$$

where

$C_{j,k}^{cap}$: Capital cost for technology j of contaminant class k, where the classes are VOC, SVOC, fuel, ordnance or metal (in this case, the contaminant class is SVOC) associated with total pumping rate ($)

$C_{j,k}^{op}$: Annual O&M cost for technology j of contaminant class k ($/year)

$C^{cap,POTW}$: Capital cost for disposing of treated groundwater to POTW (publicly-owned treatment works) associated with total pumping rate ($)

$C^{op,POTW}$: Annual O&M cost of disposing treated groundwater to POTW ($/year)

C^{ana} : Unit cost of collecting, testing and analyzing groundwater and off-gas samples for technology j of contaminant class k ($/sample)

NW : Number of remediation wells

g : Number of groundwater and off-gas samples per year

$(P \mid A, i, t_{total})$: Financial factor for converting a series of O&M costs (A) to a present value (P) at given interest rate i

X_i : Indicator variables for well installation: $X_i = 1$ if well i is installed, otherwise $X_i = 0$

The cost items: $C_{j,k}^{cap}$, $C^{cap,POTW}$, $C_{j,k}^{op}$ and $C^{op,POTW}$ are all functions of total pumping rates.

Five above-ground treatment technology configurations (air stripper-low profile tray stack, air stripper-packed tower, modular carbon adsorbers-duel bed, modular carbon adsorbers-permanent and modular carbon adsorbers-disposable) were selected for inclusion in the remediation system based on a previous analysis (Vieux (1999)). For each remediation design, the model chooses the most cost-effective technology for the total pumping rate at all wells, using the ranges shown in Table 1. These ranges were developed using the Department of Defense's Remedial Action Cost Engineering Requirements (RACER) software.

Table 1. Cost-Effective Pumping Rate Ranges for Aboveground Treatment Technologies

Technology	Effective pumping rates (gpm)	Effective pumping rates (m^3/day)
Air stripper-low profile tray stack	0 ~ 750	0 ~ 4088
Air stripper-packed tower	10 ~ 2,250	55 ~ 12,264
Modular carbon adsorbers-duel bed	0 ~ 2000	0 ~ 10,901
Modular carbon adsorbers-permanent	0 ~ 200	0 ~ 1,090
Modular carbon adsorbers-disposable	0 ~ 200	0 ~ 1,090

For more detailed information about C_{SYST}, please refer to Appendix A.

All of the objectives are subject to the following constraints:

1) The pumping rates (or injection rates) of the wells, Q_i, should be within the well capacities [$Q_{\min,i}$, $Q_{\max,i}$] for any remediation well *i*.

$$Q_{\min,i} \le |Q_i| \le Q_{\max,i}, \forall i \tag{5}$$

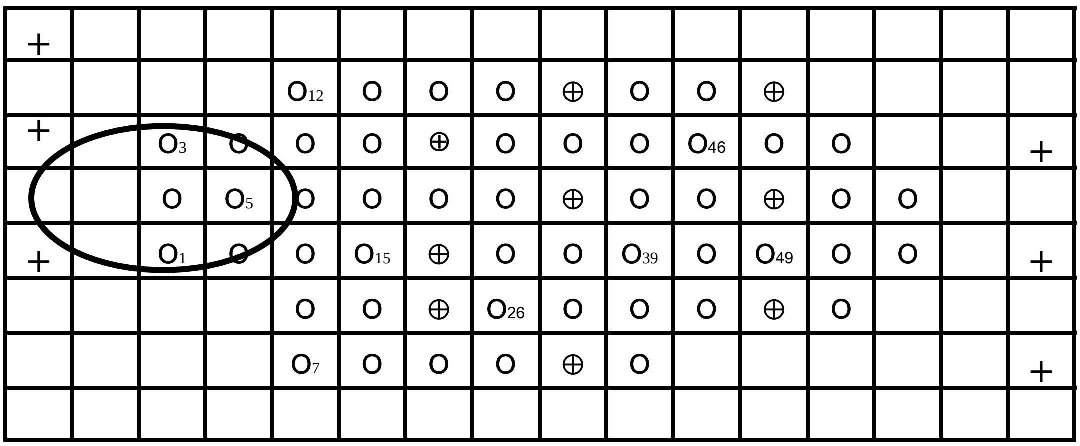
2) The hydraulic head, $h_{i,l}$, for remediation well *i* should be within the allowed head range [$h_{\min,l}, h_{\max,l}$] at any well location *l*.

$$h_{\min,l} \le h_{i,l} \le h_{\max,l}, \forall i, \forall l \tag{6}$$

3.2 Simulation Models

To evaluate the hydraulic head constraints and the cleanup duration and risk objectives, simulation models are needed. In this case study, as in several previous studies (Smalley et al 2000; Gopalakrishnan et al 2003), we model the source area using numerical models and then use the source area concentrations to predict human health risk. The numerical modeling is based on a hypothetical confined, heterogeneous and isotropic aquifer, 480m by 240m by 20m, which has been studied by Smalley et al (2000). The properties of the aquifer are based on the Borden aquifer (Mackay et al. (1986); Graham and McLaughlin (1991)). The target contaminant is BTEX. Groundwater Modeling System (GMS) modules MODFLOW (McDonald et al, 1988) and RT3D (Clement et al, 1998) were used to run the simulation model. The initial plume is shown in Fig. 2, which was created using 10 contaminant sources with contaminant concentrations varying from 50mg/l to

600mg/l. MODFLOW and RT3D ran for a stress period of 2 years to obtain the initial distribution of the plume.



+ Monitoring Wells (15)

O Possible remediation well locations (58)

BTEX Plume

Fig. 2. Plan view of the hypothetical case study

The flow of the groundwater in the aquifer is assumed to be steady state and the direction of flow is from left to right in Fig. 2. To reduce computational effort, the hydraulic conductivity values (average 2256 m/year) were obtained from one realization of a conditional simulation performed by Smalley et al (2000). The porosity of the field was assumed to be 0.3 and the soil bulk density of the aquifer was 2000 kg/m3. The longitudinal dispersivity was assumed to be 15 m with a ratio of transverse to longitudinal dispersivity of 0.2 and a ratio of vertical to longitudinal dispersivity of 1.0. The left and right boundaries of the domain in Fig. 1 are constant head boundaries with a mean hydraulic gradient of 0.00146. The upper and lower boundaries are no flow boundaries. A linear adsorption reaction is assumed with the adsorption coefficient of 0.000062 m3/ kg. The ‘no reaction/tracer transport’ chemical reaction package in RT3D was used for contaminant transport.

For the remediation model in Fig. 2, fifteen monitoring wells were used to monitor the concentrations of the contaminant in the aquifer for the whole remediation period. A maximum of three remediation wells were allowed for extraction/injection at the 58 candidate locations shown in Fig. 2. The maximum pumping capacity of each well was assumed to be 250 m^3/day.

The concentrations of the contaminant within the source zone from the two numerical models were then used to predict human health risks at an exposure point 200 m down gradient of the right boundary of Fig. 2 using a risk assessment model. For more details, please refer to Smalley et al (2000).

When this application is implemented with the NSGA-II, the decision variables include three possible well locations, each represented by 6 bits in the chromosome; pumping rates for three remediation wells, each with 8 bits; a single-bit variable to decide whether each of the three wells perform extraction or injection; a single-bit variable to determine whether each of the three wells are installed or not; and a variable for the total cleanup time, represented by 8 bits. The length of each variable was chosen based on the maximum value the variable can attain and the precision the variable requires. In total, there are 13 decision variables and the chromosome length is 56 bits.

3.3 Visualizing Tradeoffs among Objectives

The optimal solutions to three-objective problems, such as the one described by Equations 1-3, usually will form a three-dimensional surface, but if the problem is complex it can be difficult to interpret the resulting surface. In this section, we explore the following methods from Deb et al. (2001) for visualizing solutions to the three-dimensional hypothetical case study presented in the previous section:

1) *Value path method* is a popular means of showing non-dominated solutions for problems with more than two objectives and was suggested by Geoffrion et al (1972). As shown in Fig. 3, the horizontal axis represents the number of objectives. If there are N objectives, there would be N tick-marks on the axis. The vertical axis marks the normalized objective function values. The vertical shaded bar represents each objective function, with the range covering the minimum and maximum values of this objective function in the Pareto-optimal set. Each cross line connecting all the objective bars represents a solution from the non-dominated set.

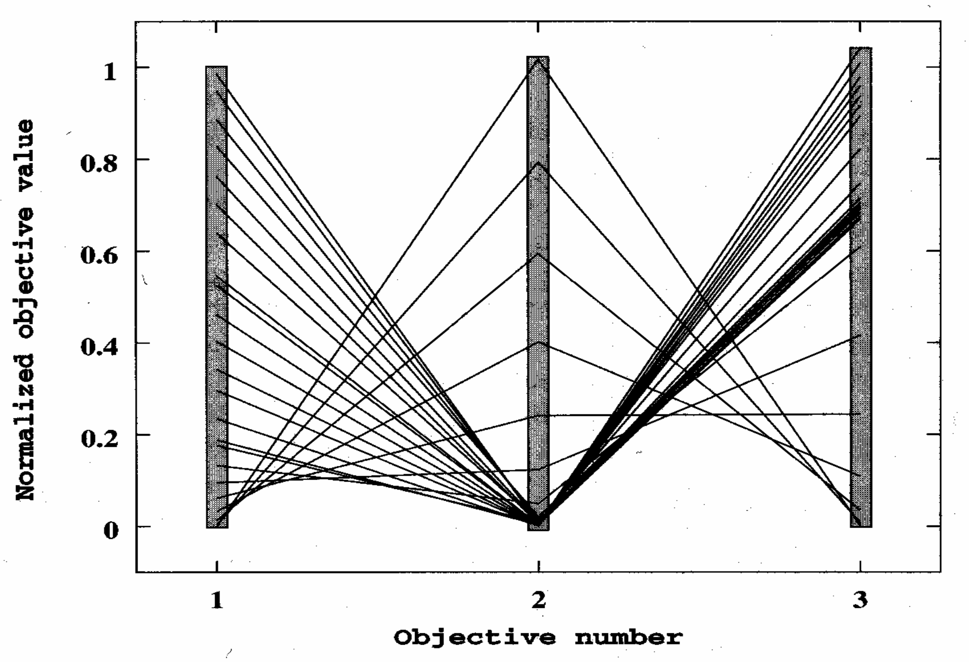


Fig. 3. The value path method (adapted from to Deb (2001))

For high-order multi-objective cases, the number of solutions is often very large and it becomes difficult to interpret the results. For this case study, the total number of solutions found by the NSGA-II is 1160. As shown in Fig. 4, it is difficult to identify any conclusions from the solutions presented in this manner. Some users avoid this difficulty by randomly sampling a portion of the solutions and showing them via this method. Fig. 5 shows a random subset of only 10% of all the solutions from Fig. 4. Not only is the graph still difficult to interpret, but the spread of the solutions over the entire optimal region is no longer represented.

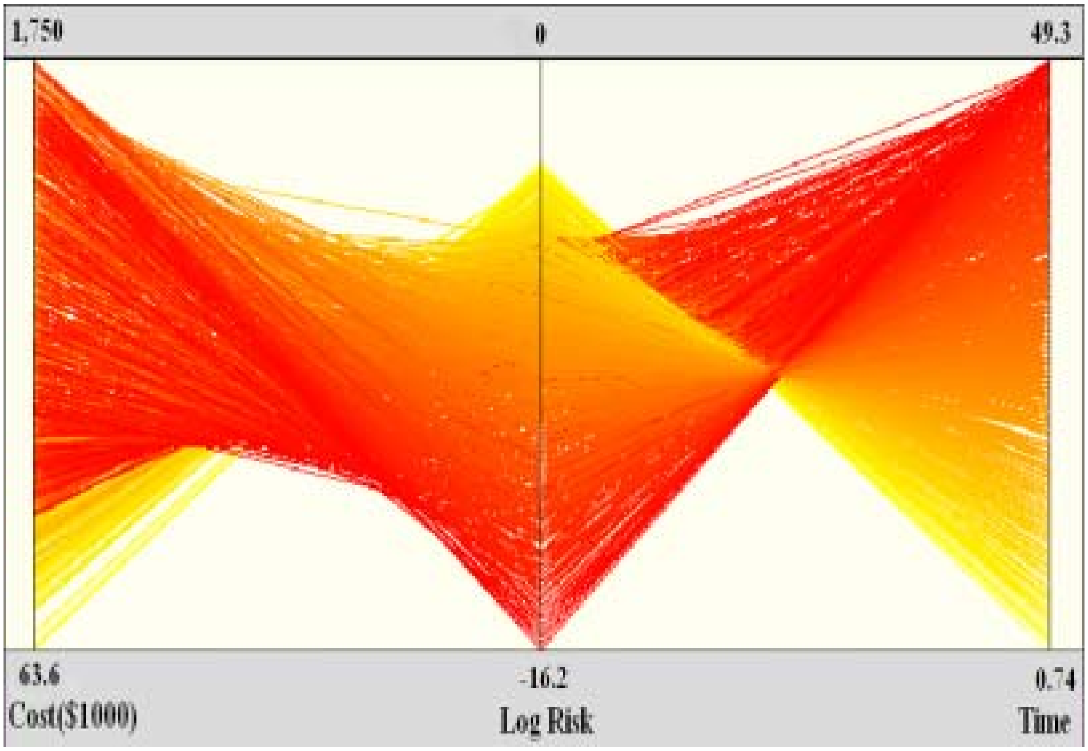


Fig. 4. All solutions shown by the value path method

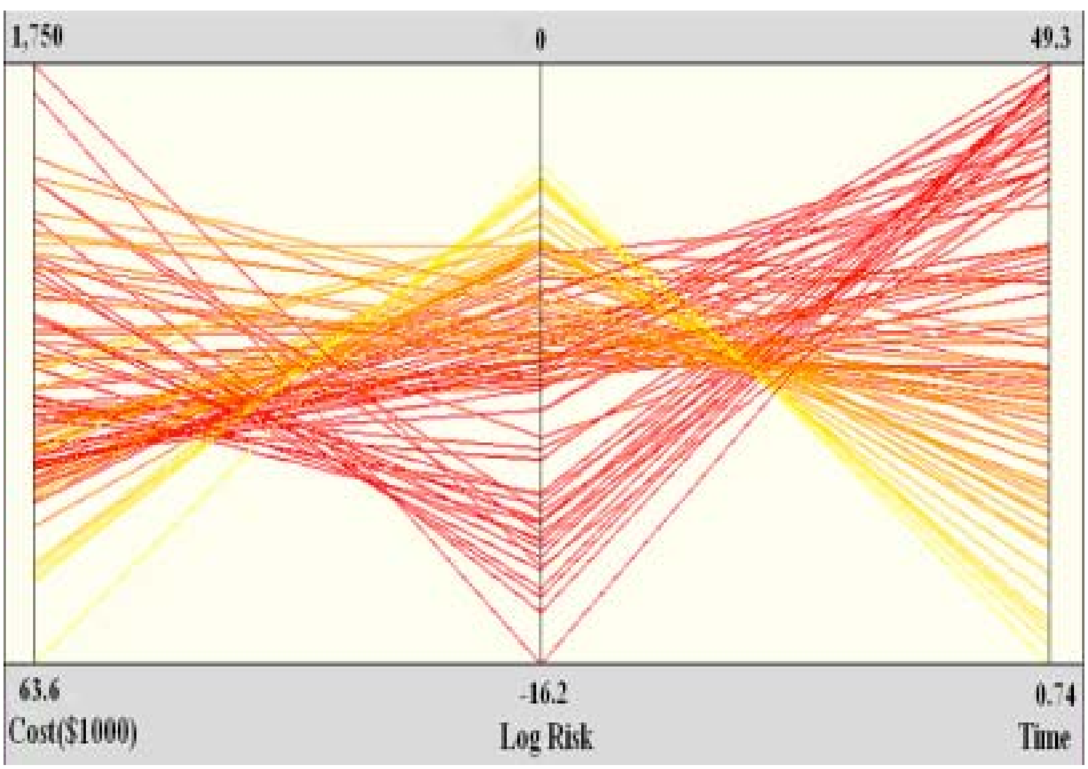


Fig. 5. 10% solutions shown by the value path method

2) *Bar chart method* is another way to present different non-dominated solutions, but is usually useful only for a small number of solutions. The objective function values, usually normalized, of each solution are plotted in a histogram in the same order. If there are N solutions, N different bars are plotted for each objective function. To illustrate this method, six solutions among the 1160 nondominated solutions to the hypothetical case study are visualized with this method in Fig. 6. Clearly it would be impossible to show all 1160 solutions with this method. Moreover, it is difficult to gain any sense of the tradeoffs among the different objective functions.

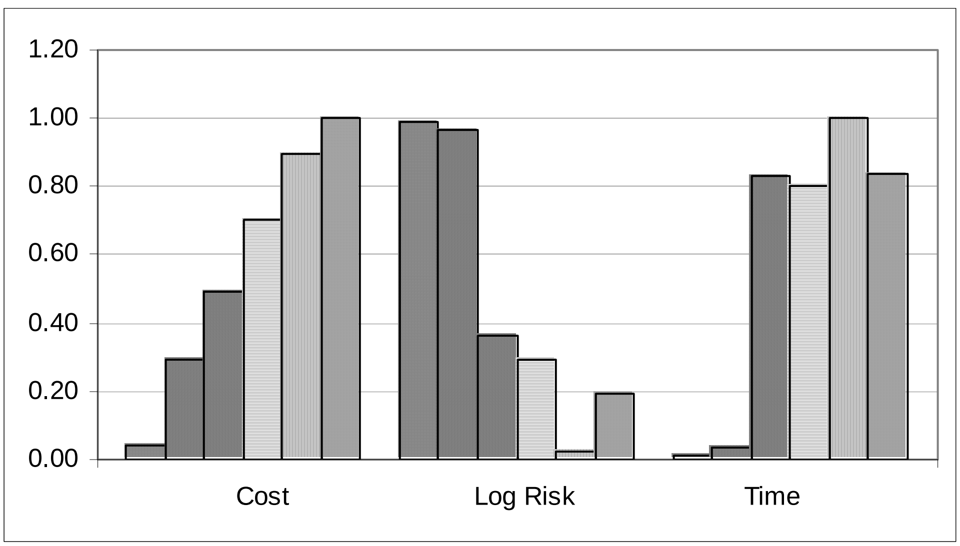
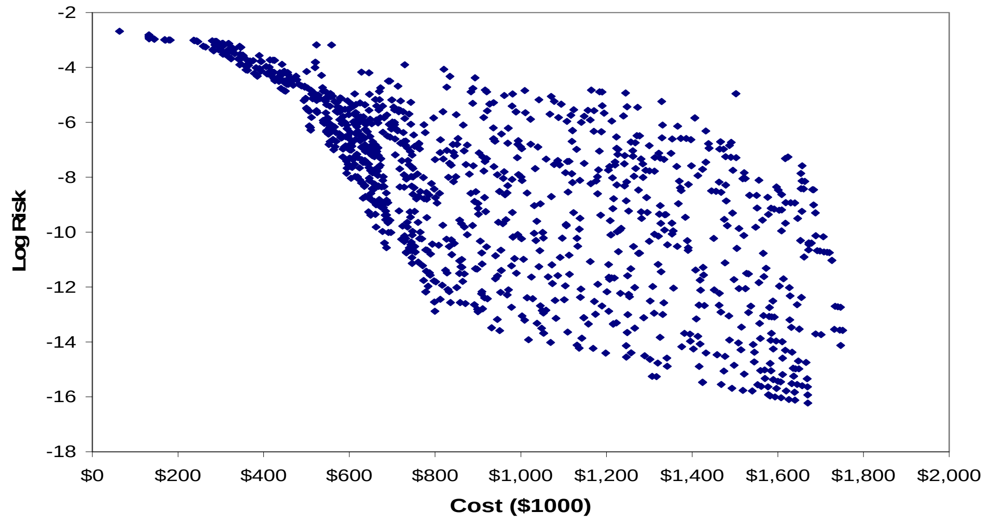


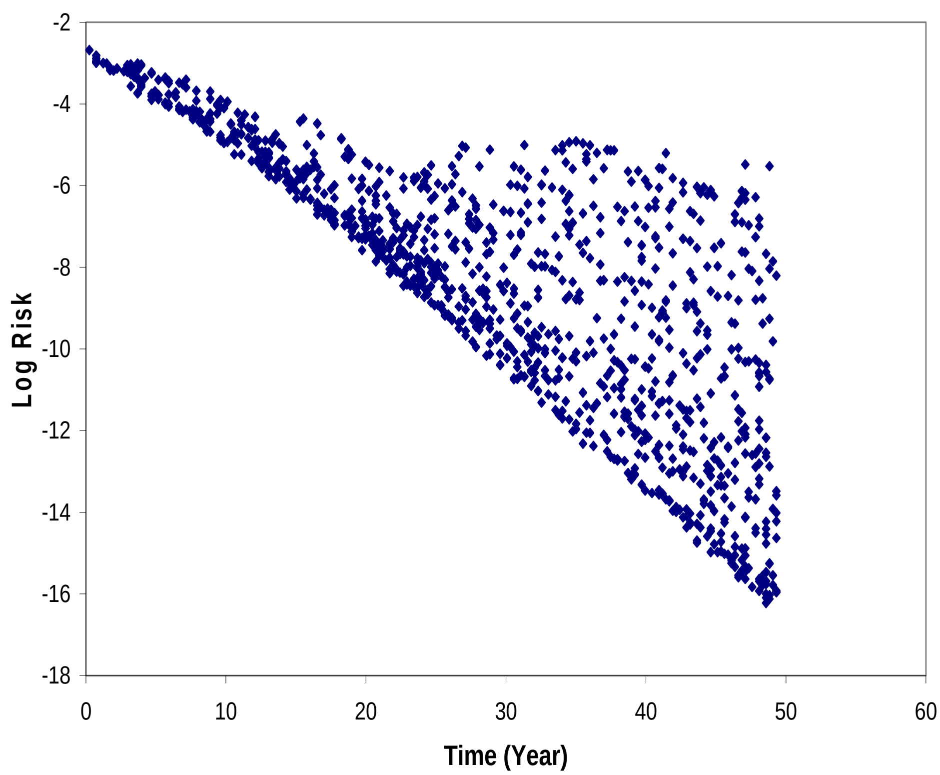
Fig. 6. Few selected solutions shown with the bar chart method

3) *Scatter-plot matrix method* involves plotting all pairs of objective functions. For example, for a three-objective problem, like the one considered here, with objectives f_1, f_2 and f_3, the three non-dominated tradeoffs between f_1 and f_2, f_1 and f_3, and f_2 and f_3

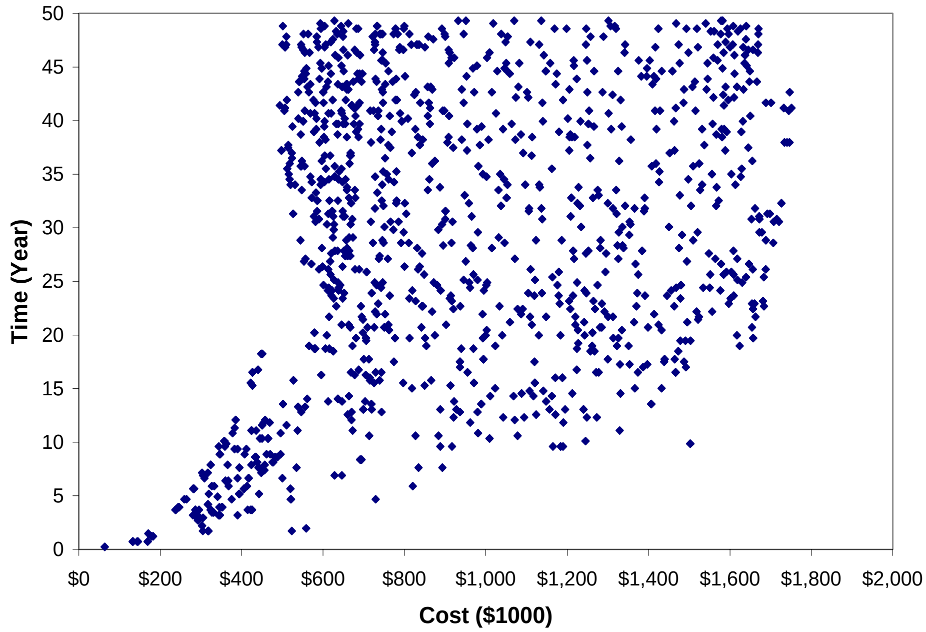
would be shown. Fig. 7 shows the results of this case study visualized with this method.



a) Tradeoff between cost and log risk



b) Tradeoff between time and log risk



c) Tradeoff between cost and time

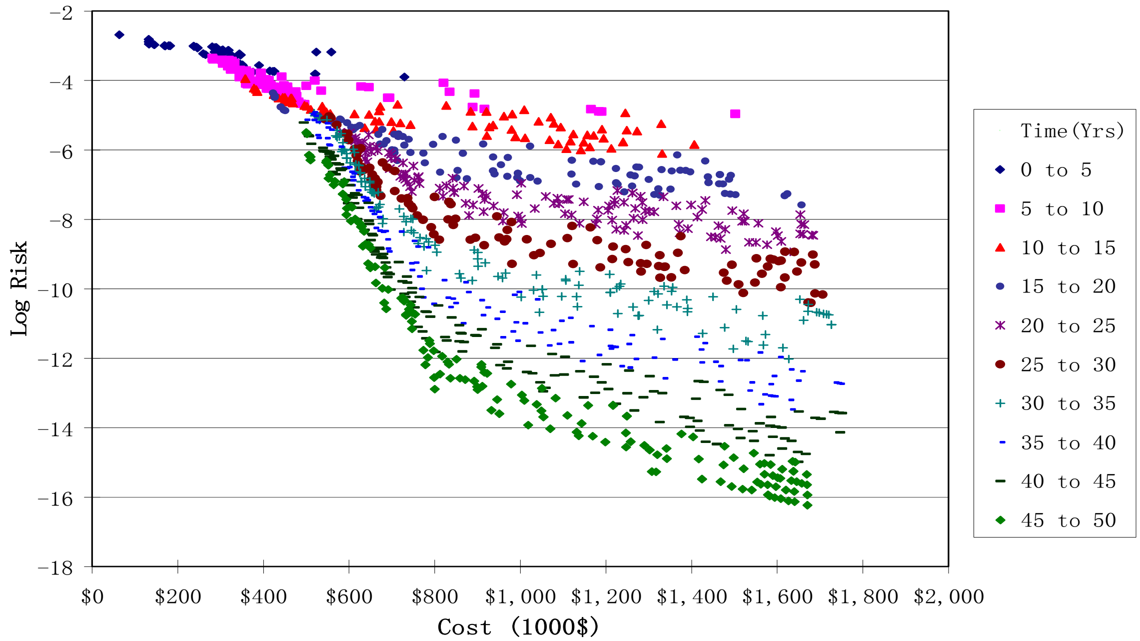
Fig. 7. Results shown with the scatter-plot matrix method

This method is useful for problems where the tradeoff surface is convex and the projection onto two objectives creates a useful tradeoff curve. For this case, though, the tradeoff surface is more complex and the two-dimensional tradeoffs are not clear.

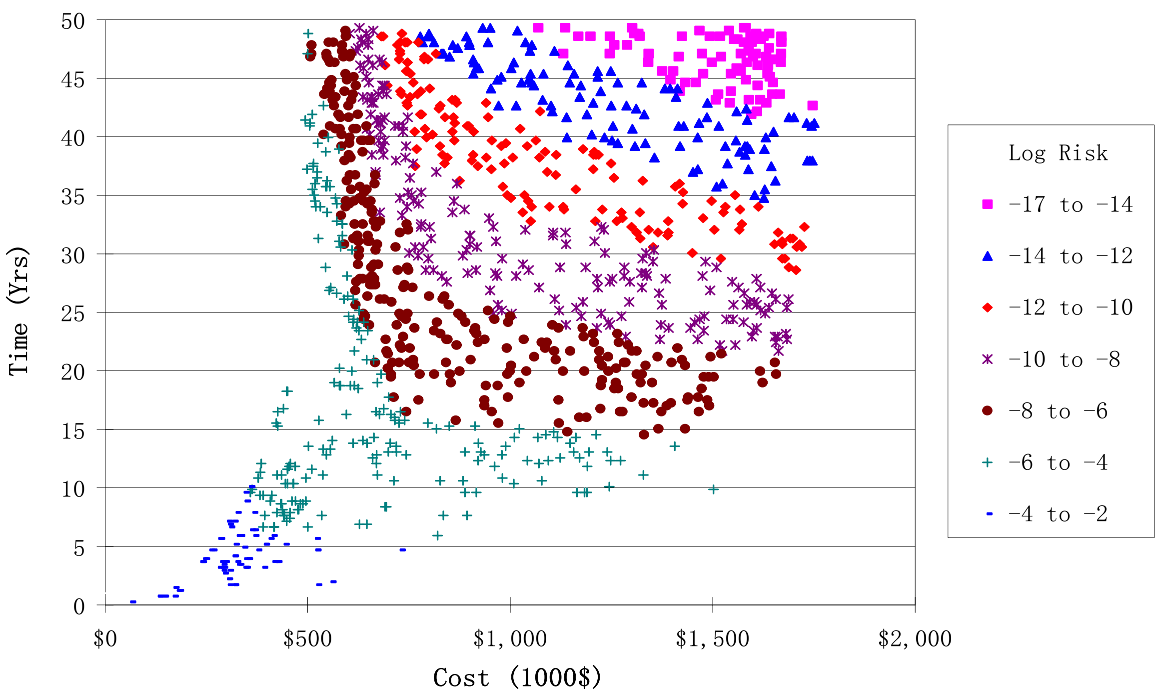
We propose a new approach to express the tradeoffs among three objectives that clearly visualizes all of the optimal solutions all of the relationships among the objectives to improve decision making. The approach is a banded scatter-plot matrix method in which the tradeoff between any two objectives are shown for different ranges of the third objective using different colors or symbols.

Fig. 8 shows the tradeoffs between two objectives based on different ranges for the third objective. Fig. 8(a) shows the tradeoffs between cost and log risk for different ranges of time, while 8(b) shows the tradeoffs between cost and time based on different ranges of log risk and 8(c) shows time and log risk tradeoffs for different cost ranges. This visualization approach is very straightforward for elucidating the relationships among the objectives.

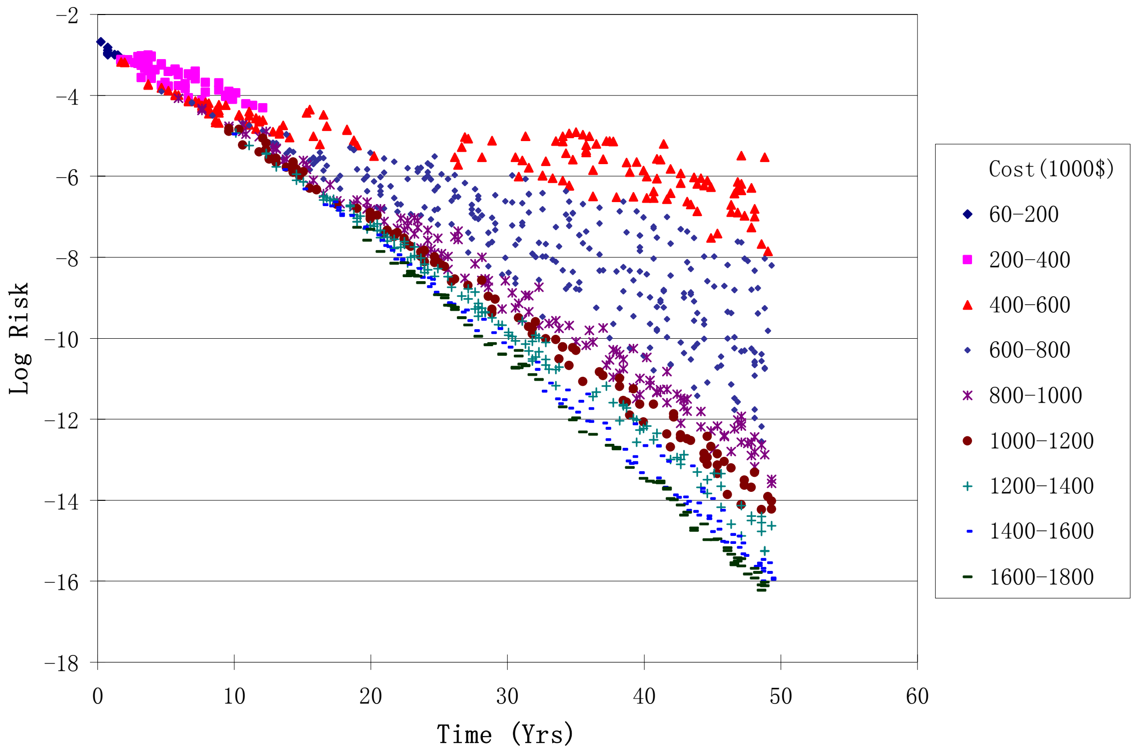
The effects of possible bounds on different objectives can also be easily seen and candidate solutions that meet the bounds identified. For example, if the project is constrained by time, Fig. 8(a) can be used to find the tradeoff between cost and risk for different ranges of cleanup time. Or if a target risk is to be set, Fig. 8(b) can be used to identify tradeoffs in cost and cleanup time. Fig. 8(b) shows that, for this case, if the required risk level is high (higher than 10^{-6}), a short term remediation (less than 15 years) is preferred. For a low risk level (especially lower than 10^{-10}), a long term remediation is more cost effective. The non-dominated solutions for risk level less than 10^{-6} are almost all solutions with cleanup time less than 15 years, while almost all the non-dominated solutions for risk level greater than 10^{-10} are gathered in the area where time is larger than 30 years.



(a) Tradeoffs between cost and log risk for different ranges of cleanup time



(b) Tradeoffs between cost and cleanup time for different ranges of log risk



(c) Tradeoffs between time and log risk for different ranges of cost

Fig. 8. Tradeoffs among objectives

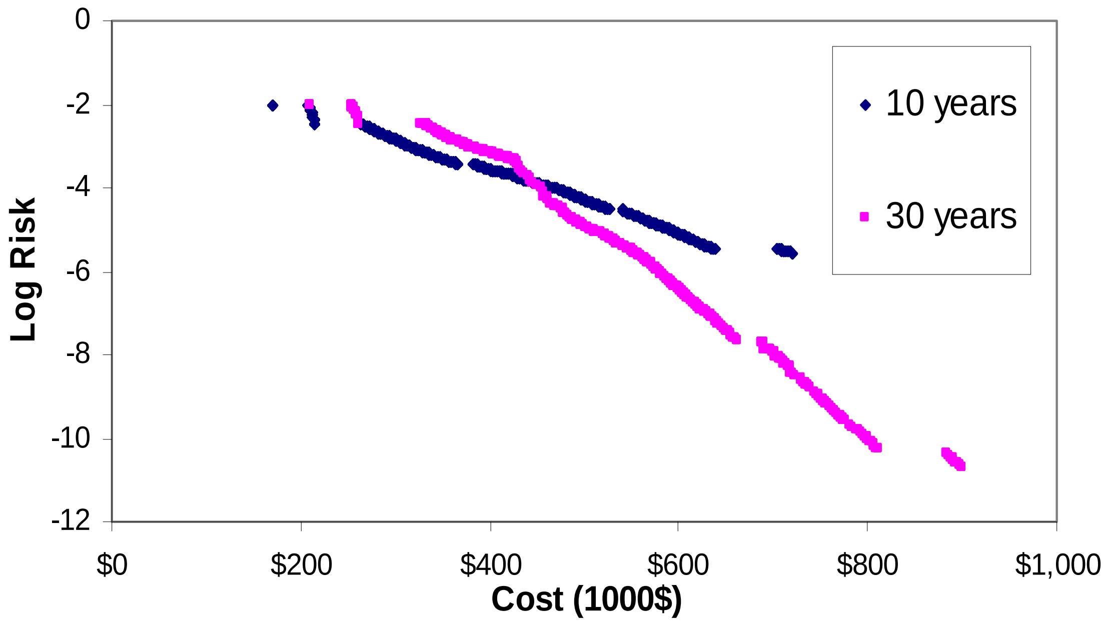
3.4 Complexity of Cost Objective Function

In this section, we will explore the tradeoffs between development efforts and cost function accuracy using four different cost functions. The cost functions, which were applied to the case study described previously, range from complex (using the function presented previously), to simple (using three functions that have been frequently used in the literature). To simplify the analysis, the study was performed for two objectives (cost and risk) with two different clean-up times (10 years and 30 years).

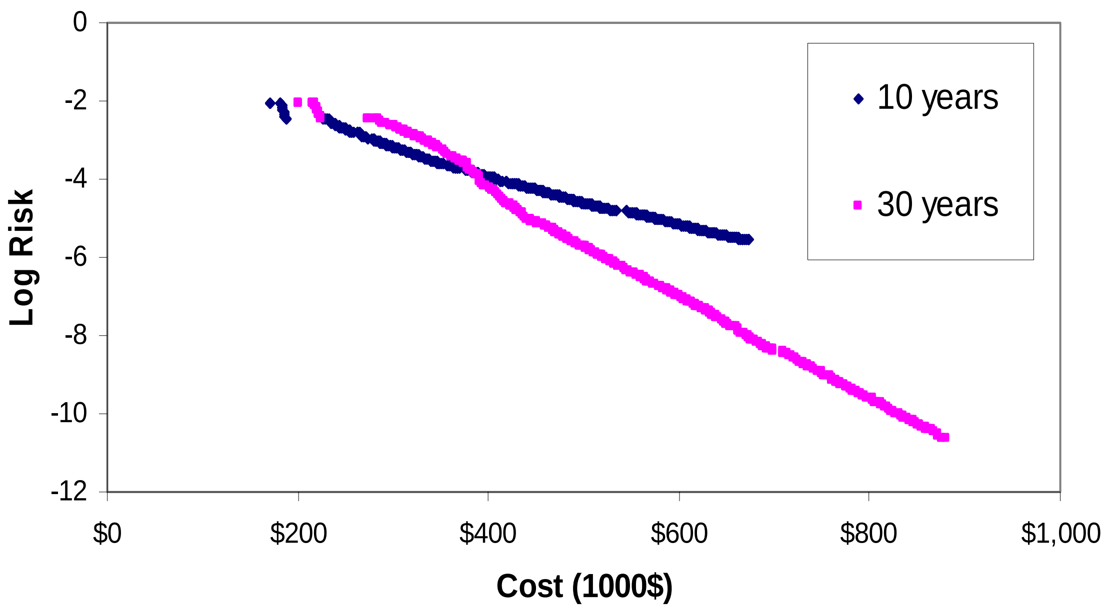
The four different cost functions tested in this study were:

1. Realistic: Fixed capital cost + variable capital cost + O&M cost for the appropriate technology (given previously in Equation 4)
2. Fixed Capital + O&M cost for a single technology, which was chosen to be the least-expensive technology at most flow rates, modular carbon adsorbers-permanent
3. O&M cost for a single technology, again using modular carbon adsorbers-permanent
4. Total pumping rates

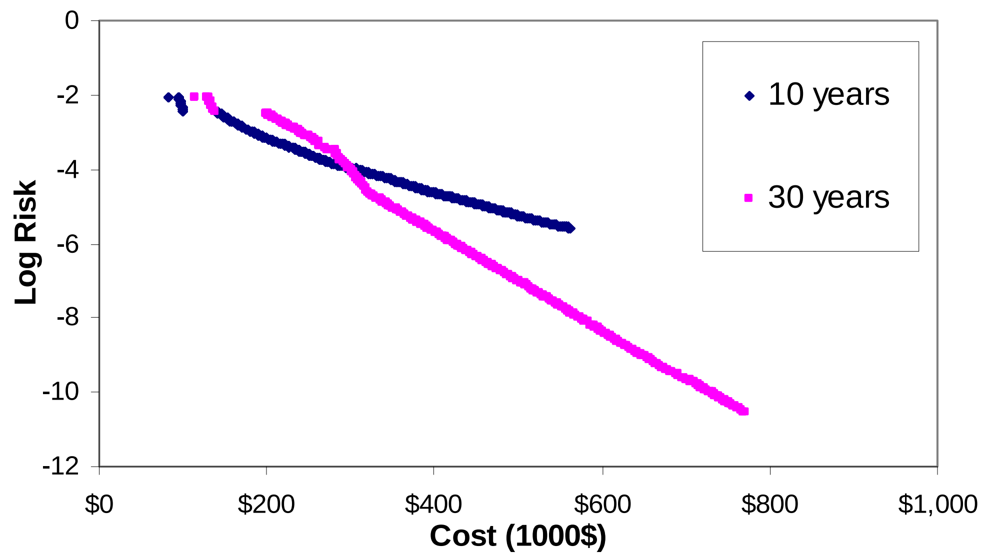
Fig. 9 compares the optimal tradeoffs for each cost function under both clean-up times. The first three cost functions indicate that for a high risk level, a short term remediation is more cost effective, as was the case for three objectives. But the result for total pumping rates, shown in Fig. 9(d), does not support the same conclusion. For a relatively high risk level project, the actual optimal solution should be a short term operation, but the optimal solution for the objective of total pumping rates is a long term operation with wells pumping at lower rates. This suggests that for this case, total pumping rates as an objective may not be a good choice, especially for higher target risks.



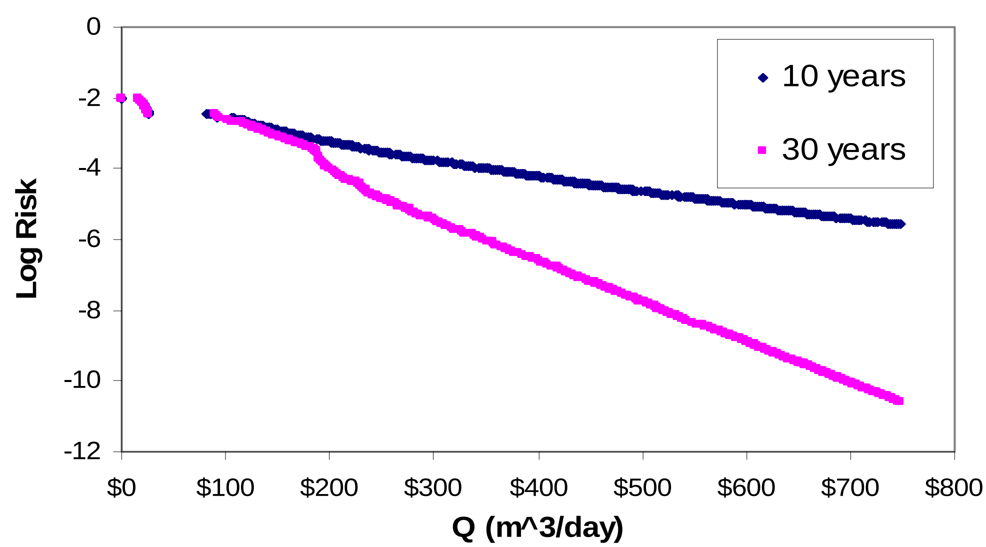
(a) Tradeoffs between cost and risk for two different remediation times using only the realistic cost function



(b) Tradeoffs between cost and risk for two different remediation times using the fixed capital + O&M cost function



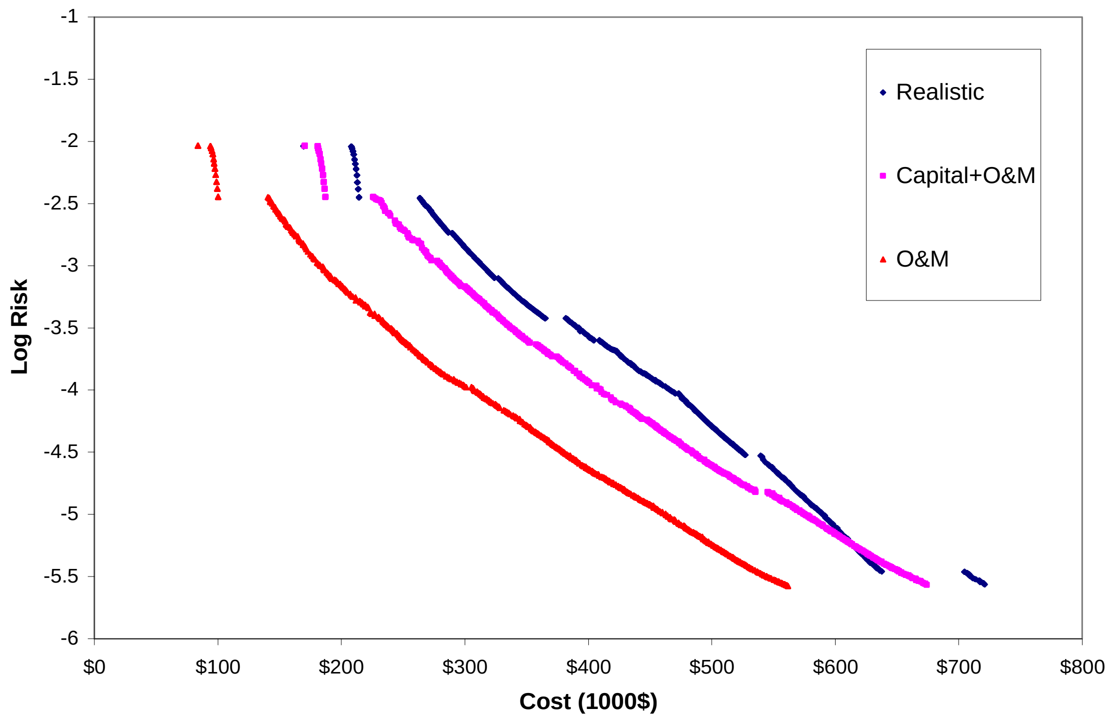
(c) Tradeoffs between cost and risk for two different remediation times using the O&M cost function



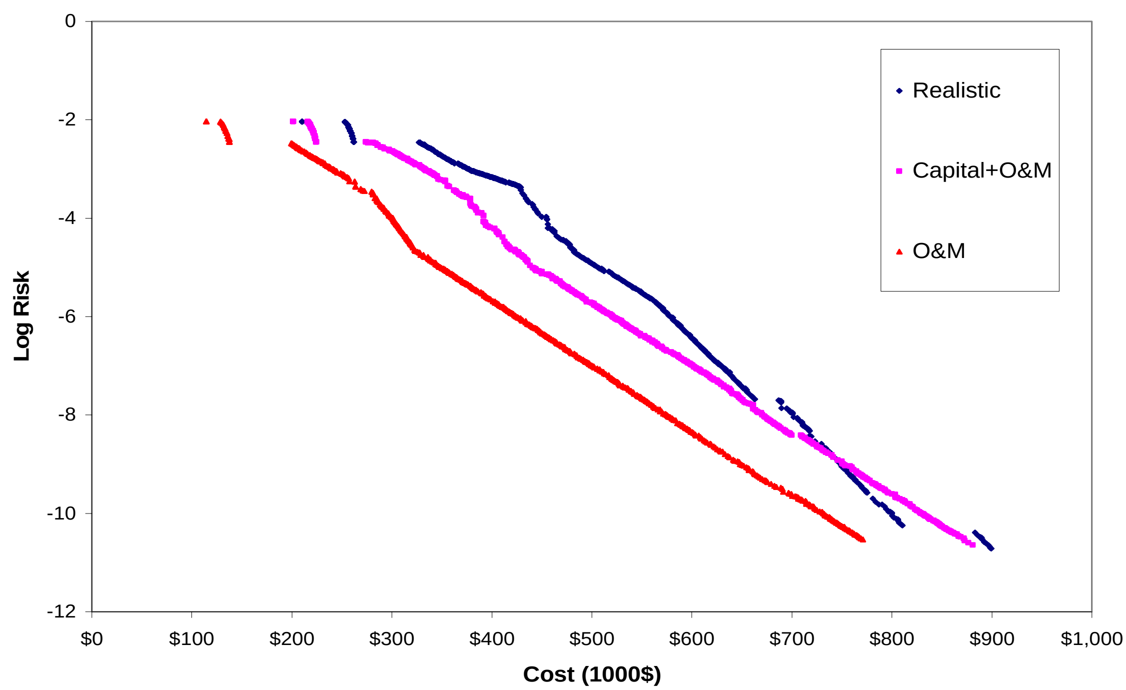
(d) Tradeoffs between cost and risk for two different remediation times using the total pumping rates function

Fig. 9. Tradeoffs between cost and risk for each cost function with two clean-up times

Fig. 10 shows a comparison of the original Pareto fronts found by the realistic cost function, fixed capital + O&M and O&M cost functions. The Pareto front of the total pumping rates function is not shown here because of the different units.



a) Short-Term Cleanup (10 years)

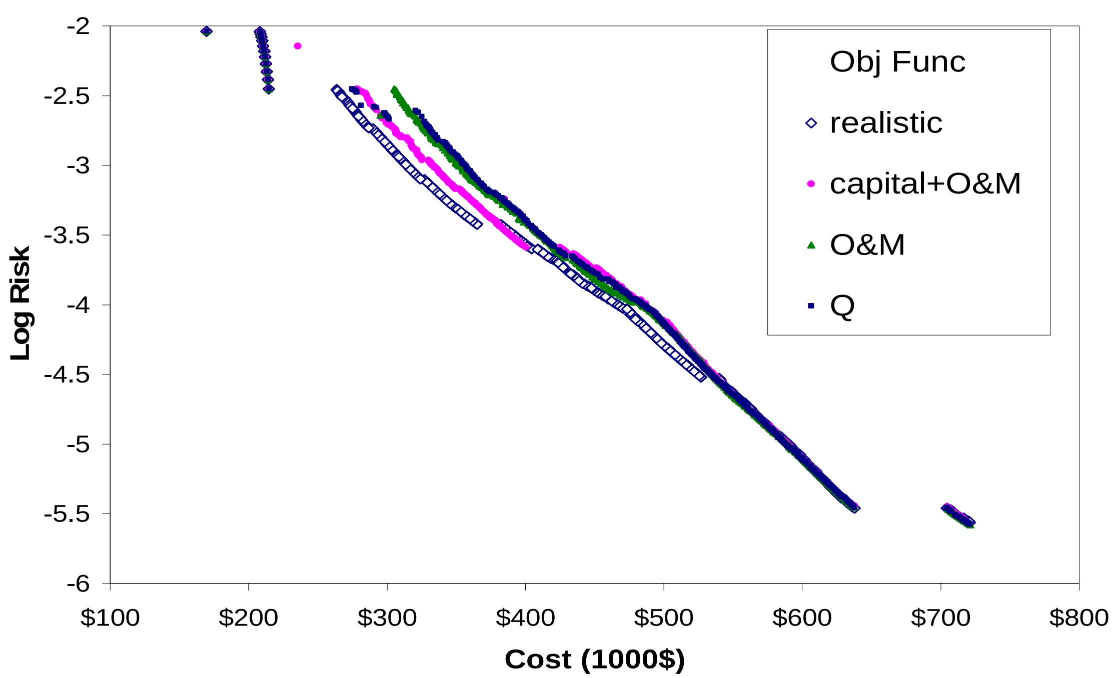


b) Long-Term Cleanup (30 years)

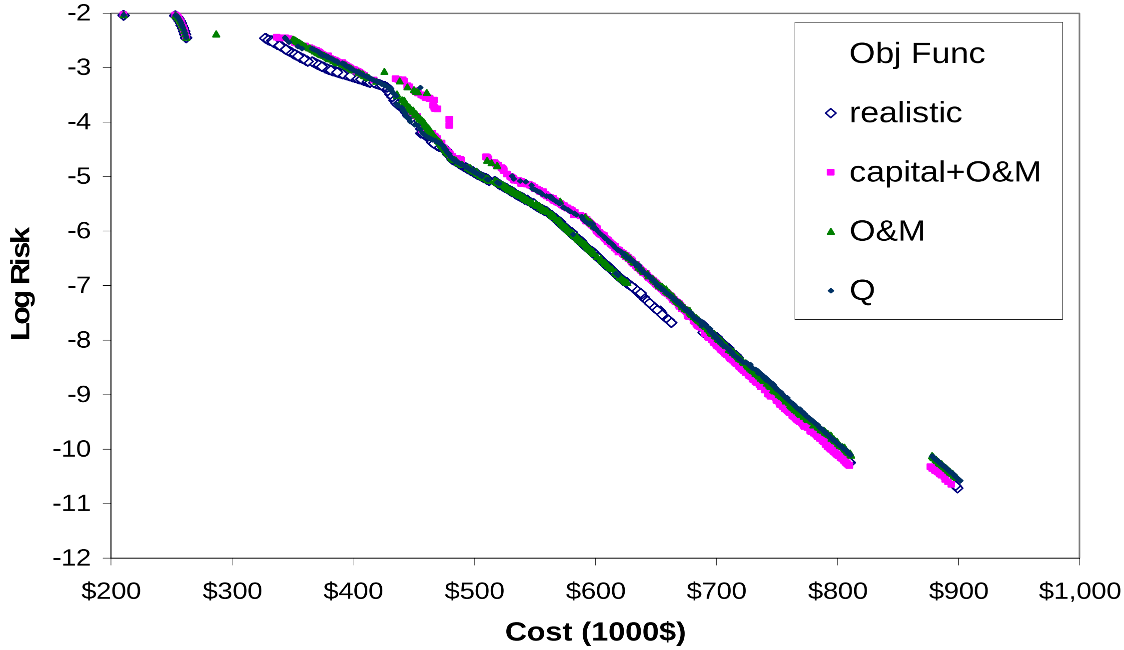
Fig. 10. Comparison of Pareto fronts identified by different cost functions

In Fig. 10, the realistic cost function actually found solutions that are even cheaper than the real value of fixed capital +O&M cost function at some risk levels for both short- and long-term cleanups even though more cost items are considered in the realistic function. There are two possible reasons for this result. One is that the realistic cost function actually found better design strategies than the simplified cost functions and the other is that the design strategies are not much different but the treatment technologies are different.

To further investigate the cause of these results and to examine the effects of choosing a simpler cost function when the real cost function is more complex, the optimal designs identified with each of the four cost functions were re-evaluated with the realistic function. Fig. 11 shows the resulting Pareto fronts for both the short- and long-term cleanups.



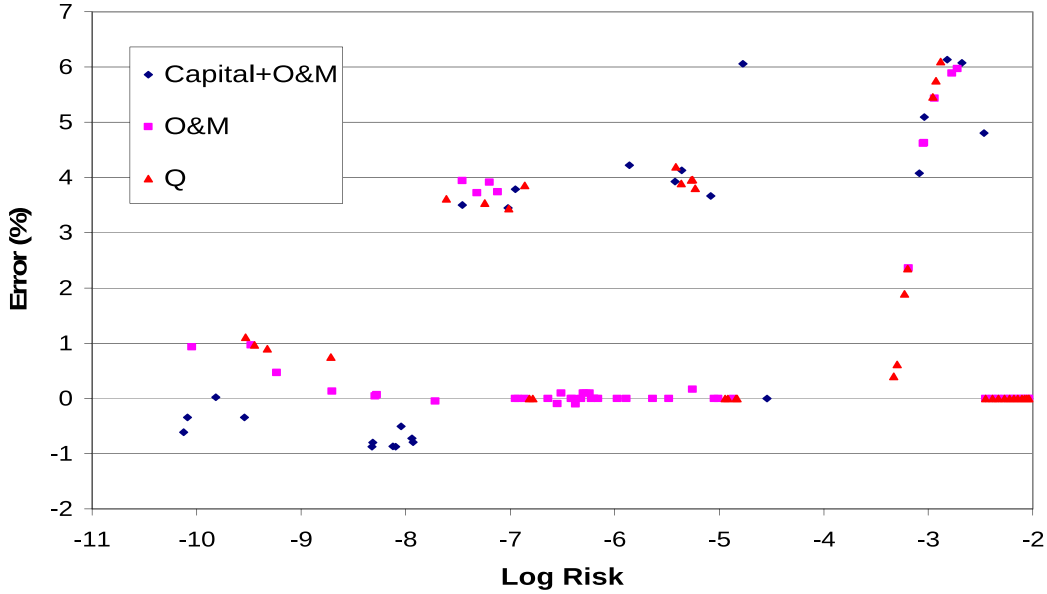
(a) Short term cleanup (10 years)



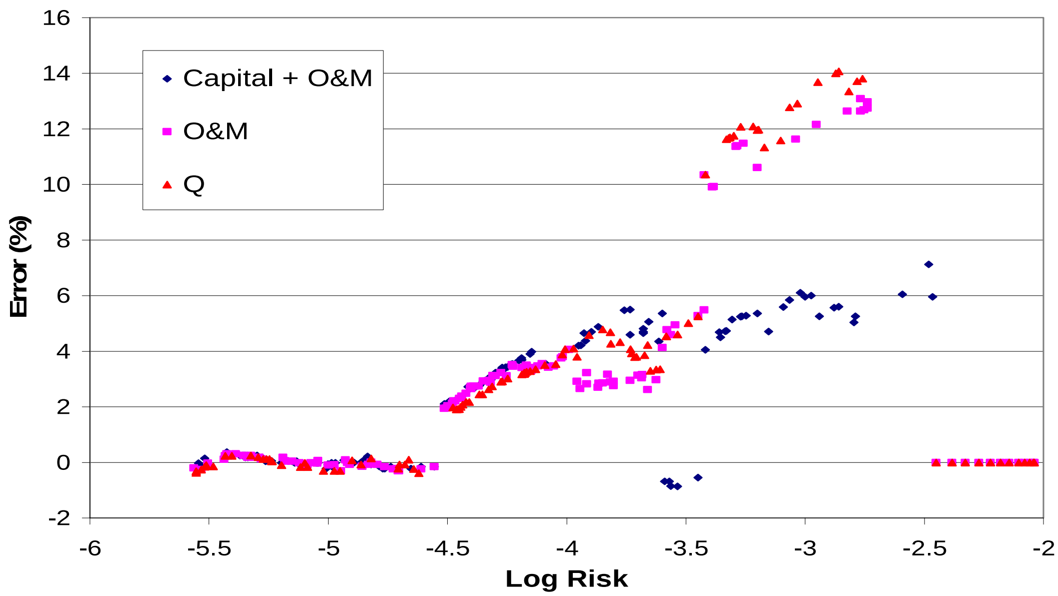
(b) Long term cleanup (30 years)

Fig. 11. Comparison of Pareto fronts from four cost functions, evaluated using the realistic cost function

Results for both short and long cleanup durations indicate that the realistic cost function performed better and identified more optimal solutions than the other functions. The differences are greater for the short-term cleanup where capital costs would represent a larger fraction of the total present worth cost.



a) Long-term cleanup



b) Short-term cleanup

Fig. 12. Difference between the re-evaluated cost and the realistic cost for different risk level

To further illustrate the extent of errors created by using simplified cost functions, Fig. 12 shows the differences between the realistic cost and the re-evaluated cost for the simplified cost functions. Because the different objective functions often generated different treatment strategies with different risks, calculating the relative cost errors from Fig. 12 across the Pareto fronts required grouping different designs by risk level. In this case, if the difference in log risk for two different designs was less than 0.0005, the risks were assumed to be the same and the cost errors were calculated.

From Fig. 12, it can be seen that the errors are much larger the for short-term cleanup (up to 14%) than for the long-term cleanup (up to 6%). In both cases, the errors increase as the risk target increases, although the trend is much clearer in the short-term case. Errors shown in Fig. 12 are generally greatest for total pumping rates and least for capital + O&M cost, although for some risk levels, O&M cost has smaller error than capital + O&M cost. For a long-term cleanup, it is difficult to tell which simplified cost function performs the best. Also, because the achievable risk range is much larger than for the short-term project, it is more difficult for different cost functions to achieve the same risk value with a slightly different pumping solution.

Note also that there are some small negative errors appearing on both the short-term and long-term cleanup results in Fig. 12, from which it would appear that the simplified cost functions (mostly capital + O&M cost) found better solutions than the realistic cost function. Most of these solutions are actually non-dominated to each other: the solution with slightly lower risk has slightly higher cost. The differences are also very small, with differences in log risk less than 0.0005 and differences in costs less than 1%. Thus we can treat them as equivalent solutions.

To further illustrate the performance of different cost functions, the optimal design strategies and re-evaluated costs of the four functions were compared at three representative risk levels for both the short- and long-term cases, with the results shown in Tables 2 to 4.

Table 2. Design Strategies for Short-Term Project When Risk = $10^{-2.86}$ (See Fig. 1 for well locations)

Objective	Well location	Pumping rate (m^3/day)	Cost ($1000)	Cost increase relative to realistic function (%)
Realistic	16	154	301	\
Fixed cap. +O&M	10 21	25 117	318	5.6
O&M	10 16 21	64 48 25	340	13
Total Q	9 16 21	15 108 19	343	14

Table 3. Design Strategies for Short-Term Project When Risk = $10^{-5.3}$

Objective	Well location	Pumping rate (m^3/day)	Cost($1000)	Cost increase relative to realistic function (%)
Realistic	16 23 25	250 237 177	619	0
Fixed cap. +O&M	16 19 23	228 193 247	621	0.24
O&M	16 19 23	240 177 250	620	0.18
Total Q	16 19 23	242 179 246	620	0.18

For the short-term cleanup case, significant differences were observed at some risk levels but not at others. At a risk level of $10^{-2.86}$, the level at which performance differed the most, the designs are completely different for the four cost functions and the solution found using the total pumping rate objective function was 14% more expensive than the one found with the realistic cost function (see Table 2). When risk is $10^{-5.3}$, the level at which performance was most similar, the costs differ by only 0.24% (see Table 3).

For a long-term cleanup, the performances of the four objective functions did not show significant differences at any risk level. When risk is $10^{-2.82}$, the level at which performance differed the most, there was only a 6.2% difference between the realistic cost function and the simplified cost function.

Table 4. Design Strategies for Long-Term Project When Risk = $10^{-2.82}$

Objective	Well location	Pumping rate (m^3/day)	Cost ($1000)	Cost increase relative to realistic function (%)
Realistic	22	130	357	\
Fixed cap. +O&M	16 22	53 74	379	6.2
O&M	16 22	75 52	379	6.2
Total Q	15 22	27 100	379	6.2

The above analysis shows that for the risk levels in Fig. 8 where the costs from the realistic cost function are lower than the real costs obtained using the capital + O&M cost function and O&M cost functions, the optimal design strategies from both functions are similar. Where the real cost differences are significant, the realistic cost function found a cheaper treatment technology (modular carbon adsorbers-duel bed or modular carbon adsorbers-disposable) for those specific designs among the five potential technologies (recall that the simpler cost functions use only one pre-selected technology: modular carbon adsorbers-permanent). Because the treatment costs make up almost 2/3 of the total cost, a cheaper technology can save up to 14.5% of the treatment costs for short-term cleanups and 15.6% for long-term cleanups. These results indicate that allowing the treatment technology to be selected appropriately for different optimal treatment flow rates can sometimes substantially improve the optimal solution, especially for longer cleanups.

When the solutions found with the other cost functions were re-evaluated using the realistic function, some of the solutions were no longer optimal and were dominated by other solutions. The numbers of solutions dominated by other solutions after re-evaluation are shown in Table 5 for each objective.

Table 5. Numbers of Optimal Solutions on the Fronts

	Objective	Realistic	Capital+O&M	O&M	Total Q
30 years	No. of Solutions in Pareto Front	501	514	545	438
	No. of Solutions After Re-Evaluation	\	442	447	390
	Relative difference in No. of Solution (%)	\	14	18	11
10 Years	No. of Solutions in Pareto Front	743	570	553	459
	No. of Solutions After Re-Evaluation	\	514	480	453
	Relative difference in No. of Solution (%)	\	9.8	13	1.3

Table 5 indicates that more solutions were dominated for the long-term cleanup than the short-term cleanup for the same objective. The O&M cost function appears to find more solutions that were not optimal for this case, regardless of the cleanup length.

Generally speaking, the fixed capital cost + O&M cost function gave better solutions than the O&M cost function, but not consistently better. For some risk levels (from $10^{-3.59}$ to $10^{-4.15}$ for short-term cleanups and $10^{-4.7}$ to 10^{-7} for long–term cleanups, as shown in Fig. 12) the O&M cost actually gave better solutions than capital + O&M cost. Further study on other cases is needed to identify whether this finding is random or a true phenomenon. The total pumping rates function performed the worst for short-term cleanups, but was almost the same as fixed capital + O&M cost for a long-term project. However, as shown in Table 5, the total pumping rate function did not identify as many solutions on the Pareto front as the other functions did.

4. UMATILLA CASE STUDY

To verify the cost function complexity findings from the hypothetical case study, a similar approach was used at a field-scale application at Umatilla Army Depot in Oregon, which was a transport optimization demonstration site in a recently completed study (Minsker et al., 2003). Umatilla Chemical Depot, established in 1941, is a 19,728 acre military reservation used as an ordnance depot for storage and handling of munitions. From the 1950s to 1965, about 85 gallons of wash water were discharged into two unlined lagoons at the site. The two major contaminants were *2,4,6-tri-nitro toluene* (TNT) and *hexahydro-1,3,5-trinitro-1,3,5-triazine* (RDX), which are the targets for cleanup in this model. This site was placed on EPA's National Priorities List (NPL) in 1984 because of the soil and groundwater contamination.

We used existing simulation models created by a modeling team at the Army Corps of Engineers (USACE, 1996 & 2000). In these models, MODFLOW (Harbaugh and McDonald, 1996) and MT3DMS (Zheng and Wang, 1999) were used to predict the groundwater flow and contaminant transport. The entire site was divided into 5 model layers with 132 rows and 125 columns. The first layer is an alluvial aquifer and the last four layers are in a silt and weathered basalt unit. The hydraulic conductivity values were obtained from pumping tests and were divided into 17 zones. There is an existing pump-and-treat system to clean up this site that includes four extraction wells (only three of which are currently functioning) and three infiltration basins, as shown in Fig. 12 with the contaminant plumes.

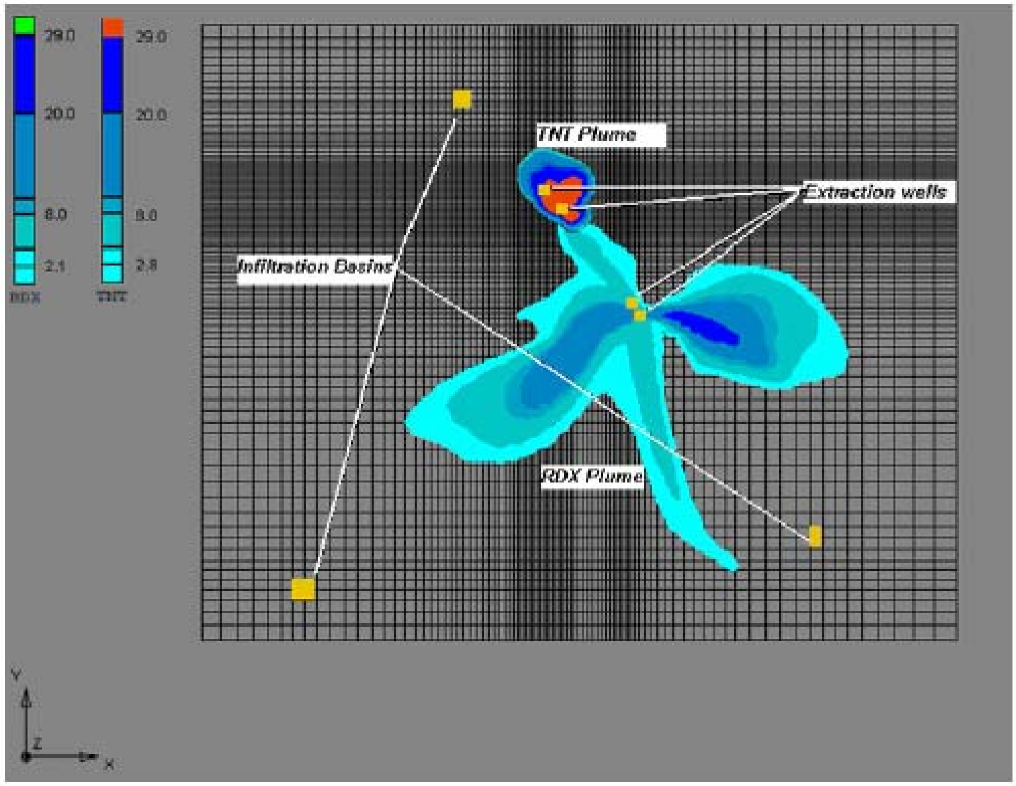


Fig. 13. Existing RDX and TNT plume at the site as of October 2000, along with the pumping wells and infiltration basins being used for cleanup

4.1 Optimization Formulation

A multi-objective optimization formulation was created for this site based on several single-objective formulations created previously (Minsker et al. 2003). For the new remediation design, a maximum of four new extraction wells and four infiltration basins could be installed. The treatment method is the same as the existing one: granular activated carbon (GAC). The total cleanup time was set to 5 years in this study. NSGA-II was then used to search for the optimal solutions to minimize the cleanup costs and maximize the total mass removal as follows:

$$\text{Min (Total Cost} = CCW + CCB + FCL + FCE + VCE + VCG + VCS) \quad (5)$$

$$\text{Min } (M_{RDX} + M_{TNT}) \quad (6)$$

where

CCW: Capital costs of new wells ($)

CCB: Capital costs of new recharge basins ($)

FCL: Fixed costs of labor ($)

FCE: Fixed costs of electricity ($)

VCE: Variable costs of electricity ($)

VCG: Variable Costs of Changing GAC Units ($)

VCS: Variable costs of sampling ($)

M_{RDX}: Total RDX mass remaining in model layer 1 that is over the water quality limit of 2.1 μg/l (kg)

M_{TNT}: Total TNT mass remaining in model layer 1 that is over the water quality limit of 2.8 μg/l (kg)

See Minsker et al. (2003) for more details on the cost functions and parameters used for each term in Equation 5.

4.2 Complexity of Cost Objective Function

To compare the performance of different cost functions, the original cost function shown in Equation 5 is treated as the most realistic function. In this case, however, the realistic function is equivalent to the Fixed Capital + O&M cost function considered for the hypothetical case, since the treatment technology is fixed. Therefore, the realistic function will be called "fixed capital + O&M cost" hereafter. The cost functions considered are then:

1. Fixed Capital + O&M cost (as shown in Equation 5)

2. O&M cost: TC = FCL + FCE + VCE + VCG + VCS

3. Total pumping rates

The optimal solutions found by different cost functions were re-evaluated by the fixed capital + O&M cost function and the results are shown in Fig. 13.

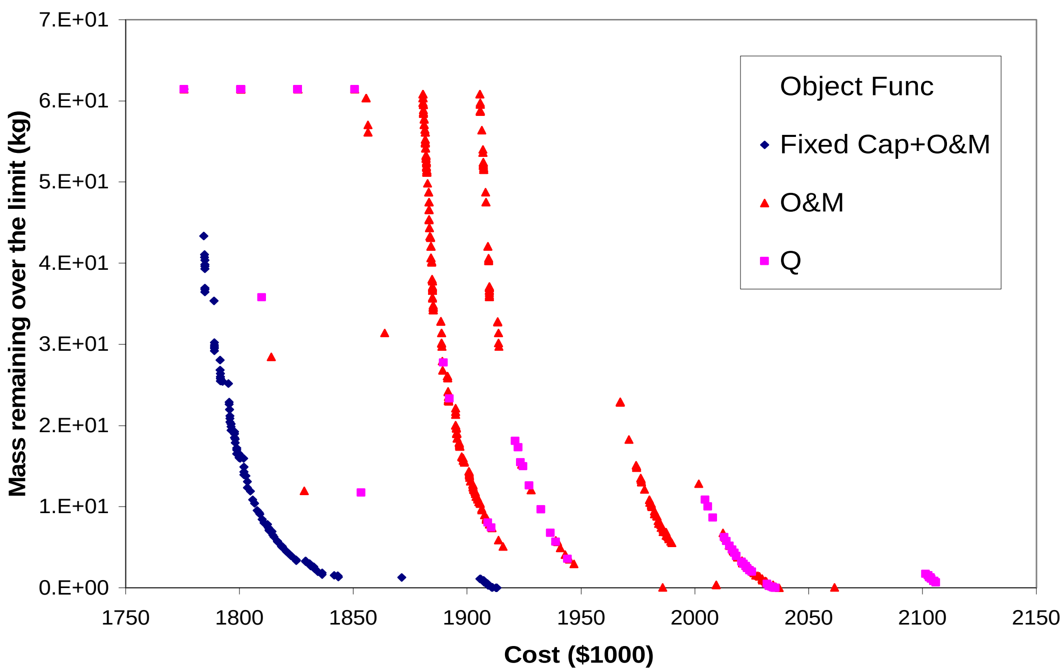


Fig. 14. Comparison of Pareto fronts from three cost functions, evaluated using fixed capital + O&M function

As previously, the most complex cost function (fixed capital + O&M cost) performs the best. The total pumping rates function performed somewhat worse than the O&M cost function. The differences between the re-evaluated costs and the optimal fixed capital + O&M costs at different mass remaining levels are shown in Fig. 15. In creating this figure, when the difference in mass remaining for two different designs was less than

0.05 kg, the mass remaining was assumed to be the same and the cost errors were calculated.

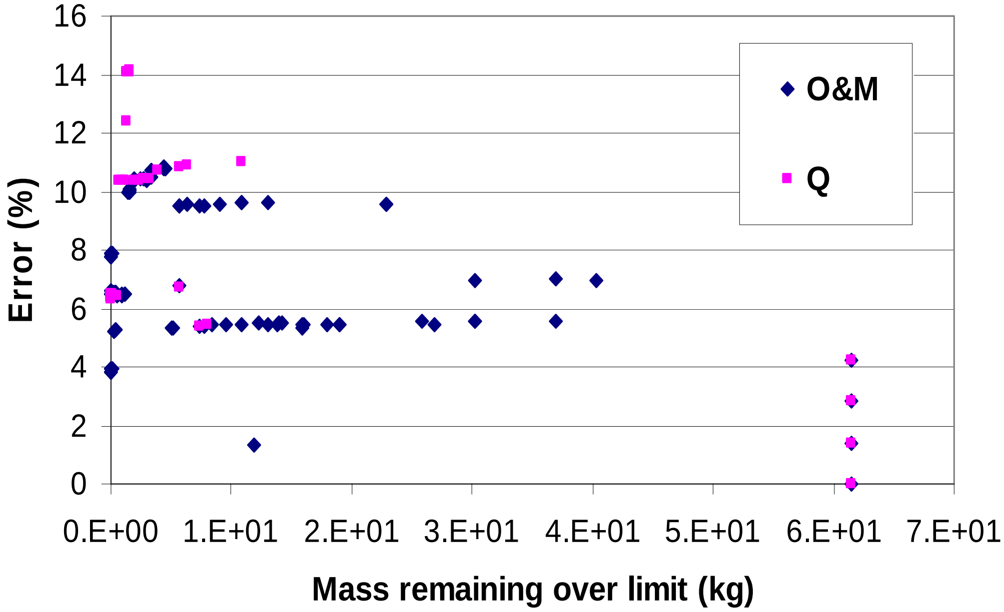


Fig. 15. Difference between the re-evaluated cost and the fixed capital + O&M cost at different levels of mass remaining

Consistent with Fig. 14, the differences are larger for the total pumping rates function than for O&M costs. The realistic cost function provided up to 11% savings over the O&M cost function and 14% savings over the total pumping rates function. The maximum difference for both simplified cost functions is observed when the mass remaining is close to 0, i.e., when the target contaminants are almost cleaned up. The design strategies representing the maximum error are compared in Table 6. We can see that fixed capital + O&M costs found the solution using only the existing wells while the solutions identified by the simplified cost functions both have new pumping wells installed that were not necessary.

Table 6. Design Strategies When Mass Remaining Over Limit = 1.5 kg

Objective Function	New extract well location	Pumping rates (m^3/day)	Existing extraction well pumping rates (m^3/day)	New injection basin location	Total pumping rates (m^3/day)	Re-evaluated cost ($1000)	Cost increased (%)
Fixed Cap + O&M	\	0	144 360 324	\	828	1842	/
O&M	18 24	252 180	252 90	10 25	774	2028	10
Total Q	2 17 18	90 90 180	252	6 31	612	2102	14

Also note in Fig. 15 that in one case, where the mass remaining is at its maximum value of 60 kg, both of the simplified cost functions found the same solutions as the fixed capital + O&M cost function. At this level of mass remaining, no pumping is implemented, similar to a natural attenuation solution, a case that results in zero treatment costs with any of the cost functions.

Note also that few comparable solutions are shown in Fig. 15 relative to the numbers shown in Fig. 14. This occurred because many solutions identified by the different cost functions do not achieve the same mass remaining level and hence cannot be compared. Also note that after re-evaluation, most solutions found with the simplified cost functions (about 92% of the solutions found with O&M cost and 63% of those found with total pumping rates function) were dominated by only a few on the re-evaluated Pareto front (see Fig. 14). This same phenomenon was observed in the hypothetical test case, but for that case, the dominated solutions represented a much smaller number relative to the whole non-dominated set (up to 18%). The lower percentage of dominated solutions for total pumping rates occurred because the total pumping rates function found fewer solutions on the Pareto front (only 49 solutions, of which only 18 were identified as optimal with the fixed capital + O&M function).

The reason that so many solutions were dominated after re-evaluation in this case is twofold. First, neither of the simplified functions adequately considered optimal solutions with injection basins, which have no O&M cost and are not included in the total pumping rates. Tables 7 and 8 show examples of this phenomenon for the O&M cost and total pumping rates functions, respectively. Table 7 shows two “optimal” design strategies identified with the O&M cost function. These two strategies are almost identical except that strategy 1 has only one injection basin while strategy 2 has two. When they were re-evaluated by the fixed capital + O&M cost function, strategy 2 was dominated by strategy 1, but this difference cannot be distinguished with the O&M cost function that does not include injection basins. Table 8 shows that the same phenomenon happened with the total pumping rates function.

The second reason that some solutions were dominated after re-evaluation is that some designs with the same mass remaining have the same total pumping rates but the distribution of pumping rates are not the same. An example is shown in Table 9. These designs are identified as the same with the total pumping rates function, but will actually cost different amounts because there is only one existing extraction well operating in strategy 1 but there are two existing extraction wells in strategy 2. This complexity cannot be captured with the total pumping rates function.

Table 7. Design Strategies identified by O&M Cost Function When Mass Remaining Over the Limit = 0.33 kg

Design Strategies	New extract well location	Pumping rates (m^3/day)	Existing extraction well pumping rates (m^3/day)	New injection basin location	Total pumping rates (m^3/day)	Re-evaluated cost ($1000)
1	16 32	360 180	360	17	900	200.9
2	16 32	360 180	360	25 27	900	203.4

Table 8. Design Strategies identified by Total Pumping Rates Function When Mass Remaining Over the Limit = 61.4 kg

Design Strategies	New extract well location	Pumping rates (m^3/day)	Existing extraction well pumping rates (m^3/day)	New injection basin location	Total pumping rates (m^3/day)	Re-evaluated cost ($1000)
1	\	0	0	26 31	0	185.065
2	\	0	0	\	0	177.565

Table 9. Design Strategies identified by Total Pumping Rates Function When Mass Remaining Over the Limit = 0

Design Strategies	New extract well location	Pumping rates (m^3/day)	Existing extraction well pumping rates (m^3/day)	New injection basin location	Total pumping rates (m^3/day)	Re-evaluated cost ($1000)
1	17 51	360 180	360	17 31	900	203.512
2	17 51	324 144	288 144	17 31	900	203.530

5. CONCLUSIONS

In this thesis, we have examined several issues regarding objective function formulation and visualization of multi-objective results. We presented a new approach to illustrate the tradeoffs among three objectives that allows easy visualization of all of the relationships among the objectives. Applying this approach to a hypothetical case study identified that for a high risk level, short-term remediation is most cost effective, but for lower risk criteria a longer-term remediation is most cost-effective. These results indicate that evaluating the full set of tradeoffs among these three objectives can be important to ensuring informed remediation decision making.

We have then compared the performance of different cost functions using two case studies. Our findings show that the results are more accurate for more complex cost functions, but the degree of loss in accuracy varies substantially for the two case studies considered in this work and for different parameter settings within each case study (such as cleanup length, risk level, or mass remaining).

For the hypothetical case study, the realistic cost function found better solutions than the simplified ones, especially for short-term cleanups. Total pumping rates performed the worst for both cleanup durations studied. If the ex-situ treatment technology has already been set, the fixed capital cost + O&M cost function performed almost as well as the realistic one for the entire range of risks for a long-term remediation project. The O&M cost function could also be used at some risk levels. For a short term project, if the target risk is set at a low risk level, the simplified cost function may do as well as the realistic one. However, if the optimal tradeoffs are desired at all cleanup durations and risk levels, or the treatment technology needs to be selected, the realistic function appears to improve performance, with as much as 14% improvement in the total cost of the solutions found and 16% improvement in the treatment costs of the solutions found.

For the Umatilla case, the fixed capital + O&M cost function (which in this case is the realistic cost function) performs the best, with as much as 11% improvement relative to the O&M cost function and 14% improvement relative to the total pumping rates function. In this case, the simplified cost functions were not able to capture important features that were needed for identifying the correct Pareto front, including the facts that injection basins had no O&M costs and O&M costs will vary depending on the distribution of pumping rates among the wells.

Overall, realistic cost functions are able to identify more and better solutions than simplified cost functions. In some circumstances, simplified cost functions can be substituted for the realistic cost function with only minor effects on the results, but it would be difficult to predict a priori when the substitution would result in minimal errors. Given that the optimal solutions found with the simplified cost functions were as much as 14% more costly, which can be a substantial amount at complex sites, the time and effort required to develop cost functions that realistically reflect the actual remediation costs appears to be worthwhile.

REFERENCES

Aly, A. and Peralta, R.C. (1999). “Optimal design of aquifer cleanup systems under uncertainty using a neural network and a genetic algorithm.” *Water Resources Research*, 35(8), 2523-2532.

Andricevic, R., and Kitanidis, P.K. (1990). “Optimization of the pumping schedule in aquifer remediation under uncertainty.” *Water Resources Research, 26*(5), 875-885.

Babbar, M. (2002). “Multiscale parallel genetic algorithms for optimal groundwater remediation design.” Master Thesis, University of Illinois.

Beckford, O.M and Chan Hilton, A.B. (2002). “Development of multiobjective robust genetic algorithm for groundwater remediation design under uncertainty.” 2002 Conference on Water Resources Planning and Management, May 19-22.

Chan, N. (1994). “Partial infeasibility method of chance constrained aquifer management.” *Journal of Water Resources Planning and Management*, 120(1), 70-89.

Cieniawski, S.E., Eheart J. W., and Ranjithan S. (1995). “Using genetic algorithms to solve a multiobjective groundwater monitoring problem.” *Water Resources Research*, 31(2), 399-409.

Clement, T. P. (1997). “RT3D - A modular computer code for simulating reactive multi-species transport in 3-Dimensional groundwater aquifers.” *Battelle Pacific Northwest National Laboratory Research Report*, PNNL-SA-28967. (http://bioprocesses.pnl.gov/rt3d.htm.)

Clement, T. P, Sun, Y., Hooker, B. S., and Petersen, J. N. (1998). “Modeling multi-species reactive transport in groundwater.” *Ground Water Monitoring and Remediation*, 18(2), 79-92.

Coello, C.A. (1999). “A comprehensive survey of evolutionary-based multiobjective optimization techniques.” *Knowledge Information System*, 1(3), 269-308.

Culver, T.B., and Shenk, G.W. (1998). “Dynamic optimal groundwater remediation by granular activated carbon.” *Journal of Water Resources Planning and Management*, 124(1), 59-64.

Culver, T.B., and Shoemaker, C.A. (1992). “Dynamic optimal control for groundwater remediation with flexible management periods.” *Water Resources Research*, 28(3), 629-641.

Culver, T.B., and Shoemaker, C.A. (1997). "Dynamic optimal groundwater reclamation with treatment capital costs." *Journal of Water Resources Planning and Management,* 123(1), 23-29.

Deb, K., Agrawal, S., Pratap, A. and Meyarivan, T. (2000). "A fast elitist non-Dominated sorting genetic algorithm for multi-objective optimization: NSGA-II." Kanpur Genetic Algorithm Laboratory (KanGAL) Report 200001, Indian Institute of Technology, Kanpur, India.

Deb, K., Thiele, L., Laumanns, M. and Zitzler, E. (2001). "Scalable test problems for evolutionary multi-objective optimization." Computer Engineering and Networks laboratory Report (TIK-112), Department of Electrical Engineering, Swiss Federal Institute of Technology, Zurich, Switzerland.

Deb, K. (2001). "Multi-objective optimization using evolutionary algorithms." *John Wiley & Sons, Ltd.*

Erickson, M., Mayer, A. and Horn, J. (2002). "Multi-objective optimal design of groundwater remediation systems: application of the niched Pareto genetic algorithm (NPGA)." *Advances in Water Resources,* 25 (2002), 51–65.

Geoffrion, A.M., Dyer, J.S. and Feinberg, A. (1972). "An interactive approach for multi-criterion optimization with an application to the operation of an academic department." *Management Science*, 19(4), 357-368.

Gopalakrishnan, G., Minsker, B., and Goldberg D.E. (2003). "Optimal sampling in a noisy genetic algorithm for risk-based remediation design." *Journal of Hydroinformatics*, 05.1, 11-25.

Gorelick, S.M., Voss, C.I, Gill, P.E. (1984). "Murray, W., Saunders, M.A., and Wright, M.H, Aquifer reclamation design: The use of contaminant transport simulation combined with nonlinear programming." *Water Resources Research*, 20(4), 415-427.

Graham, W.D., and McLaughlin, D.B. (1991). "A Stochastic model of solute transport in groundwater: Application to the Borden, Ontario, tracer test." *Water Resources Research*, 27(6), 1345-1359.

Harbaugh, A.W., and McDonald, M.G. (1996). "User's documentation for MODFLOW-96, an update to the U.S. geological survey modular finite-difference ground-water flow model, U.S. Geological Survey Open-File Report 96-485.

Hsiao, C.-T., and Chang, L.-C. (2002). "Dynamic optimal groundwater management with inclusion of fixed costs." *Journal of Water Resources Planning and Management,* 128(1), 57-65.

Huang, C., and Mayer, A.S. (1997). “Pump-and-treat optimization using well locations and pumping rates as decision variables.” *Water Resources Research*, 33(4), 1001-1012.

Karatzas, G.P., and Pinder, G.F. (1996). “The solution of groundwater quality management problems with a nonconvex feasible region using a cutting plane optimization technique.” *Water Resources Research*, 32(4), 1091-1100.

Kwanyuen, B. and Fontane, D.G. (1998). “Heuristic branch-and-bound method for ground water development planning**.”** *Journal of Water Resources Planning and Management*, 124(3), 140-148.

Johnson V.M. and Rogers, L.L. (2000) “Accuracy of neural network spproximators in simulation-optimization.” *Journal of Water Resources Planning and Management*, 126(2), 48-56.

Lee, S.I., and Kitanidis, P.K. (1991). “Optimal estimation and scheduling in aquifer remediation with incomplete information.” *Water Resources Research*, 27(9), 2203-2217.

Marryot, R.A., Dougherty, D.E., and Stoller, R.L. (1993). “Optimal groundwater management. II: Application of simulated annealing to a field-scale contamination site.” *Water Resources Research*, 29(4), 847-860.

Mackay, D. M., Freyberg, D. L., Roberts, P. V. and Cherry, J. A. (1986). “A natural gradient experiment on solute transport in a sand aquifer; 1. Approach and overview of plume movement.” *Water Resources Research*, 22(13), 2017-2029.

Maskey, S., Jonoski, A., and Solomatine, D.P. (2002). “Groundwater remediation strategy using global optimization algorithms.” *Journal of Water Resources Planning and Management*, 128(6), 431-440.

McDonald, M.G., and Harbaugh, A.W. (1988). “A modular three-dimensional finite-difference ground-water flow model.” *Techniques of Water Resources Investigations 06-A1, United States Geological Survey*.

McKinney, D. C., and Lin, M. D. (1995). ‘‘Approximate mixed-integer nonlinear programming methods for optimal aquifer remediation design.’’ *Water Resources Research*, 31(3), 731–740.

McKinney, D.C., and Lin, M. (1996). “Pump-and-treat ground-water remediation system optimization.” *Journal of Water Resources Planning and Management*, 122(2), 128-136.

Medina, M.A.Jr. (2002). “Integration of parameter estimation, optimization and transport for remedial strategies.” 2002 Conference on Water Resources Planning and Management, May 19-22.

Minsker, B.S., and Shoemaker, C.A. (1998). “Dynamic optimal control of in situ bioremediation of groundwater.” *Journal of Water Resources Planning and Management,* 124(3), 149-161.

Minsker, B., Y. Zhang, R. Greenwald, R. Peralta, C. Zheng, K. Harre, D. Becker, L. Yeh, and K.Yager (2003). *Final Technical Report for Application of Flow and Transport Optimization Codes to Groundwater Pump and Treat Systems*, Environmental Security Technology Certification Program. Available at http://www.frtr.gov/estcp/.

Misirli, F., and Yazicigil, H. (1997). “Optimal ground-water pollution plume containment with fixed charges.” *Journal of Water Resources Planning and Management*, 123(1), 2-14.

Reed, P., Minsker, B. S., and Goldberg, D. E. (2000). “Designing a competent simple genetic algorithm for search and optimization.” *Water Resources Research,* 36(12), 3757-3761.

Reed, P., Minsker, B. S., and Goldberg, D. E. (2001) “A multiobjective approach to cost effective long-term groundwater monitoring using an elitist nondominated sorted genetic algorithm with historical data.” *Journal of Hydroinformatics*, 3(2), 71-89.

Reed, P. and Minsker, B.S. (2003). “Striking the balance: long-term groundwater monitoring design for multiple conflicting objectives.” *Journal of Water Resources and Planning Management,* in press.

Ritzel, B.J., Eheart, J.W., and Ranjithan, S. (1994). “Using genetic algorithms to solve a multiple objective groundwater pollution containment problem.” *Water Resources Research,* 30(5), 1589-1603.

Rizzo, D.M. and Dougherty D.E. (1996). “Design optimization for multiple management period groundwater remediation” *Water Resources Research*, 32(8), 2549-2561.

Sawyer, C.S., Ahlfeld, D.P., and King, A.J. (1995). “Groundwater remediation design using a threedimensional simulation model and mixed integer programming.” *Water Resources Research,* 31(5), 1373-1385.

Smalley, J. B., Minsker B. S., and Goldberg, D. E. (2000). “Risk-based In Situ bioremeditation design using a noisy genetic algorithm.” *Water Resources Research,* 36(20), 3043-3052.

Sun, Y.-H., Davert, M.W., and Yeh, W.W.-G. (1996). “Soil vapor extraction system design by combinatorial optimization.” *Water Resources Research,* 32(6), 1863-1873.

Tiedeman, C., and Gorelick, S.M. (1993). “Analysis of uncertainty in optimal groundwater containment capture design.” *Water Resources Research,* 29(7), 2139-2153.

U.S. Army Corps of Engineering (USACE). (1996). “Final remedial design submittal, contaminated groundwater remediation, explosives washout lagoons”, Umatilla Depot Activity, Hermiston, OR.

U.S. Army Corps of Engineering (USACE). (2000). “Explosives washout lagoons groundwater model revision (preliminary draft)”, Umatilla Chemical Depot, Hermiston, OR.

Van Veldhuizen, D.A., and Lamont, G.B. (2000). “Multiobjective evolutionary algorithms: analyzing the state-of-the-art.” *Evolutionary Computation*, 8(2), 125-147.

Vieux, M.A. (1999). “Developing an objective and cost equation for Ex Situ treatment echnologies.” Special Project, Department of Civil and Environmental Engineering, University of Illinois at Urbana-Champaign.

Wagner, B.J., and Gorelick, S.M. (1987). “Optimal groundwater remediation with well location as a decision variable.” *Water Resources Research*, 23(7), 1162-1174.

Yoon, J.H. and Shoemaker, C.A. (1999). “Comparison of optimization methods for ground-water bioremediation.” *Journal of Water Resources Planning and Management*, 125(1), 54-63.

Zhen, C., and Uber, J.G. (1996). “Reliability of remediation designs in presence of modeling error.” *Journal of Water Resources Planning and Management*, 122(4), 253-261.

Zheng, C. and Wang, P.P. (1999). “MT3DMS: Documentation and User’s Guide”. Report to the US Army Corps of Engineers Waterways Experiment Station. (available at http://hydro.geo.ua.edu).

Zheng, C. and Wang, P.P. (2003). “Application of flow and transport optimization codes to groundwater pump-and-Treat systems: Umatilla Army Depot, Oregon.” Environmental Security Technology Certification Program, draft 2003.

APPENDIX A. DEVELOPMENT OF REMEDIAL SYSTEM COSTS, C_{SYST}

This appendix is focusing on the development of the remediation system cost: C_{SYST}. C_{SYST} is the total cost for the remedial system, which in this case is an ex situ groundwater treatment system. The detailed equation for C_{SYST} is as follows (based on *Vieux* (1999)):

$$C_{SYST} = C_{j,k}^{cap} X_i + C^{cap,POTW} X_i + (C_{j,k}^{op} + C^{ana} g + C^{op,POTW}) * (P \mid A, i, t_{total}) \quad \text{(A-1)}$$

where

$C_{j,k}^{cap}$: Capital cost for technology j of contaminant class k, where the classes are VOC, SVOC, fuel, ordnance or metal (in this case, the contaminant class is SVOC) associated with total pumping rate ($)

$C_{j,k}^{op}$: Annual O&M cost for technology j of contaminant class k ($/year)

$C^{cap,POTW}$: Capital cost for disposing of treated groundwater to POTW (publicly-owned treatment works) associated with total pumping rate ($)

$C^{op,POTW}$: Annual O&M cost of disposing treated groundwater to POTW ($/year)

C^{ana} : Unit cost of collecting, testing and analyzing groundwater and off-gas samples for technology j of contaminant class k ($/sample)

NW : Number of remediation wells

g : Number of groundwater and off-gas samples per year

$(P \mid A, i, t_{total})$: Financial factor for converting a series of O&M costs (A) to a present value (P) at given interest rate i

X_i : Indicator variables for well installation: $X_i = 1$ if well i is installed, otherwise $X_i = 0$

Five contaminant classes were taken into consideration: Volatile Organic Compounds (VOC), Semi-Volatile Organic Compounds (SVOC), fuels, ordnance and metal. *Vieux* (1999) showed that carbon adsorption using granular activated carbon (GAC) and air stripping are the least cost technologies for all applicable contaminant classes except metals. Both technologies have different configurations, given in Table 1. Applicable technologies for metals are coagulation/flocculation and media filtration. The technology configurations considered for each contaminant class and range of influent flow rates (which would be the sum of the pumping rates at all wells operating during the remediation) are listed in Table 10.

All of the cost data for these technologies were obtained from Remedial Action Cost Engineering and Requirement 2001(RACER 2001), a parametric modeling system. The cost database RACER uses is a duplicate of the ECHOS (Environmental Cost Handling Options and Solutions) database that was developed by Talisman Partners, Ltd. and R.S. Means Company. The cost given by RACER includes material, equipment and labor costs.

Table 10. Applicable Technologies for Contaminant Classes and Pumping Rate Ranges

	Contaminant classes					Influent flow	
	VOC	SVOC	Fuels	Ordnance	Metal	(gpm)	(m^3/d)
Air Stripper Packed Tower	X	X	X			0 ~ 750	0 ~ 4088
Air Stripper Low Profile Tray	X	X	X			10 ~ 2250	55~ 12264
Modular Carbon Adsorbers, Duel Bed – Single Pass	X	X	X	X		0 ~ 2000	0 ~ 10901
Modular Carbon Adsorbers, Permanent - Single Pass Redundancy	X	X	X	X		0 ~ 200	0 ~ 1090
Modular Carbon Adsorbers, Disposable - Single Pass Redundancy	X	X	X	X		0 ~ 200	0 ~ 1090
Modular Carbon Adsorbers, Duel Bed – 2 in series	X	X	X	X		0 ~ 2000	0 ~ 10901
Modular Carbon Adsorbers, Permanent - 2 in series	X	X	X	X		0 ~ 200	0 ~ 1090
Modular Carbon Adsorbers, Disposable - 2 in series	X	X	X	X		0 ~ 200	0 ~ 1090
Coagulation/ Flocculation					X	0 ~ 1645	0 ~ 8965
Media Filtration					X	0 ~ 250	0 ~ 1362

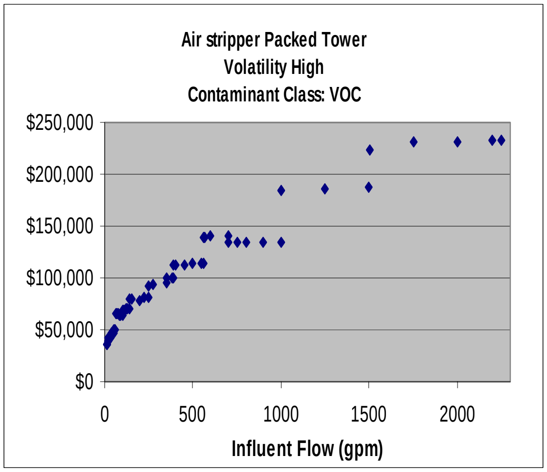
To estimate the cost terms in Equation A-1 from RACER, a number of required and secondary parameters had to be set for each technology. The primary parameters differ with different technologies, but for all technologies, influent flow and safety level are both required. The safety level, which refers to four different levels, A, B, C and D are defined by OSHA regulations, specifically CFR Part 1910. Each level identifies a certain amount and type of Personal Protective Equipment (PPE) required for on-site workers. Different safety levels have different capital and O&M costs. Safety level D, the least protective one, which includes disposable latex gloves and coveralls as part of the O&M costs, was assumed for all contaminant classes and all technologies to maintain simplicity and consistency. Higher levels include the costs of latex gloves, overalls and respirator cartridges. The influent flow rate, measured in gallons per minute (gpm) determines the capacity of the system and the required maintenance level. Other required parameters include volatility of the contaminant and removal percentage for Air Stripper and the total organic carbon (TOC) concentration for Carbon Adsorption. The volatility of VOC was assumed to be high, while Fuels and SVOC were assumed to be moderately high. Removal percentage was assumed to be 99% for all contaminant classes. TOC concentration was set to be 5 ppm.

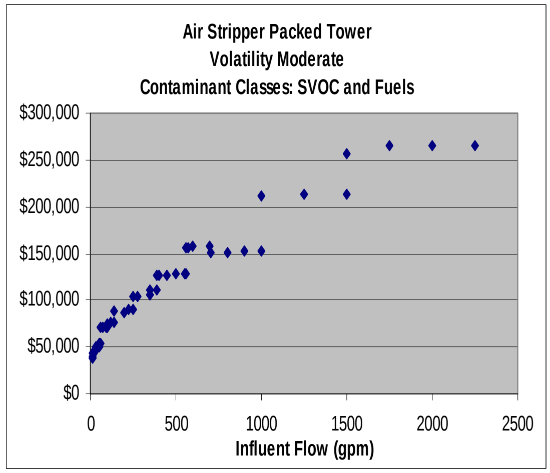
Secondary parameters, which are automatically calculated by RACER based on the primary parameters, generally specify the size of the system. For all technologies, a default electricity cost of $0.07 per kilowatts-hours (KWH) is applied by RACER 2001. The influent flow rate (equal to total pumping rates in this case) is assumed to be constant over time and the treatment facility is assumed to operate 97% of the time during any given year.

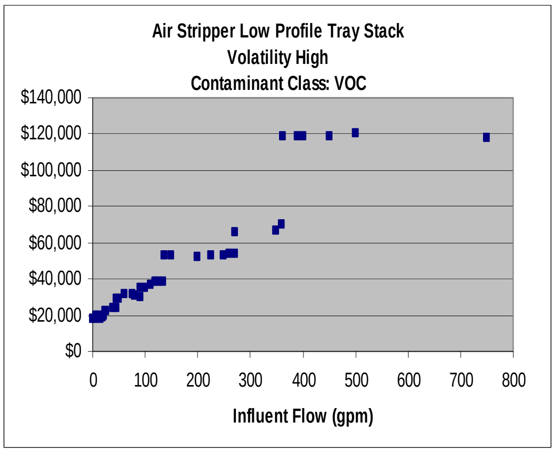
After treatment, the groundwater was assumed to discharge to a POTW (publicly-owned treatment works), which was assumed to be located off-site and the distance to the sewer connection was assumed to be 50 feet. Some other default parameters include: the connection fee is $1000, the wastewater disposal fee is $2 per thousand gallons, the discharge operates 20 hours per day, and the flow rate is equal to the treatment influent flow rate.

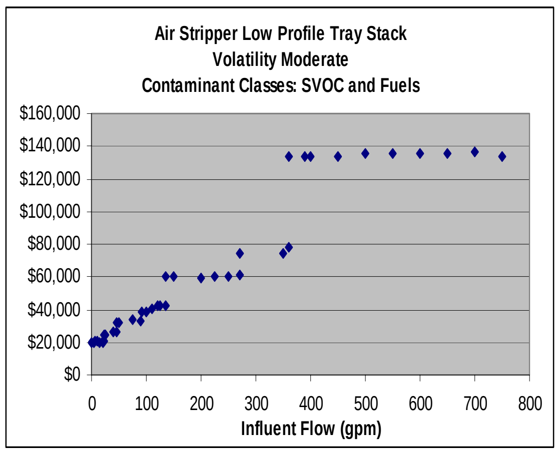
A range of influent flow rates were used to obtain a cost data set for developing cost functions of capital and annual O&M costs. Capital costs (shown in Fig. 16) were obtained directly from RACER 2001. To get the annual O&M cost (shown in Fig. 17), the variable O&M costs over a 15-year remediation period were obtained from RACER 2001 and then annualized.

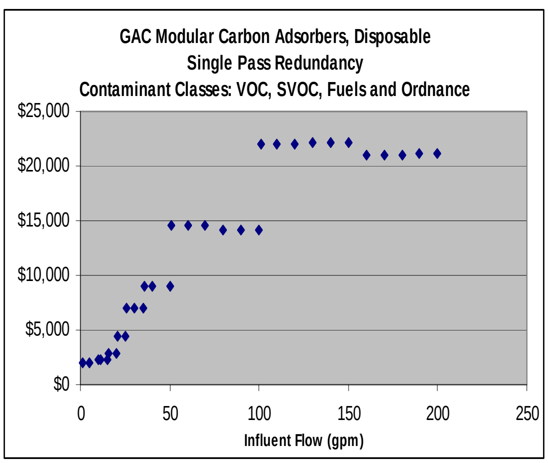
Fig. 16 indicates that capital costs for most technologies are constant within certain flow ranges for all contaminant classes. The discontinuity in capital costs reflects the fact that a given size treatment facility can handle a range of influent flows for a fixed cost. For coagulation/flocculation and media filtration, the relationships fit better to a quadratic function. Capital costs for different influent flow ranges, technologies, and contaminant classes are detailed in Table 11. In contrast, the annual O&M costs, as in Fig. 17, showed a linear relationship within different flow ranges, except for coagulation/flocculation and media filtration, which showed a quadratic relationship. All of the O&M cost equations for different technologies and contaminant classes are listed in Table 12.

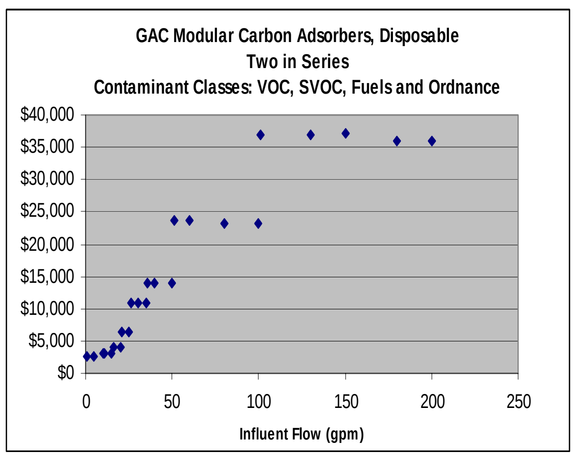












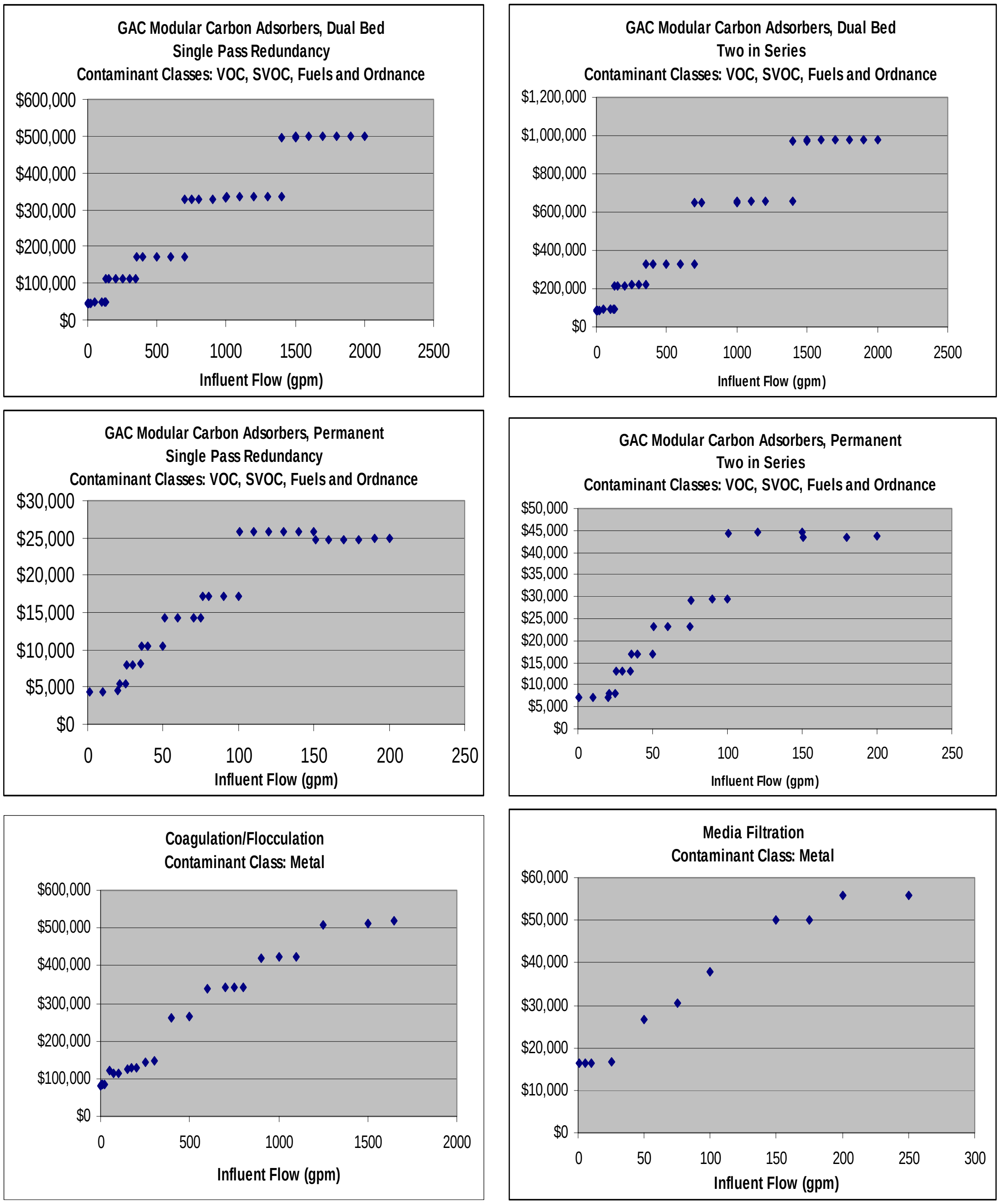
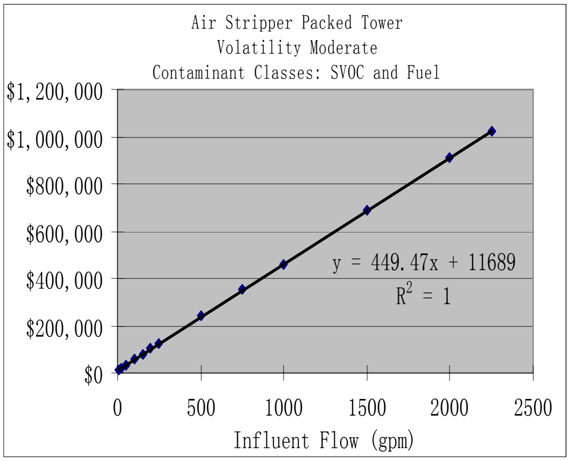
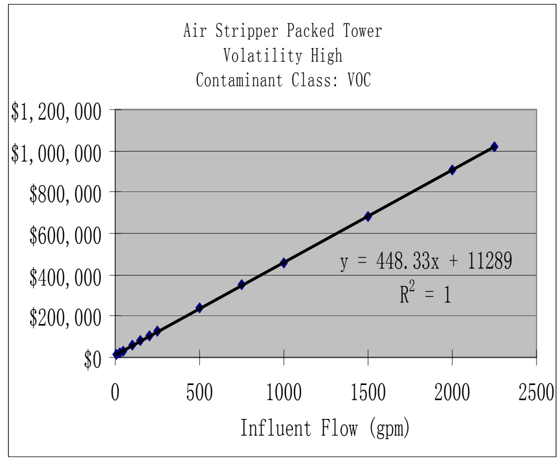
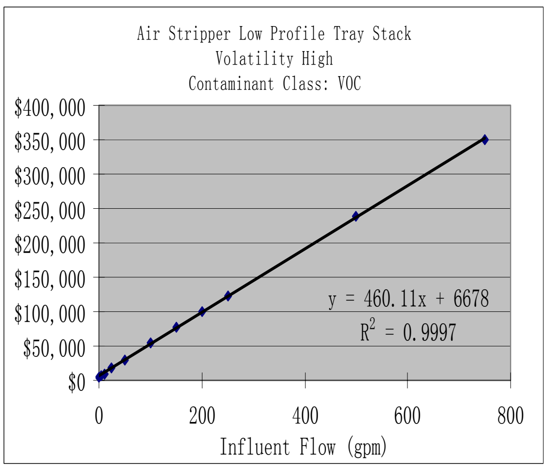
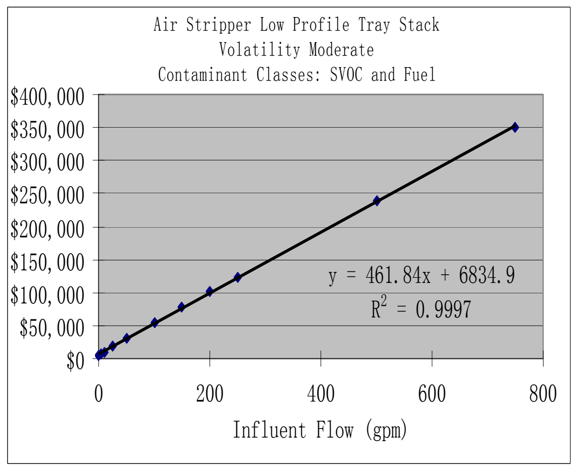


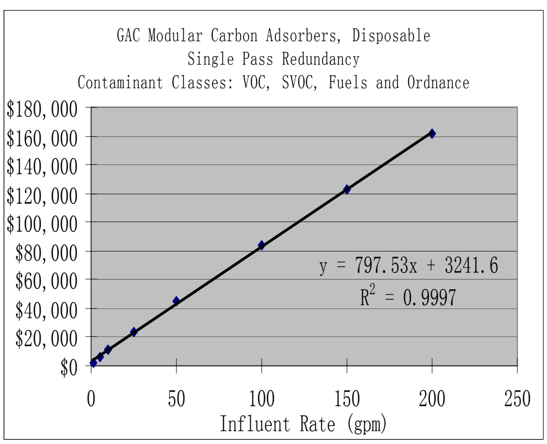
Fig. 16. Capital costs versus influent flow rate for different contaminant classes with different technologies

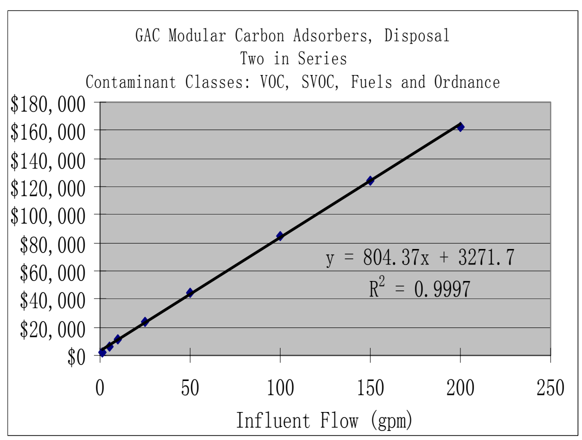

Air Stripper Packed Tower
Volatility Moderate
Contaminant Classes: SVOC and Fuel
$1,200,000
$1,000,000
$800,000
$600,000
$400,000
$200,000
$0
0
500
1000
1500
2000
2500
Influent Flow (gpm)
y = 449.47x + 11689
R2 = 1


Air Stripper Packed Tower
Volatility High
Contaminant Class: VOC
$1,200,000
$1,000,000
$800,000
$600,000
$400,000
$200,000
$0
0
500
1000
1500
2000
2500
Influent Flow (gpm)
y = 448.33x + 11289
R2 = 1


Air Stripper Low Profile Tray Stack
Volatility High
Contaminant Class: VOC
$400,000
$350,000
$300,000
$250,000
$200,000
$150,000
$100,000
$50,000
$0
0
200
400
600
800
Influent Flow (gpm)
y = 460.11x + 6678
R2 = 0.9997


Air Stripper Low Profile Tray Stack
Volatility Moderate
Contaminant Classes: SVOC and Fuel
$400,000
$350,000
$300,000
$250,000
$200,000
$150,000
$100,000
$50,000
$0
0
200
400
600
800
Influent Flow (gpm)
y = 461.84x + 6834.9
R2 = 0.9997


GAC Modular Carbon Adsorbers, Disposable
Single Pass Redundancy
Contaminant Classes: VOC, SVOC, Fuels and Ordnance
$180,000
$160,000
$140,000
$120,000
$100,000
$80,000
$60,000
$40,000
$20,000
$0
0
50
100
150
200
250
Influent Rate (gpm)
y = 797.53x + 3241.6
R2 = 0.9997


GAC Modular Carbon Adsorbers, Disposal
Two in Series
Contaminant Classes: VOC, SVOC, Fuels and Ordnance
$180,000
$160,000
$140,000
$120,000
$100,000
$80,000
$60,000
$40,000
$20,000
$0
0
50
100
150
200
250
Influent Flow (gpm)
y = 804.37x + 3271.7
R2 = 0.9997

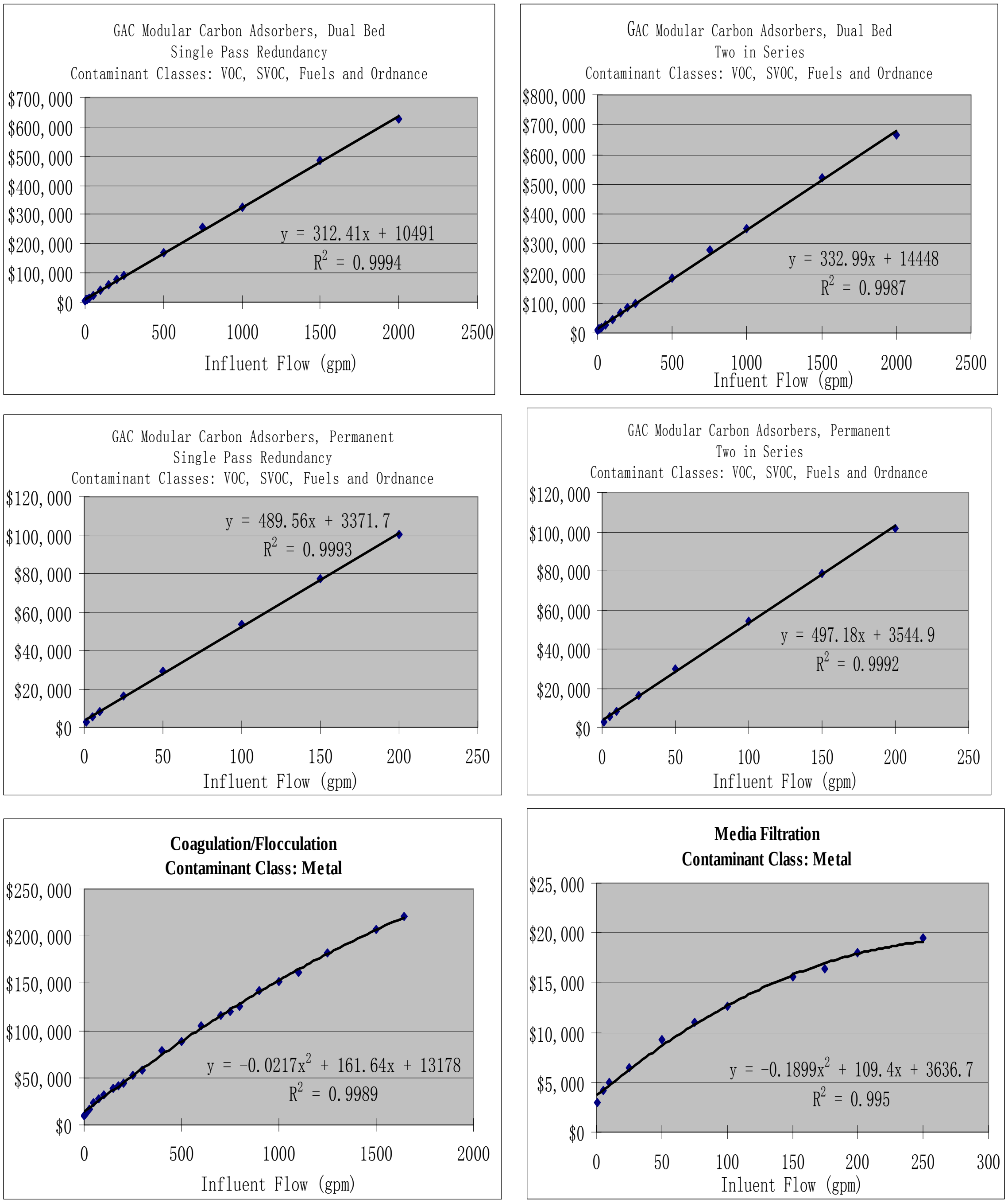


Fig. 17. Annual O&M costs versus influent flow rate for different contaminant classes with different technologies

Table 11. Equations for $C_{j,k}^{cap}$

Contaminant Class and Technology Configuration	Flow Range (gpm)	$C_{j\,k}^{cap}$ ($)
VOCs		
Air Stripper Packed Tower - Volatility high	10 to 20 21 to 35 36 to 50 51 to 60 61 to 100 101 to 140 141 to 250 251 to 350 351 to 390 391 to 560 561 to 700 701 to 1000 1001 to 1500 1501 to 2250	37460 42160 46687 49715 64881 69183 79995 93512 100711 113884 139345 134532 185802 229897
Air Stripper Low Profile Tray Stack – Volatility high	less than 20 20 to 45 46 to 90 91 to 135 136 to 270 271 to 360 361 to 750	19760 23343 30341 36981 52874 67393 118713
Modular Carbon Adsorbers, Dual Bed - Single Pass Redundancy	Less than 130 131 to 350 351 to 700 701 to 1000 1001 to 1400 1401 to 2000	46552 112662 171384 329230 336039 499185
Modular Carbon Adsorbers, Permanent - Single Pass Redundancy	less than 20 21 to 25 26 to 35 36 to 50 51 to 75 76 to 100 101 to 150 151 to 200	4340 5360 8022 10482 14321 17162 25831 24821

Modular Carbon Adsorbers, Disposable - Single Pass Redundancy	less than 5 6 to 15 16 to 20 21 to 25 26 to 35 36 to 50 51 to 100 101 to 200	2051 2303 2888 4486 6946 8952 14374 21606
Modular Carbon Adsorbers, Dual Bed – 2 in series	Less than 100 101 to 130 131 to 350 351 to 700 701 to 1000 1001 to 1400 1401 to 2000	88212 92653 217844 330743 647906 654576 977260
Modular Carbon Adsorbers, Permanent - 2 in series	less than 20 21 to 25 26 to 35 36 to 50 51 to 75 76 to 100 101 to 150 151 to 200	7165 8179 12985 17011 23150 29339 44550 43552
Modular Carbon Adsorbers, Disposable - 2 in series	less than 5 6 to 15 16 to 20 21 to 25 26 to 35 36 to 50 51 to 100 101 to 200	2634 3114 4129 6431 10833 13952 23503 36629

Contaminant Class and Technology Configuration	Flow Range (gpm)	$C_{j\,k}^{cap}$ ($)
SVOCs and Fuels		
Air Stripper Packed Tower - Volatility moderate	10 to 15	39177
	16 to 20	43271
	21 to 35	45549
	36 to 50	50229
	51 to 60	53257
	61 to 100	71162
	101 to 140	75840
	141 to 250	88982
	251 to 350	104340
	351 to 390	111539
	391 to 560	126862
	561 to 700	156505
	701 to 1000	151728
	1001 to 1500	213064
	1501 to 2250	262994
Air Stripper Low Profile Tray Stack - Volatility moderate	less than 22	20039
	23 to 45	25111
	46 to 90	32499
	91 to 135	40546
	136 to 270	60238
	271 to 360	75524
	361 to 750	134675
Modular Carbon Adsorbers, Dual Bed - Single Pass Redundancy	Less than 130	46552
	131 to 350	112662
	351 to 700	171384
	701 to 1000	329230
	1001 to 1400	336039
	1401 to 2000	499185
Modular Carbon Adsorbers, Permanent - Single Pass Redundancy	less than 20	4340
	21 to 25	5360
	26 to 35	8022
	36 to 50	10482
	51 to 75	14321
	76 to 100	17162
	101 to 150	25831
	151 to 200	24821

Modular Carbon Adsorbers, Disposable - Single Pass Redundancy	less than 5 6 to 15 16 to 20 21 to 25 26 to 35 36 to 50 51 to 100 101 to 200	2051 2303 2888 4486 6946 8952 14374 21606
Modular Carbon Adsorbers, Dual Bed – 2 in series	Less than 100 101 to 130 131 to 350 351 to 700 701 to 1000 1001 to 1400 1401 to 2000	88212 92653 217844 330743 647906 654576 977260
Modular Carbon Adsorbers, Permanent - 2 in series	less than 20 21 to 25 26 to 35 36 to 50 51 to 75 76 to 100 101 to 150 151 to 200	7165 8179 12985 17011 23150 29339 44550 43552
Modular Carbon Adsorbers, Disposable - 2 in series	less than 5 6 to 15 16 to 20 21 to 25 26 to 35 36 to 50 51 to 100 101 to 200	2634 3114 4129 6431 10833 13952 23503 36629
Ordnance		
Modular Carbon Adsorbers, Dual Bed - Single Pass Redundancy	Less than 130 131 to 350 351 to 700 701 to 1000 1001 to 1400 1401 to 2000	46552 112662 171384 329230 336039 499185
Modular Carbon Adsorbers, Permanent - Single Pass Redundancy	less than 20 21 to 25 26 to 35 36 to 50 51 to 75 76 to 100 101 to 150 151 to 200	4340 5360 8022 10482 14321 17162 25831 24821

Modular Carbon Adsorbers, Disposable - Single Pass Redundancy	less than 5 6 to 15 16 to 20 21 to 25 26 to 35 36 to 50 51 to 100 101 to 200	2051 2303 2888 4486 6946 8952 14374 21606
Modular Carbon Adsorbers, Dual Bed – 2 in series	Less than 100 101 to 130 131 to 350 351 to 700 701 to 1000 1001 to 1400 1401 to 2000	88212 92653 217844 330743 647906 654576 977260
Modular Carbon Adsorbers, Permanent - 2 in series	less than 20 21 to 25 26 to 35 36 to 50 51 to 75 76 to 100 101 to 150 151 to 200	7165 8179 12985 17011 23150 29339 44550 43552
Modular Carbon Adsorbers, Disposable - 2 in series	less than 5 6 to 15 16 to 20 21 to 25 26 to 35 36 to 50 51 to 100 101 to 200	2634 3114 4129 6431 10833 13952 23503 36629
Metals		
Coagulation/Flocculation where q is influent flow rate (R^2 = 0.9801)	$C_{j\,k}^{cap}$ = $-0.1038q^2 + 452.82q + 69578$	
Media Filtration (R^2 = 0.9829)	$C_{j\,k}^{cap}$ = $-0.4668q^2 + 293.98q + 13471$	

Table 12. Equations for $C^{op}_{j,k}$

VOC Air Stripper Packed Tower - Volatility high $C_{j\,k}^{op} = 448.33x + 11289$ Air Stripper Low Profile Tray Stack - Volatility high $C_{j\,k}^{op} = 460.11x + 6678$ Modular Carbon Adsorbers, Duel Bed – Single Pass $C_{j\,k}^{op} = 312.41x + 10491$ Modular Carbon Adsorbers, Permanent - Single Pass Redundancy $C_{j\,k}^{op} = 489.56x + 3371.7$ Modular Carbon Adsorbers, Disposable - Single Pass Redundancy $C_{j\,k}^{op} = 797.53x + 3241.6$ Modular Carbon Adsorbers, Duel Bed – 2 in series $C_{j\,k}^{op} = 332.99x + 14448$ Modular Carbon Adsorbers, Permanent - 2 in series $C_{j\,k}^{op} = 497.18x + 3544.9$ Modular Carbon Adsorbers, Disposable - 2 in series $C_{j\,k}^{op} = 804.37x + 3271.7$
SVOC and Fuels Air Stripping packed Tower -Volatility moderate $C_{j\,k}^{op} = 449.47x + 11689$ Air Stripping Low Profile Tray Stack -Volatility moderate $C_{j\,k}^{op} = 461.84x + 6834.9$ Modular Carbon Adsorbers, Duel Bed – Single Pass $C_{j\,k}^{op} = 312.41x + 10491$ Modular Carbon Adsorbers, Permanent - Single Pass Redundancy $C_{j\,k}^{op} = 489.56x + 3371.7$ Modular Carbon Adsorbers, Disposable - Single Pass Redundancy $C_{j\,k}^{op} = 797.53x + 3241.6$ Modular Carbon Adsorbers, Duel Bed – 2 in series $C_{j\,k}^{op} = 332.99x + 14448$ Modular Carbon Adsorbers, Permanent - 2 in series $C_{j\,k}^{op} = 497.18x + 3544.9$ Modular Carbon Adsorbers, Disposable - 2 in series $C_{j\,k}^{op} = 804.37x + 3271.7$
Ordnance Modular Carbon Adsorbers, Duel Bed – Single Pass $C_{j\,k}^{op} = 312.41x + 10491$ Modular Carbon Adsorbers, Permanent - Single Pass Redundancy $C_{j\,k}^{op} = 489.56x + 3371.7$

Modular Carbon Adsorbers, Disposable - Single Pass Redundancy $C_{j\,k}^{op} = 797.53x + 3241.6$ Modular Carbon Adsorbers, Duel Bed – 2 in series $C_{j\,k}^{op} = 332.99x + 14448$ Modular Carbon Adsorbers, Permanent - 2 in series $C_{j\,k}^{op} = 497.18x + 3544.9$ Modular Carbon Adsorbers, Disposable - 2 in series $C_{j\,k}^{op} = 804.37x + 3271.7$
Metals Coagulation/Flocculation $C_{j\,k}^{op} = -0.0217x2 + 161.64x + 13178$ media filtration $C_{j\,k}^{op} = -0.1899x2 + 109.4x + 3636.7$