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Environmental Technology Verification Report

Environmental Decision Support Software

University of Tennessee Research Corporation

Spatial Analysis and Decision Assistance (SADA)

THE ENVIRONMENTAL TECHNOLOGY VERIFICATION PROGRAM

U.S. Environmental Protection Agency

Oak Ridge National Laboratory

ETV Joint Verification Statement

TECHNOLOGY TYPE:	**ENVIRONMENTAL DECISION SUPPORT SOFTWARE**
APPLICATION:	**INTEGRATION, VISUALIZATION, SAMPLE OPTIMIZATION, COST-BENEFIT, AND RISK ANALYSIS OF ENVIRONMENTAL DATA SETS**
TECHNOLOGY NAME:	**Spatial Analysis and Decision Assistance (SADA)**
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The U.S. Environmental Protection Agency (EPA) has created the Environmental Technology Verification Program (ETV) to facilitate the deployment of innovative or improved environmental technologies through performance verification and dissemination of information. The goal of the ETV Program is to further environmental protection by substantially accelerating the acceptance and use of improved and cost-effective technologies. ETV seeks to achieve this goal by providing high-quality, peer-reviewed data on technology performance to those involved in the design, distribution, financing, permitting, purchase, and use of environmental technologies.

ETV works in partnership with recognized standards and testing organizations and stakeholder groups consisting of regulators, buyers, and vendor organizations, with the full participation of individual technology developers. The program evaluates the performance of innovative technologies by developing test plans that are responsive to the needs of stakeholders, conducting field or laboratory tests (as appropriate), collecting and analyzing data, and preparing peer-reviewed reports. All evaluations are conducted in accordance with rigorous quality assurance protocols to ensure that data of known and adequate quality are generated and that the results are defensible.

The Site Characterization and Monitoring Technologies Pilot (SCMT), one of 12 technology areas under ETV, is administered by EPA's National Exposure Research Laboratory (NERL). With the support of the U.S. Department of Energy's (DOE's) Environmental Management (EM) program, NERL selected a team from Brookhaven National Laboratory (BNL) and Oak Ridge National Laboratory (ORNL) to perform the verification of environmental decision support software. This verification statement provides a summary of the test results of a demonstration of the University of Tennessee Research Corporation's (UTRC's) Spatial Analysis and Decision Assistance (SADA)™ environmental decision support software product.

DEMONSTRATION DESCRIPTION

In September 1998, the performance of five decision support software (DSS) products were evaluated at the New Mexico Engineering Research Institute located in Albuquerque, New Mexico. In October 1998, a sixth DSS product was tested at BNL in Upton, New York. Each technology was independently evaluated by comparing its analysis results with measured field data and, in some cases, known analytical solutions to the problem.

Depending on the software, each was assessed for its ability to evaluate one or more of the following endpoints of environmental remediation problems: visualization, sample optimization, and cost-benefit analysis. The capabilities of the DSS were evaluated in the following areas: (1) the effectiveness of integrating data and models to produce information that supports the decision, and (2) the information and approach used to support the analysis. Secondary evaluation objectives were to examine the DSS for its reliability, resource requirements, range of applicability, and ease of operation. The verification study focused on the developers' analysis of multiple test problems with different levels of complexity. Each developer analyzed a minimum of three test problems. These test problems, generated mostly from actual environmental data from six real remediation sites, were identified as Sites A, B, D, N, S, and T. The use of real data challenged the software systems because of the variability in natural systems.

The University of Tennessee Research Corporation (UTRC) demonstrated Spatial Analysis and Decision Assistance (SADA) by performing visualization, sample optimization, and cost-benefit analysis for Sites N and S. Site N had two separate problems, and both were evaluated using SADA. The Site N problems were two-dimensional (2-D) soil contamination problems for three heavy metals (arsenic, chromium, and cadmium). In the Site N sample optimization problem, data were supplied over a limited area of the site, and the analyst was asked to develop a sampling strategy that characterized the remainder of the 125-acre site while taking only 80 additional samples. The Site N cost-benefit problem contained 524 data points on a 14-acre region of the site and required the analyst to perform a cost-benefit analysis of the remediation costs vs cleanup goal for each of the three contaminants. In addition, the analyst was asked to estimate the human health risks based on current conditions. The Site S test problem was a three-dimensional (3-D) groundwater contamination cost-benefit problem for a single contaminant (chlordane). The analyst was provided with a series of wells containing chlordane concentrations as a function of depth. The analyst was asked to define the region, mass, and volume of the plume at contaminant threshold concentrations of 5 and 500 μg/L. Based on this information and groundwater flow rates, estimates of current and future human health risks were requested.

SADA was used to integrate large quantities of data into a visual framework for assistance in understanding a site's contamination problem. For the Site N sample optimization problem, the data were used to develop a sampling scheme to characterize the site. Upon completion of the data-collection phase of the problem, maps with the probability of exceeding threshold concentrations were provided. For the Site N cost-benefit problem, SADA was used to estimate the cost of cleanup versus the cleanup threshold. Human health risks were evaluated on the basis of current conditions. For the Site S problem, SADA was used to estimate the volume of contamination above threshold levels and human health risks based on current conditions.

Details of the demonstration, including an evaluation of the software's performance, may be found in the report entitled *Environmental Technology Verification Report: University of Tennessee Research Corporation, Spatial Analysis and Decision Assistance (SADA),* EPA/600/R-00/036.

TECHNOLOGY DESCRIPTION

SADA is an environmental software product that incorporates tools from various fields — including visualization, geospatial analysis, statistical analysis, human health risk assessment, cost-benefit analysis, sampling design, and decision analysis — into a dynamic and interactive environment. Each of these modules can be used independently or in an integrated fashion to address site-specific concerns in the characterization and remedial action design. SADA was designed to simplify and streamline several of the processes in environmental characterization, risk assessment, and cost-benefit analysis to bring the information together in a way that can help users make decisions about their particular site in a quick and cost-effective manner. SADA is designed to assist environmental professionals who need to examine the data within a spatial context. SADA runs on Windows 95, 98, and NT platforms.

VERIFICATION OF PERFORMANCE

The following performance characteristics of SADA were observed:

Decision Support: SADA was designed as a decision support tool and directly addresses environmental questions such as (1) the location and size of the area of contamination, (2) the size of the cleanup zone at a specified contaminant threshold concentration or risk level, (3) the confidence in predicting the area of contamination or cleanup zone, (4) the costs for remediating the cleanup zone, (5) the human health risks, and (6) the optimal location for the next set of samples to best define the extent of contamination. In the demonstration, UTRC was able to use SADA to quickly import data on contaminant concentrations, overlay site maps, and integrate this information on a single platform. SADA demonstrated the ability to place the information in a visual context and produced 2-D and 3-D maps that support data interpretation and decision making. SADA was used in the demonstration to automatically generate maps showing contaminant concentration, recommended cleanup zones, cost-benefit curves, and human health risk. These maps can be based on the probability of exceeding specified contaminant threshold concentrations or risk levels and at specified probability levels. SADA was also used to predict new sample locations based on statistical and/or geostatistical analyses of the existing data.

Documentation of the SADA Analysis: UTRC staff used SADA to generate reports that provided an adequate explanation of the process and parameters used to analyze each problem. Documentation of data transfer, manipulations of the data (e.g., how to treat contamination data as a function of depth in a well), and analyses were included. Model selection and parameters for statistical analysis and contouring were also provided in the exportable documentation.

Comparison with Baseline Analysis and Data: SADA was able to generate 2-D and 3-D maps of contaminant concentrations, human health risk, probability of exceeding contaminant threshold concentrations as a function of degree of probability, and remedial zone maps for specified contaminant thresholds and probability levels. The maps included posting of data at the sample location, color coding of sample points to represent a parameter (concentration or risk), contaminant concentration contours, human health point risks, and human health risk contours. SADA also generated cost-benefit curves for the cost of remediation vs the cleanup threshold. These curves could be calculated for varying degrees of probability in the data. For the Site N sample optimization problem, the SADA analysis generated an acceptable match to the data and the baseline analysis. When compared with the baseline geostatistical analysis that used the entire data set, SADA identified approximately 75% of the site that had arsenic contamination above 125 mg/kg with the constraint of an additional 80 samples to characterize the entire 125-acre site. For the Site N cost-benefit problem, contaminant contour and probability maps were consistent with the baseline interpolation and geostatistical analysis. Estimates of the area where the contamination exceeded the threshold concentrations matched, to within 21%, the baseline interpolation and geostatistical analyses at the 50% probability levels. Likewise, the area estimates at the 90% probability level were within 21% of the baseline analyses and geostatistical analysis. The slight differences between SADA and the baseline analysis were due to the different parameters used for interpolation. For the Site S cost-benefit test problem, at the 50% probability level there is good agreement between SADA, the baseline analysis using Surfer™, and the baseline geostatistical analysis. In fact, all three area estimates are within 13% of each other, indicating agreement. For the 10% probability level, the SADA area estimates are 6% less at the 5-µg/L threshold and 9% less at 500-µg/L than the baseline area estimates. The difference between the SADA results and the baseline analysis is due to the slightly different selection of boundaries of contamination and kriging parameters selected for the analyses. Overall, there is close agreement among the area estimates produced by SADA and the baseline geostatistical analysis. Both the noncarcinogenic and carcinogenic risks calculated by SADA for Site N and Site S were accurate and consistent with the baseline analysis and EPA's risk assessment guidance for Superfund for all of the test problems.

Multiple Lines of Reasoning: UTRC staff conducted multiple data explorations and evaluations that were supported by the statistical and geostatistical functions in SADA. This information provided a quantitative measure of the confidence that could be placed in the decision. Several data interpolation routines were considered on a problem-specific basis before UTRC staff selected the best one for data analysis. Several sample optimization schemes are available for use. Selection of a particular scheme depends on the objectives of the analysis and the amount of data.

In addition to performance criteria, the following secondary criteria were evaluated:

Ease of Use: The demonstration showed that SADA was easy to use. The SADA graphical user interface has a logical structure to facilitate use of the options in the software package. SADA accepts database files in comma-delimited format; however, database files were supplied in .dbf format. The analyst imported the .dbf files into another software program (Microsoft Excel) and converted them into comma-delimited files. Drawing and map files could be read in .dxf format. Other common image file formats such as .jpg and .bmp were not supported. Visualization results can be output to any other Windows application that supports the use of the Clipboard, including commonly available software (e.g., Microsoft PowerPoint, Word, and WordPerfect).

Efficiency and Range of Applicability: SADA relies on a flexible database format with user-defined inputs. This provides a flexible platform that addresses problems efficiently and is tailored to the problem under study. The database permits filtering on the contaminant identifier and location. SADA has an auxiliary database that contains contaminants identified by name and Chemical Abstract Service (CAS) number. This feature facilitates data checking. SADA also has databases containing toxicological and exposure scenario parameters. These databases facilitate human health risk assessment. The software provides analysis on spatially correlated data and can simulate a wide range of environmental media and conditions (e.g., contaminant in groundwater, soil, sediment, or surface water; multiple contaminants on a single site) to be evaluated.

Training and Technical Support: SADA requires training for efficient and proper use. An analyst with a background in environmental problems and a basic knowledge of database operations, human health risk assessment, and statistics/geostatistics can be using SADA after one or two days of training. A detailed on-line help system is supplied with the software package. The on-line help provides examples of how to conduct analysis and gives recommendations on approaches to statistical/geostatistical modeling. Examples of software applications are provided as part of the software packages. A two-day training course is available. Technical support is available through e-mail.

Operator Skill Base: Effective use of all of the features of SADA requires that the operator possess a thorough understanding of the use of geospatial modeling in analyzing environmental problems and human health risk assessment. This includes an understanding of interpolation algorithms and geostatistics along with a fundamental knowledge of database manipulations, sample optimization, and cost-benefit analysis.

Platform: During the demonstration, SADA Beta Version 3.0 was operated on a Windows 95 operating system using a laptop with a 266-MHz Pentium processor, 128 MB of RAM, and 4 MB of video memory.

Cost: SADA will be distributed free over the Internet.

Overall Evaluation: The technical team concluded that the main strength of SADA is its technical approach to assist environmental decision-makers by defining areas of concern based on user-defined contaminant concentrations or human health risks. SADA's use of a geostatistical approach provides an estimate of the degree of uncertainty in the prediction that provides key information to assist in the selection of future sample locations and in determining cost-risk tradeoffs. The incorporation of databases of risk parameters, coupled with the pull-down menus in SADA, make risk calculations easy to perform. The integration of geostatistical analysis, human health risk assessment, cost-benefit analysis, sampling design, and decision analysis into a single software product makes SADA a powerful tool for analyzing spatially correlated data. SADA demonstrated the capability to accurately perform sample optimization analysis, estimate areas and volumes of contamination for cost-benefit analysis, and estimate the probability of exceeding threshold levels in concentration or risk.

The technical team did not notice any major limitations in SADA. Several minor limitations were noted. The 3-D visualizations provided only a qualitative depiction of the plume because a frame of reference (axis scale or surface maps) was not provided. Maps and drawings could be imported only as .dxf files; the capability to

import other graphic formats would be beneficial. Finally, data files could be imported only in comma-delimited format, which requires reformatting in another software product.

A credible computer analysis of environmental problems requires good data, reliable and appropriate software, adequate conceptualization of the site, and a technically defensible problem analysis. The results of the demonstration show that the SADA software can be used to generate reliable and useful analyses for evaluating environmental contamination problems. This is the only component of a credible analysis that can be addressed by the software. The results of a SADA analysis can support decision making. Although SADA has been demonstrated to have the capability to produce reliable and useful analyses, improper use of the software can cause the results of the analysis to be misleading or inconsistent with the data. As with any complex environmental DSS product, the quality of the output is directly dependent on the skill of the operator.

As with any technology selection, the user must determine if this technology is appropriate for the application and the project data quality objectives. For more information on this and other verified technologies visit the ETV web site at http://www.epa.gov/etv.

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Spatial Analysis and Decision Assistance (SADA)

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Notice

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Foreword

The U.S. Environmental Protection Agency (EPA) is charged by Congress with protecting the nation's natural resources. The National Exposure Research Laboratory (NERL) is EPA's center for the investigation of technical and management approaches for identifying and quantifying risks to human health and the environment. NERL's research goals are to (1) develop and evaluate technologies for the characterization and monitoring of air, soil, and water; (2) support regulatory and policy decisions; and (3) provide the science support needed to ensure effective implementation of environmental regulations and strategies.

EPA created the Environmental Technology Verification (ETV) Program to facilitate the deployment of innovative technologies through performance verification and information dissemination. The goal of the ETV Program is to further environmental protection by substantially accelerating the acceptance and use of improved and cost-effective technologies. The ETV Program is intended to assist and inform those involved in the design, distribution, permitting, and purchase of environmental technologies. This program is administered by NERL's Environmental Sciences Division in Las Vegas, Nevada.

The U.S. Department of Energy's (DOE's) Environmental Management (EM) program has partnered with EPA to provide cooperative technical management and funding support. DOE EM realizes that its goals for rapid and cost-effective cleanup hinge on the deployment of innovative environmental characterization and monitoring technologies. To this end, DOE EM shares the goals and objectives of the ETV.

Candidate technologies for these programs originate from the private sector and must be commercially ready. Through the ETV Program, developers are given the opportunity to conduct rigorous demonstrations of their technologies under realistic field conditions. By completing the evaluation and distributing the results, EPA establishes a baseline for acceptance and use of these technologies.

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Abbreviations and Acronyms

As	arsenic
.bmp	bitmap file
BNL	Brookhaven National Laboratory
CAS	Chemical Abstract Service
Cd	cadmium
CD-ROM	compact disk — read only memory
Cr	chromium
CTC	carbon tetrachloride
DBCP	dibromochloroproprane
.dbf	database file
DCA	dichloroethane
DCE	dichloroethene
DCP	dichloropropane
DOE	U.S. Department of Energy
DSS	decision support software
.dxf	data exchange format file
EDB	ethylene dibromide
EM	Environmental Management Program (DOE)
EPA	U.S. Environmental Protection Agency
ESRI	Environmental Systems Research Institute
ETV	Environmental Technology Verification Program
FTP	file transfer protocol
Geo-EAS	Geostatistical Environmental Assessment Software
GIS	geographic information system
GUI	graphical user interface
GSLIB	Geostatistical Software Library (software)
HTML	Hypertext Markup Language
IDW	inverse distance weighting
MB	megabyte
MHz	megahertz
NAMP	National Analytical Management Program (DOE)
NERL	National Exposure Research Laboratory (EPA)
NMERI	New Mexico Engineering Research Institute
ORD	Office of Research and Development (EPA)
ORNL	Oak Ridge National Laboratory
PCE	perchloroethene or tetrachloroethene
ppm	parts per million
QA	quality assurance
QC	quality control
RAM	random access memory
SADA	Spatial Analysis and Decision Assistance (software)
SCMT	Site Characterization and Monitoring Technology
SVGA	super video graphics adapter
TCA	trichloroethane
TCE	trichlorethene
Tc-99	technetium-99
UTRC	University of Tennessee Research Corporation

VC	vinyl chloride
VOC	volatile organic compound
2-D	two-dimensional
3-D	three-dimensional

Section 1 — Introduction

Background

The U.S. Environmental Protection Agency (EPA) has created the Environmental Technology Verification Program (ETV) to facilitate the deployment of innovative or improved environmental technologies through performance verification and dissemination of information. The goal of the ETV Program is to further environmental protection by substantially accelerating the acceptance and use of improved and cost-effective technologies. ETV seeks to achieve this goal by providing high-quality, peer-reviewed data on technology performance to those involved in the design, distribution, financing, permitting, purchase, and use of environmental technologies.

ETV works in partnership with recognized standards and testing organizations and stakeholder groups consisting of regulators, buyers, and vendor organizations, with the full participation of individual technology developers. The program evaluates the performance of innovative technologies by developing test plans that are responsive to the needs of stakeholders, conducting field or laboratory tests (as appropriate), collecting and analyzing data, and preparing peer-reviewed reports. All evaluations are conducted in accordance with rigorous quality assurance (QA) protocols to ensure that data of known and adequate quality are generated and that the results are defensible.

ETV is a voluntary program that seeks to provide objective performance information to all of the actors in the environmental marketplace and to assist them in making informed technology decisions. ETV does not rank technologies or compare their performance, label or list technologies as acceptable or unacceptable, seek to determine "best available technology," nor approve or disapprove technologies. The program does not evaluate technologies at the bench or pilot scale and does not conduct or support research.

The program now operates 12 pilots covering a broad range of environmental areas. ETV has begun with a 5-year pilot phase (1995–2000) to test a wide range of partner and procedural alternatives in various pilot areas, as well as the true market demand for and response to such a program. In these pilots, EPA utilizes the expertise of partner "verification organizations" to design efficient processes for conducting performance tests of innovative technologies. These expert partners are both public and private organizations, including federal laboratories, states, industry consortia, and private sector facilities. Verification organizations oversee and report verification activities based on testing and QA protocols developed with input from all major stakeholder/customer groups associated with the technology area. The demonstration described in this report was administered by the Site Characterization and Monitoring Technology (SCMT) Pilot. (To learn more about ETV, visit ETV's Web site at http://www.epa.gov/etv.)

The SCMT pilot is administered by EPA's National Exposure Research Laboratory (NERL). With the support of the U.S. Department of Energy's (DOE's) Environmental Management (EM) program, NERL selected a team from Brookhaven National Laboratory (BNL) and Oak Ridge National Laboratory (ORNL) to perform the verification of environmental decision support software. Decision support software (DSS) is designed to integrate measured or modeled data (such as soil or groundwater contamination levels) into a framework that can be used for decision-making purposes. There are many potential ways to use such software, including visualization of the nature and extent of contamination, locating optimum future samples, assessing costs of cleanup versus benefits obtained, or estimating human health risks. The primary objective of this demonstration was to conduct an independent evaluation of each software's capability to evaluate three common endpoints of environmental remediation problems: visualization, sample optimization, and cost-benefit analysis. These endpoints were defined as follows.

- *Visualization* — using the software to organize and display site and contamination data in ways that promote understanding of current conditions, problems, potential solutions, and eventual cleanup choices;
- *Sample optimization* — selecting the minimum number of samples needed to define a contaminated area within a predetermined statistical confidence;

- *Cost-benefit analysis* — assessment of either the size of the zone to be remediated according to cleanup goals, or estimation of human health risks due to the contaminants. These can be related to costs of cleanup.

The developers were permitted to select the endpoints that they wished to demonstrate because each piece of software had unique features and focused on different aspects of the three endpoints. Some focused entirely on visualization and did not attempt sample optimization or cost-benefit analysis, while others focused on the technical aspects of generating cost-benefit or sample-optimization analysis, with a minor emphasis on visualization. The evaluation of the DSS focused only on the analyses conducted during the demonstration. No penalty was assessed for performing only part of the problem (e.g., performing only visualization).

Evaluation of software that is used for complex environmental problems is by necessity primarily qualitative in nature. It is not meaningful to quantitatively evaluate how well predictions match at locations where data have not been collected. (This is discussed in more detail in Appendix B.) In addition, the selection of a software product for a particular application relies heavily on the user's background, personal preferences (for instance, some people prefer Microsoft Word, while others prefer Corel WordPerfect for word processing), and the intended use of the software (for example, spreadsheets can be used for managing data; however, programs specifically designed for database management would be a better choice for this type of application). The objective of these reports is to provide sufficient information to judge whether the DSS product has the analysis capabilities and features that will be useful for the types of problems typically encountered by the reader.

Demonstration Overview

In September 1998, a demonstration was conducted to verify the performance of five environmental software programs: Environmental Visualizations System (C Tech Development Corp.), ArcView and associated software extenders [Environmental Systems Research Institute (ESRI)], Groundwater*FX* (Decision*FX* Corp.), Sampling*FX* (Decision*FX* Corp.), and SitePro (Environmental Software Corp.). In October, a sixth software package from the University of Tennessee Research Corporation (UTRC), Spatial Analysis and Decision Assistance (SADA), was tested. This report contains the evaluation of SADA.

Each developer was asked to use their own software to address a minimum of three test problems. In preparation for the demonstration, ten sites were identified as having data sets that might provide useful test cases for the demonstration. All of this data received a quality control review to screen out sites that did not have adequate data sets. After the review, ten test problems were developed from field data at six different sites. Each site was given a unique identifier (Sites A, B, D, N, S, and T). Each test problem focused on different aspects of environmental remediation problems. From the complete data sets, test problems that were subsets of the entire data set were prepared. The demonstration technical team performed an independent analysis of each of the ten test problems to ensure that the data sets were complete.

All developers were required to choose either Site S or Site N as one of their three problems because these sites had the most data available for developing a quantitative evaluation of DSS performance.

Each DSS was evaluated on its own merits based on the evaluation criteria presented in Section 3. Because of the inherent variability in soil and subsurface contamination, most of the evaluation criteria are qualitative. Even when a direct comparison is made between the developer's analysis and the baseline analysis, different numerical algorithms and assumptions used to interpolate data between measured values at known locations make it almost impossible to make a quantitative judgement as to which technical approach is superior. The comparisons, however, do permit an evaluation of whether the analysis is consistent with the data supplied for the analysis and therefore useful in supporting remediation decisions.

Summary of Analysis Performed by SADA

SADA is a Windows 95, 98, or NT environmental software product that incorporates tools from various fields — including visualization, geospatial analysis, statistical analysis, human health risk assessment, cost-benefit analysis, sampling design, and decision analysis — into an interactive environment. SADA relies mainly on statistical and geostatistical algorithms to quantify the nature and extent of uncertainties in environmental data and various

cost-risk methods to provide objective guidance on key decision analysis needs. SADA provides the information in a visual form, as two-dimensional (2-D) and three-dimensional (3-D) graphics, to assist the user in data interpretation and provides statistical information about the contamination (e.g., area or volume of contamination, standard deviation, probability of exceeding cleanup goals).

UTRC staff chose to use SADA to perform all three endpoints (visualization, sample optimization, and cost-benefit analysis) using data from the Site N sample optimization problem, the Site N cost-benefit problem, and the Site S cost-benefit problem. Visualization results were presented on all three problems. The three problems were analyzed using a statistical approach that permitted the evaluation to be defined in terms of probability of exceeding a threshold in risk or concentration.

The Site N sample optimization problem involved soil contamination from three heavy metals — arsenic, cadmium, and chromium. Data were provided from a small section of the 125-acre site, and the analyst was required to define contamination throughout the site using only 80 additional samples. SADA was used in an iterative fashion to select a few sample locations for further data collection. This information was used to generate the next set of sample locations, and the process continued until 80 sample locations had been specified. Using the final data set, SADA generated contaminant concentration contour maps and remediation zone maps based on contaminant threshold levels and the probability level of the interpolation results. These maps were overlain with site features (roads and surface waterways).

The Site N cost-benefit problem also involved soil contamination from the three heavy metals. SADA was used to generate maps for each contaminant with sample locations color-coded by concentration and suggested cleanup areas for each contaminant at two threshold levels. These cleanup maps were calculated based on the probability of exceeding the threshold concentration for two probability levels. SADA was then used to produce cost-benefit curves of remediation cost vs cleanup goal for each contaminant at the two probability levels. Finally, SADA was used to estimate human health risks based on current conditions for all contaminants. The risks were summed to obtain total risk, and SADA generated maps of human health risk. In addition, SADA generated maps with sample points that had contamination levels exceeding a threshold health risk inscribed in a square to facilitate location of these points.

The Site S cost-benefit problem involved groundwater contamination by chlordane. SADA was used to define the 3-D volume of groundwater contamination above specified contamination levels and to estimate human health risks from drinking the contaminated water. SADA was used to divide the data into a series of 5-ft vertical strata based on depth below ground surface. The data were analyzed in these strata to generate a series of 2-D maps for concentration contours, cleanup zones based on threshold concentration levels, and carcinogenic and noncarcinogenic health risks. The maps were prepared at two probability levels. The 2-D representations of each stratum were combined to provide a 3-D depiction of the concentration, cleanup zone, and risks.

Section 2 contains a brief description of the capabilities of SADA. Section 3 outlines the approach used to develop the test problems, a summary description of the ten test problems, the approach used to perform the baseline analyses used for comparison with the developers analyses, and the evaluation criteria. Section 4 presents the technical review of the analyses performed by SADA. This includes a detailed discussion of the problems attempted, comparisons of the SADA analyses and the baseline results, and an evaluation of SADA against the criteria established in Section 3. Section 5 presents an update on the SADA technology and provides examples of representative applications of SADA in environmental problem-solving.

Section 2 — SADA Technology Description

The following section provides a general overview of the capabilities of UTRC's SADA software product. The information was supplied by UTRC.

SADA Features

Spatial Analysis Decision Assistance (SADA) is an environmental software product for Windows NT 4 (Service Pack 4 or higher) and Windows 95/98 that incorporates tools from various fields — including visualization, geospatial analysis, statistical analysis, human health risk assessment, cost-benefit analysis, sampling design, and decision analysis — into a dynamic and interactive environment. Each of these modules can be used independently or in an integrated fashion to address site-specific concerns in the characterization and remedial action design. SADA was designed to simplify and streamline several of the processes in environmental characterization and to bring the information together in a way that can help users make decisions about their particular site in a quick and cost-effective manner. SADA may be found useful by anyone who needs to look at data within a spatial context. These users include

- statisticians,
- human health risk assessors,
- GIS/visualization users,
- project managers, and
- stakeholders.

SADA was developed by UTRC and can be accessed through the SADA website at http://www.sis.utk.edu/cis/SADA. Technical assistance is contained in SADA's on-line help and on the SADA website. Formal training modules are currently being developed.

SADA provides 2-D and 3-D visualization. The visualization techniques in SADA were designed to be simple to use and easy to understand and to facilitate the data-exploration, modeling, and decision analysis components. Two-dimensional information is presented as simple *xy* plots. Three-dimensional information is presented through two different methods. The first is by 2-D slices (layers) in the third dimension. The user can easily set the depth of each of these layers. The layer approach, while not a true 3-D visualization, provides a way to see results quickly in daily application. In addition, environmental data are often categorized by depth (e.g., surface, subsurface, 0–1 ft, 0–2 ft) during remedial investigations, and SADA was designed to fit into this type of framework. The second method allows the user to view true 3-D volume rendering. All the standard methods for viewing 3-D information are available.

SADA can accept any map layer from a geographic information system (GIS) if saved in a data exchange format (.dxf) file. Multiple layers can be imported into SADA, and the user can control the layer order and coloring scheme.

In addition, the user can select a subregion of the site to conduct the analysis. This region is defined by a user-defined polygon with only the interior region considered in the analysis.

SADA provides methods for quick and easy data exploration. Tools include statistical analysis, visual database queries, and basic data screening exercises. All these tools can be applied to the entire site or to any subset of the site. Similarly, they may be applied to all or some of the contaminants. In addition, the user may select any region of the site and immediately view the human health risk results for that region.

For most applications, minimum system requirements for SADA are a Pentium computer with 32 MB of RAM, a clock speed of 120 MHz, a disk drive with 50 MB of free space, and a super video graphics adapter (SVGA) monitor. For more involved modeling, particularly for 3-D geospatial models, a higher-performance computer is recommended. As an example, SADA has performed well under these conditions on a 266-MHz Pentium Pro with 128 MB of RAM and 100 MB of free disk space. To visualize true 3-D volumes a minimum of 16 million colors is required.

SADA Assessment Capabilities

Human Health Risk

SADA provides the user with a full human health risk assessment module and associated databases. The risk models follow EPA's *Risk Assessment Guidance for Superfund* (EPA 1989) and can be

customized to fit site-specific exposure conditions. Updated toxicological databases and default scenario parameters can be downloaded over the web directly from SADA. For radioactive and nonradioactive contaminants, SADA simulates five land-use scenarios (residential, industrial, agricultural, recreational, and excavation) and five exposure pathways [ingestion, inhalation, dermal contact, external (radiation), and food consumption]. The exposures resulting from different pathways and contaminants can be summed to provide total exposure from all contaminants.

Geospatial Analysis

SADA provides several tools for performing geospatial analysis. These include methods for measuring spatial correlation among data, modeling spatial correlation, and producing concentration, risk, probability, variance, and cleanup maps. Among these tools are four geospatial interpolators: ordinary kriging, indicator kriging, inverse distance, and nearest neighbor. With these tools, the user can generate concentration-contour, probability, risk, and remedial design maps.

Decision Analysis

SADA's decision support tools include cost-benefit analysis, defining areas of concern, and sampling optimization. SADA produces cost-benefit curves that demonstrate the relationship between the cleanup goal (concentration- or risk-based) and the cost of remediation. Based on the decision rule, SADA estimates the location of areas of concern. The decision rule includes components such as the cleanup goal, the level of confidence, and whether the goal applies to the entire site or any part of the site. These areas of concern can then serve as a basis for remedial action design. SADA allows the user to choose from a variety of strategies for determining where to collect data in the next round of sampling. Depending on the chosen geospatial interpolator, the following five strategies are available: adaptive fill, estimate rank, variance rank, percentile rank, and uncertainty rank.

Section 3 — Demonstration Process and Design

Introduction

The objective of this demonstration was to conduct an independent evaluation of the capabilities of several DSSs in the following areas: (1) effectiveness in integrating data and models to produce information that supports decisions pertaining to environmental contamination problems, and (2) the information and approach used to support the analysis. Specifically, three endpoints were evaluated:

- *Visualization* — Visualization software was evaluated in terms of its ability to integrate site and contamination data in a coherent and accurate fashion that aids in understanding the contamination problem. Tools used in visualization can range from data display in graphical or contour form to integrating site maps and aerial photos into the results.
- *Sample optimization* — Sample optimization was evaluated for soil and groundwater contamination problems in terms of the software's ability to select the minimum number of samples needed to define a contaminated region with a specified level of confidence.
- *Cost-benefit analysis* — Cost-benefit analysis involved either defining the size of remediation zone as a function of the cleanup goal or evaluating the potential human health risk. For problems that defined the contamination zone, the cost could be evaluated in terms of the size of the zone, and cost-benefit analysis could be performed for different cleanup levels or different statistical confidence levels. For problems that calculated human health risk, the cost-benefit calculation would require computing the cost to remediate the contamination as a function of reduction in health risk.

Secondary evaluation objectives for this demonstration were to examine the reliability, resource requirements, range of applicability, and ease of operation of the DSS. The developers participated in this demonstration in order to highlight the range and utility of their software in addressing the three endpoints discussed above. Actual users might achieve results that are less reliable, as reliable, or more reliable than those achieved in this demonstration, depending on their expertise in using a given software to solve environmental problems.

Development of Test Problems

Test Problem Definition

A problem development team was formed to collect, prepare, and conduct the baseline analysis of the data. A large effort was initiated to collect data sets from actual sites with an extensive data collection history. Literature review and contact with different government agencies (EPA field offices, DOE, the U.S. Department of Defense, and the U.S. Geological Survey) identified ten different sites throughout the U.S which had the potential for developing test problems for the demonstration. The data from these ten sites were screened for completeness of data, range of environmental conditions covered, and potential for developing challenging and defensible test problems for the three endpoints of the demonstration. The objective of the screening was to obtain a set of problems that covered a wide range of contaminants (metals, organics, and radionuclides), site conditions, and source conditions (spills, continual slow release, and multiple releases over time). On the basis of this screening, six sites were selected for development of test problems. Of these six sites, four had sufficient information to provide multiple test problems. This provided a total of ten test problems for use in the demonstration.

Summary of Test Problems

A detailed description of the ten test problems was supplied to the developers as part of the demonstration (Sullivan, Armstrong, and Osleeb 1998). A general description of each of the problems can be found in Appendix A. This description includes the operating history of the site, the contaminants of concern, and the objectives of the test problem (e.g., define the volume over which the contaminant concentration exceeds 100 μg/L). The test problems analyzed by UTRC are discussed in Section 4 as part of the evaluation of SADA's performance.

Table 1 summarizes the ten problems by site identifier, location of contamination (soil or groundwater), problem endpoints, and contaminants

Table 1. Summary of test problems

Site identifier	Media	Problem endpoints	Contaminants
A	Groundwater	Visualization, sample optimization	Dichloroethene, trichloroethene
A	Groundwater	Visualization, cost-benefit	Perchloroethene, trichloroethane
B	Groundwater	Visualization, sample optimization, cost-benefit	Trichloroethene, vinyl-chloride, technetium-99
D	Groundwater	Visualization, sample optimization, cost-benefit	Dichloroethene, dichloroethane, trichloroethene, perchloroethene
N	Soil	Visualization, sample optimization	Arsenic, cadmium, chromium
N	Soil	Visualization, cost-benefit	Arsenic, cadmium, chromium
S	Groundwater	Visualization, sample optimization	Carbon tetrachloride
S	Groundwater	Visualization, cost-benefit	Chlordane
T	Soil	Visualization, sample optimization	Ethylene dibromide, dibromochloropropane, dichloropropane, carbon tetrachloride
T	Groundwater	Visualization, cost-benefit	Ethylene dibromide, dibromochloropropane, dichloropropane, carbon tetrachloride

of concern. The visualization endpoint could be performed on all ten problems. In addition, there were four sample optimization problems, four cost-benefit problems, and two problems that combined sample optimization and cost-benefit issues. The range of contaminants considered included metals, volatile organic compounds (VOCs), and radionuclides. The range of environmental conditions included two- and three-dimensional soil and groundwater contamination problems over varying geologic, hydrologic, and environmental settings. Table 2 provides a summary of the types of data supplied with each problem.

Analysis of Test Problems

Prior to the demonstration, the demonstration technical team performed a quality control examination of all data sets and test problems. This involved reviewing database files for improper data (e.g., negative concentrations), removing information that was not necessary for the demonstration (e.g., site descriptors), and limiting the data to the contaminants, the region of the site, and the time frame covered by the test problems (e.g., only data from one year for three contaminants). For sample optimization problems, a limited data set was prepared for the developers as a starting point for the analysis. The remainder of the data was reserved to provide input concentrations to developers for their sample optimization analysis. For cost-benefit problems, the analysts were provided with an extensive data set for each test problem with a few data points reserved for checking the DSS analysis. The data quality review

Table 2. Data supplied for test problems

Site history	Industrial operations, environmental settings, site descriptions
Surface structure	Road and building locations, topography, aerial photos
Sample locations	x, y, z coordinates for soil surface samples soil borings groundwater wells
Contaminants	Concentration data as a function of time and location (x, y, and z) for metals, inorganics, organics, radioactive contaminants
Geology	Soil boring profiles, bedrock stratigraphy
Hydrogeology	Hydraulic conductivities in each stratigraphic unit; hydraulic head measurements and locations
Transport parameters	Sorption coefficient (K_d), biodegradation rates, dispersion coefficients, porosity, bulk density
Human health risk	Exposure pathways and parameters, receptor location

also involved importing all graphics files (e.g., .dxf and .bmp) that contained information on surface structures such as buildings, roads, and water bodies to ensure that they were readable and useful for problem development. Many of the drawing files were prepared as ESRI shape files compatible with ArcView™. ArcView was also used to examine the graphics files.

Once the quality control evaluation was completed, the test problems were developed. The test problems were designed to be manageable within the time frame of the demonstration and were often a subset of the total data set. For example, in some cases, test problems were developed for a selected region of the site. In other cases, the database could have contained information for tens of contaminants, while the test problems themselves were limited to the three or four principal contaminants. At some sites, data were available over time periods exceeding 10 years. For the DSS test problems, the analysts were typically supplied chemical and hydrologic data for a few sampling periods.

Once the test problems were developed, the demonstration technical team conducted a complete analysis of each test problem. These analyses served as the baseline for evaluating results from the developers. Each analysis consisted of taking the entire data set and obtaining an estimate of the plume boundaries for the specified threshold contaminant concentrations and estimating the area of contamination above the specified thresholds for each contaminant.

The independent data analysis was performed using Surfer™ (Golden Software 1996). Surfer was selected for the task because it is a widely used, commercially available software package with the functionality necessary to examine the data. This functionality includes the ability to import drawing files to use as layers in the map, and the ability to interpolate data in two dimensions. Surfer has eight different interpolation methods, each of which can be customized by changing model parameters, to generate contours. These different contouring options were used to generate multiple views of the interpolated regions of contamination and hydrologic information. The best fit to the data was used as the baseline analysis. For 3-D problems, the data were grouped by elevation to provide a series of 2-D slices of the problem. The distance between slices ranged between 5 and 10 ft depending on the availability of data. Compilation of vertical slices generated 3-D depictions of the data sets. Comparisons of the baseline analysis to the SADA results are presented in Section 4.

In addition to Surfer, two other software packages were used to provide an independent analysis of the data and to provide an alternative representation for comparison with the Surfer results. The Geostatistical Software Library Version 2.0 (GSLIB) and Geostatistical Environmental Assessment Software Version 1.1 (Geo-EAS) were selected because both provide enhanced geostatistical routines that assist in data exploration and selection of modeling parameters to provide extensive evaluations of the data from a spatial context (Deutsch and Journel 1992; Englund and Sparks 1991). These three analyses provide multiple lines of reasoning, particularly for the test problems that involved geostatistics. The results from Surfer, GSLIB, and Geo-EAS were compared and contrasted to determine the best fit of the data, thus providing a more robust baseline analysis for comparison to the developers' results.

Under actual site conditions, uncertainties and natural variability make it impossible to define plume boundaries exactly. In these case studies, the baseline analyses serve as a guideline for evaluating the accuracy of the analyses prepared by the developers. Reasonable agreement should be obtained between the baseline and the developer's results. A discussion of the technical approaches and limitations to estimating physical properties at locations that are between data collection points is provided in Appendix B.

To minimize problems in evaluating the software associated with uncertainties in the data, the developers were required to perform an analysis of one problem from either Site N or Site S. For Site N, with over 4000 soil contamination data points, the baseline analysis reflected the actual site conditions closely; and if the developers performed an accurate analysis, the correlation between the two should be high. For Site S, the test problems used actual contamination data as the basis for developing a problem with a known solution. In both Site S problems, the data were modified to simulate a constant source term to the aquifer in which the movement of the contaminant can be described by the classic advective-dispersive transport equation. Transport parameters were based on the actual data. These assumptions permitted release to the aquifer and subsequent transport to be represented by a

partial differential equation that was solved analytically. This analytical solution could be used to determine the concentration at any point in the aquifer at any time. Therefore, the developer's results can be compared against calculated concentrations with known accuracy.

After completion of the development of the ten test problems, a predemonstration test was conducted. In the predemonstration, the developers were supplied with a problem taken from Site D that was similar to test problems for the demonstration. The objective of the predemonstration was to provide the developers with a sample problem with the level of complexity envisioned for the demonstration. In addition, the predemonstration allowed the developers to process data from a typical problem in advance of the demonstration and allowed the demonstration technical team to determine if any problems occurred during data transfer or because of problem definition. The results of the predemonstration were used to refine the problems used in the demonstration.

Preparation of Demonstration Plan

In conjunction with the development of the test problems, a demonstration plan (Sullivan and Armstrong 1998) was prepared to ensure that all aspects of the demonstration were documented and scientifically sound and that operational procedures were conducted within quality assurance (QA)/quality control (QC) specifications. The demonstration plan covered

- the roles and responsibilities of demonstration participants;
- the procedures governing demonstration activities such as data collection to define test problems and data preparation, analysis, and interpretation;
- the experimental design of the demonstration;
- the evaluation criteria against which the DSS would be judged; and
- QA and QC procedures for conducting the demonstration and for assessing the quality of the information generated from the demonstration.

All parties involved with implementation of the plan approved and signed the demonstration plan prior to the start of the demonstration.

Summary of Demonstration Activities

On September 14–25, 1998, the Site Characterization and Monitoring Technology Pilot, in cooperation with DOE's National Analytical Management Program, conducted a demonstration to verify the performance of five environmental DSS packages. The demonstration was conducted at the New Mexico Engineering Research Institute, Albuquerque, New Mexico. An additional software package was tested on October 26–29, 1998, at Brookhaven National Laboratory, Upton, New York.

The first morning of the demonstration was devoted to a brief presentation of the ten test problems, a discussion of the output requirements to be provided from the developers for evaluation, and transferring the data to the developers. The data from all ten test problems — along with a narrative that provided a description of the each site, the problems to be solved, the names of data files, structure of the data files, and a list of output requirements — were given to the developers. The developers were asked to address a minimum of three test problems for each software product.

Upon completion of the review of the ten test problems and the discussion of the outputs required from the developers, the developers received data sets for the problems by file transfer protocol (FTP) from a remote server or on a high-capacity removable disk. Developers downloaded the data sets to their own personal computers, which they had supplied for the demonstration. Once the data transfers of the test problems were complete and the technical team had verified that each developer had received the data sets intact, the developers were allowed to proceed with the analysis at their own pace. During the demonstration, the technical team observed the developers, answered questions, and provided data as requested by the developers for the sample optimization test problems. The developers were given 2 weeks to complete the analysis for the test problems that they selected.

The third day of the demonstration was visitors' day, an open house during which people interested in DSS could learn about the various products being tested. During the morning of visitors' day, presenters from EPA, DOE, and the demonstration technical team outlined the format and content of the demonstration. This was followed by a presentation

from the developers on the capabilities of their respective software products. In the afternoon, attendees were free to meet with the developers for a demonstration of the software products and further discussion.

Prior to leaving the test facility, the developers were required to provide the demonstration technical team with the final output files generated by their software. These output files were transferred by FTP to an anonymous server or copied to a zip drive or compact disk–read only memory (CD-ROM). The technical team verified that all files generated by the developers during the demonstration were provided and intact. The developers were given a 10-day period after the demonstration to provide a written narrative of the work that was performed and a discussion of their results.

Evaluation Criteria

One important objective of DSS is to integrate data and models to produce information that supports an environmental decision. Therefore, the overriding performance goal in this demonstration was to provide a credible analysis. The credibility of a software and computer analysis is built on four components:

- good data,
- adequate and reliable software,
- adequate conceptualization of the site, and
- well-executed problem analysis (van der Heijde and Kanzer 1997).

In this demonstration, substantial efforts were taken to evaluate the data and remove data of poor quality prior to presenting it to the developers. Therefore, the developers were directed to assume that the data were of good quality. The technical team provided the developers with detailed site maps and test problem instructions on the requested analysis and assisted in site conceptualization. Thus, the demonstration was primarily to test the adequacy of the software and the skills of the analyst. The developers operated their own software on their own computers throughout the demonstration.

Attempting to define and measure credibility makes this demonstration far different from most demonstrations in the ETV program in which measurement devices are evaluated. In the typical ETV demonstrations, quality can be measured in a quantitative and statistical manner. This is not true for DSS. While there are some quantitative measures, there are also many qualitative measures. The criteria for evaluating the DSS's ability to support a credible analysis are discussed below. In addition a number of secondary objectives, also discussed below, were used to evaluate the software. These included documentation of software, training and technical support, ease of use of the software, efficiency, and range of applicability.

Criteria for Assessing Decision Support

The developers were asked to use their software to answer questions pertaining to environmental contamination problems. For visualization tools, integration of geologic data, contaminant data, and site maps to define the contamination region at specified concentration levels was requested. For software tools that address sample optimization questions, the developers were asked to suggest optimum sampling locations, subject to constraints on the number of samples or on the confidence with which contamination concentrations were known. For software tools that address cost-benefit problems, the developers were asked either to define the volume (or area) of contamination and, if possible, supply the statistical confidence with which the estimate was made, or to estimate human health risks resulting from exposure to the contamination.

The criterion for evaluation was the credibility of the analyses to support the decision. This evaluation was based on several points, including

- documentation of the use of the models, input parameters, and assumptions;
- presentation of the results in a clear and consistent manner;
- comparison of model results with the data and baseline analyses;
- evaluation of the use of the models; and
- use of multiple lines of reasoning to support the decision.

The following sections provide more detail on each of these topics.

Documentation of the Analysis and Evaluation of the Technical Approach

The developers were requested to supply a concise description of the objectives of the analysis, the procedures used in the analysis, the conclusions of

the analysis with technical justification of the conclusions, and a graphical display of the results of the analysis. Documentation of key input parameters and modeling assumptions was also requested. Guidance was provided on the quantity and type of information requested to perform the evaluation.

Based on observations obtained during the demonstration and the documentation supplied by the developers, the use of the models was evaluated and compared to standard practices. Issues in proper use of the models include selection of appropriate contouring parameters, spatial and temporal discretization, solution techniques, and parameter selection. This evaluation was performed as a QA check to determine if standard practices were followed. This evaluation was useful in determining whether the cause of discrepancies between model projections and the data resulted from operator actions or from the model itself and was instrumental in understanding the role of the operator in obtaining quality results.

Comparison of Projected Results with the Data and Baseline Analysis

Quantitative comparisons between DSS-generated predictions and the data or baseline analyses were performed and evaluated. In addition, DSS-generated estimates of the mass and volume of contamination were compared to the baseline analyses to evaluate the ability of the software to determine the extent of contamination. For visualization and cost-benefit problems, developers were given a detailed data set for the test problem with only a few data points held back for checking the consistency of the analysis. For sample optimization problems, the developers were provided with a limited data set to begin the problem. In this case, the data not supplied to the developers were used for checking the accuracy of the sample optimization analysis. However, because of the inherent variability in environmental systems and the choice of different models and parameters by the analysts, quantitative measures of the accuracy of the analysis are difficult to obtain and defend. Therefore, qualitative evaluations of how well the model projections reproduced the trends in the data were also performed.

A major component of the analysis of environmental data sets involves predicting physical or chemical properties (contaminant concentrations, hydraulic head, thickness of a geologic layer, etc.) at locations between measured data. This process, called interpolation, is often critical in developing an understanding of the nature and extent of the environmental problem. The premise of interpolation is that the estimated value of a parameter is a weighted average of measured values around it. Different interpolation routines use different criteria to select the weights. Due to the importance of obtaining estimates of data between measured data points in many fields of science, a wide number of interpolation routines exist. Three classes of interpolation routines commonly used in environmental analysis are nearest neighbor, inverse distance, and kriging. These three classes of interpolation, and their strengths and limitations, are discussed in detail in Appendix B.

Use of Multiple Lines of Reasoning

Environmental decisions are often made with uncertainties because of an incomplete understanding of the problem and lack of information, time, and/or resources. Therefore, multiple lines of reasoning are valuable in obtaining a credible analysis. Multiple lines of reasoning may incorporate statistical analyses, which in addition to providing an answer provide an estimate of the probability that the answer is correct. Multiple lines of reasoning may also incorporate alternative conceptual models or multiple simulations with different parameter sets. The DSS packages were evaluated on their capabilities to provide multiple lines of reasoning.

Secondary Evaluation Criteria

Documentation of Software

The software was evaluated in terms of its documentation. Complete documentation includes detailed instructions on how to use the software package, examples of verification tests performed with the software package, a discussion of all output files generated by the software package, a discussion of how the output files may be used by other programs (e.g., ability to be directly imported into an Excel spreadsheet), and an explanation of the theory behind the technical approach used in the software package.

Training and Technical Support

The developers were asked to list the necessary background knowledge necessary to successfully operate the software package (i.e., basic understanding of hydrology, geology, geostatistics, etc.) and the auxiliary software used by the software package (e.g., Excel). In addition, the operating

systems (e.g., Unix, Windows NT) under which the DSS can be used was requested. A discussion of training, software documentation, and technical support provided by the developers was also required.

Ease of Use

Ease of use is one of the most important factors to users of computer software. Ease of use was evaluated by an examination of the software package's operation and on the basis of adequate on-line help, the availability of technical support, the flexibility to change input parameters and databases used by the software package, the time required for an experienced user to set up the model and prepare the analysis (that is, input preparation time, time required to run the simulation, and the time required to prepare graphical output).

The demonstration technical team observed the operation of each software product during the demonstration to assist in determining the ease of use. These observations documented operation and the technical skills required for operation. In addition, several members of the technical team were given a 4-hour tutorial by each developer on their respective software to gain an understanding of the training level required for software operation as well as the functionalities of each software.

Efficiency and Range of Applicability

Efficiency was evaluated on the basis of the resources that were necessary to evaluate the test problems. This was assessed through the number of problems completed as a function of time required for the analysis and computing capabilities.

Range of applicability is defined as a measure of the software's ability to represent a wide range of environmental conditions and was evaluated through the range of conditions over which the software was tested and the number of problems analyzed.

Section 4 — SADA Evaluation

SADA Technical Approach

For sample optimization and quantification of uncertainties in predicted values, the technical approach applied in SADA is based on geostatistics. Geostatistical methods are based on the premise that measured variables located close to each other will have similar values, while variables far apart will have little correlation between their corresponding values. A statistical measure for this interrelationship is summarized by the correlation between measured variables measured at different points in space. This measure or related measures, such as the variogram and covariance, form the central idea around which linear estimation methods in geostatistics operate. The use of correlation measures also separates this estimation method from other interpolation algorithms such as inverse distance, nearest neighbor, linear interpolation, splines, and quadrature methods. Using a statistical estimator allows the estimation error to be calculated along with the estimate. Thus, a geostatistical method provides both the most likely value and an estimate of the range of other possible values for a given location. This is important information because the spatial variability present in most variables is such that error-free estimation is not possible. In fact, often there are many possible solutions to the estimation problem that agree with the measurements (Appendix B). Ordinary and indicator kriging, which are estimation methods available in SADA, represent the more common geostatistical methods used to provide smoothed estimates of variables.

For human-health risk analysis, SADA has toxicological exposure databases and databases for five land-use scenarios and multiple exposure pathways. Default values for the different land-use scenarios (residential, agricultural, recreational, and excavation) and exposure pathways (ingestion, inhalation, dermal contact, external radiation, and food consumption) used in the risk assessment calculations follow EPA guidance (EPA 1989) and can be modified by the user for site-specific applications. The exposure concentrations used in the risk assessment can be based on interpolated estimates of the measured values and adjusted for probability level.

SADA Implementation of Geostatistical Approach

SADA imports measured data, defines a grid (i.e., divides the area of concern into a number of 2-D rectangular blocks), provides algorithms to calculate the spatial correlation of the data in 2-D (i.e., generates a variogram), and from the variogram obtains estimates for the parameters necessary for kriging interpolation of the data. The kriging process provides an estimate of the most likely value of the variable and a statistical measure of the variability expected at that location. SADA help files provide guidance for calculating the spatial correlation and kriging parameters. For 3-D problems, the data is sliced into vertical sections and a 2-D analysis is performed for each vertical layer and then summarized into 3-D images.

In estimating the volume of contaminated media that contains contamination at levels above the cleanup level as a function of probability levels, SADA performs an analysis for each vertical layer defined by the analyst. In this approach, SADA determines the contamination volume as a function of probability by using one of the two available geostatistical interpolation algorithms (indicator kriging or ordinary kriging) to calculate the nominal value and associated standard deviation at every location in the model. For the case of the 90% probability level, at each model location an estimate of the concentration is obtained such that 90% of the time, the actual value is expected to be greater than the estimated value for that nominal concentration and standard deviation. Thus, the resulting estimate of contamination is the region in which there is a 90% probability that contamination region is at least that large. The approach used in SADA is consistent with the EPA data quality objectives guidance (EPA 1994).

The objective in sample optimization is to collect samples at the locations that will provide the maximum amount of information to define the extent of contamination. Depending on the interpolation scheme used, five schemes may be used to select sample locations: adaptive fill, estimate rank, variance rank, percentile rank, and uncertainty rank. Adaptive fill is useful during early

stages of analysis when data are sparsely located and the statistics of the data are not well defined. As more data are collected, the other techniques, which use the data and its statistical properties, can be used to assist in selection of sample locations.

Description of Test Problems

SADA is an environmental decision support software product that incorporates tools from various fields — including visualization, geospatial analysis, statistical analysis, human health risk assessment, cost-benefit analysis, sampling design, and decision analysis — into a dynamic and interactive environment. UTRC used SADA to analyze problems for Sites N and S; SADA addressed all three endpoints of the demonstration. As part of the demonstration, several dozen visualization outputs were generated. A few examples that display the range of SADA's capabilities and features are included in this report. A general description of each test problem and the analysis performed using SADA follows. Detailed descriptions of all test problems are provided in Appendix A and in Sullivan, Armstrong, and Osleeb (1998).

Site N Sample Optimization Problem

The objective of the Site N sample optimization problem was to challenge the software's ability to develop a sample optimization scheme to characterize a 125-acre site. The Site N data set contained the most extensive and reliable data set for evaluating the accuracy of the analysis for a soil contamination problem. To focus only on the accuracy of the soil sample optimization analysis, the test problem was simplified by removing information regarding groundwater contamination at this site and by limiting the problem to three contaminants.

This test problem considers surface soil contamination (2-D) for three contaminants — arsenic (As), cadmium (Cd), and chromium (Cr).The analyst was given an extensive data set for a small region of the site (<10 acres) that was highly contaminated and asked to develop a sample optimization scheme to define the extent of contamination on the entire site as defined by two threshold concentrations for each contaminant (Table 3). Budgetary restraints limited the number of additional sample locations to 80. Because of the limited number of samples, the analyst was asked to supply estimates of the extent of contamination based on the confidence in their results.

SADA was used to perform an iterative analysis in which several suggested sample locations were requested. Data from these locations were supplied to the analyst, and this information was used to define the next set of sample locations. The process continued until data at the 80 additional sample locations were provided. SADA was used to produce a site map with all sample locations color-coded by concentration, concentration contour maps for each contaminant, and maps of the probability of exceeding the arsenic threshold concentration of 500 mg/kg.

Site N Cost-Benefit Problem

The objective of the Site N cost-benefit problem was to challenge the software's ability to perform cost-benefit analysis as defined in terms of area of contaminated soil above two threshold concentrations for three contaminants. The Site N data set contained the most extensive and reliable data set for evaluating the accuracy of the analysis for a soil contamination problem. To focus only on the accuracy of the soil cost-benefit analysis, the problem was simplified by removing information regarding groundwater contamination at this site and by limiting the problem to three contaminants.

This test problem considers surface soil contamination (2-D) for three contaminants — As, Cd, and Cr. The developers were given an extensive

Table 3. Site N soil contamination threshold concentrations for the sample optimization problem

Contaminant	Minimum threshold concentration (mg/kg)	Maximum threshold concentration (mg/kg)
Arsenic (As)	125	500
Cadmium (Cd)	70	700
Chromium (Cr)	370	3700

data set for a small region of the site and asked to conduct a cost-benefit analysis to evaluate the area and cost for remediation to achieve specified threshold concentrations provided in Table 4.

SADA estimated the areal extent of the soil contamination by taking the supplied contaminant concentration data and interpolating over the region. The following output was generated for this problem:

- for each contaminant (As, Cd, and Cr), a map with roads, water bodies, and buildings overlain with concentration contours at the specified threshold concentrations;
- a map with the contaminated areas defined as a function of the probability of exceeding specified threshold concentrations at defined probability levels of 10, 50, and 90%;
- an estimate of the area of contamination of each contaminant above its minimum threshold concentration at defined probability levels of 10, 50, and 90%;
- curves of remediation costs for each contaminant's minimum threshold concentration and probability levels of 10, 50, and 90%; and
- noncarcinogenic and carcinogenic risk maps for each contaminant as well as summed noncarcinogenic and carcinogenic risk maps (i.e., sum of risks from As, Cd, and Cr).

Site S Cost-Benefit Problem

The Site S cost-benefit problem was designed as a method for assessing the accuracy with which the software can predict the volume and area of contamination to assist in cost-benefit analysis as a function of cleanup goals. Site S contains the most extensive and reliable data set for evaluating the accuracy of the analysis for a 3-D groundwater problem. To focus only on the accuracy of the analysis, the problem was simplified by removing information regarding surface structures (e.g., buildings and roads) and selecting only one contaminant for the test problem.

This test problem was a 3-D groundwater contamination cost-benefit problem for a single contaminant, chlordane. The data consisted of a series of wells containing chlordane concentrations as a function of depth. The analyst was asked to define the region, mass, and volume of the plume at contamination concentrations of 5 and 500 μg/L. The analysis could be extended to include definition of the plume volumes as a function of three probability levels, 10, 50, and 90%.

SADA estimated the extent of the plume by dividing the data into strata that were 5 ft thick and analyzing the contaminant data in each stratum. Then, each stratum was combined to produce 3-D depictions of the chlordane contamination. The analysis by SADA produced the 2-D region contaminated by chlordane as well as 3-D plume maps. SADA was used to generate the following output for this problem:

- graphics of chlordane contours for each 5-ft interval (2-D depiction);
- a 3-D chlordane contour plume map;
- chlordane-concentration contour maps for specified threshold concentrations of 5 and 500 μg/L;
- maps (2-D and 3-D) indicating areas where the 5-μg/L chlordane threshold concentration was exceeded at 90% probability; and
- maps (2-D and 3-D) of carcinogenic risk estimates based on ingestion of chlordane-contaminated groundwater for a residential scenario.

Table 4. Site N soil contamination threshold concentrations for the cost-benefit problem

Contaminant	Minimum threshold concentration (mg/kg)	Maximum threshold concentration (mg/kg)
Arsenic (As)	75	500
Cadmium (Cd)	70	700
Chromium (Cr)	370	3700

Evaluation of SADA

Decision Support

During the demonstration, SADA was able to quickly import data on contaminant concentrations and site maps and integrate this information on a single platform. SADA demonstrated the ability to place the information in a visual context and generated 2-D and 3-D maps that support data interpretation and decision-making. SADA was used in the demonstration to automatically generate contaminant concentration maps, recommended cleanup zones, cost-benefit curves, and human health risk maps. These maps can be based on the probability of exceeding specified contaminant threshold concentrations or risk levels and at specified probability levels. SADA was also used to predict new sample locations based on geostatistical analysis of the existing data. The accuracy of the analysis is discussed in the section on comparison of SADA results with baseline data and analysis.

Documentation of the SADA Analysis and Evaluation of the Technical Approach

For each analysis, UTRC provided a step-by-step description of the SADA manipulations necessary to import data provided and perform the desired analysis. The steps proceeded logically and in a straightforward manner. Manipulations to format the data within the SADA architecture were relatively simple. Files containing data were supplied to the analyst using a .dbf format. Prior to using these files in SADA, these files were imported into another program (Microsoft Excel) and saved using ASCII comma-delimited file format (.csv). Discussions occurred on the choice of the different model approaches (adaptive fill, rank uncertainty, etc.) used in performing the sample optimization problem. Model selection and parameters for contouring, human health risk assessment, and cost-benefit analysis were also provided in the output files and documentation. The technical approach used by UTRC followed standard practices.

Comparison of SADA Results with the Baseline Analysis and Data

Site N Sample Optimization Problem

For the Site N sample optimization test problem, data from soil samples from the southwest corner of the site, which indicated contamination above the threshold concentrations, were provided to the analyst. Figure 1 presents a site map with overlays of roads, ponds, and creeks. Initial sample locations are marked with the symbol + and arsenic contours are shown for threshold concentrations of 125 and 500 mg/kg. Since this initial region contained data covering only a small area of the entire site, the test problem required that additional sample locations be determined to characterize contamination for the entire site. UTRC initiated the analysis by using SADA to plot sample locations and contaminant data for As, Cd, and Cr. Although UTRC evaluated all three contaminants, only the results for arsenic are presented in this report. Next, SADA was used to predict additional sampling locations to define the boundary of arsenic contamination in the initial region in the southwest corner. SADA required four rounds of sampling and a total of 19 additional samples to bound the initial small region of contamination. Next, the UTRC analyst used the adaptive fill model in SADA to obtain an additional 40 sample locations throughout the entire site. Using this information, the analyst performed rank uncertainty analysis (in which locations with the highest uncertainty in exceeding the threshold concentration are selected for sampling) to select the final 21 sampling locations. During the analysis, UTRC examined the effect of model parameters (correlation length and probability level) for the area predicted to exceed the threshold concentration.

Figure 2 shows the final sample locations selected by UTRC using SADA for the area of concern at Site N. Color-coded circles denote sample locations. The highest arsenic concentrations are denoted in red and the lowest concentrations in purple. From the SADA-generated map, it can be seen that the entire area of concern has been evaluated with more samples taken in the regions of higher concentrations. Figure 3 presents the final nominal arsenic concentration contour map as determined using SADA and the data obtained through the 80 additional samples. The map is color-coded based on default concentrations and the maximum concentration. This makes it extremely difficult to judge the location of the regions above the threshold concentrations of 125 and 500 mg/kg, which are not displayed directly on the map. In addition, the choice of dark purple for the regions of low concentration makes it difficult to see the base site map containing streets and other points of reference. During the demonstration, the UTRC analyst showed that the default parameters used in generating the contour maps could be updated, thus incorporating user-specified parameters. Updating to user-specified parameters would have been helpful in comparing the areal extent of predicted contamination with the baseline data, but this was not done for this map.

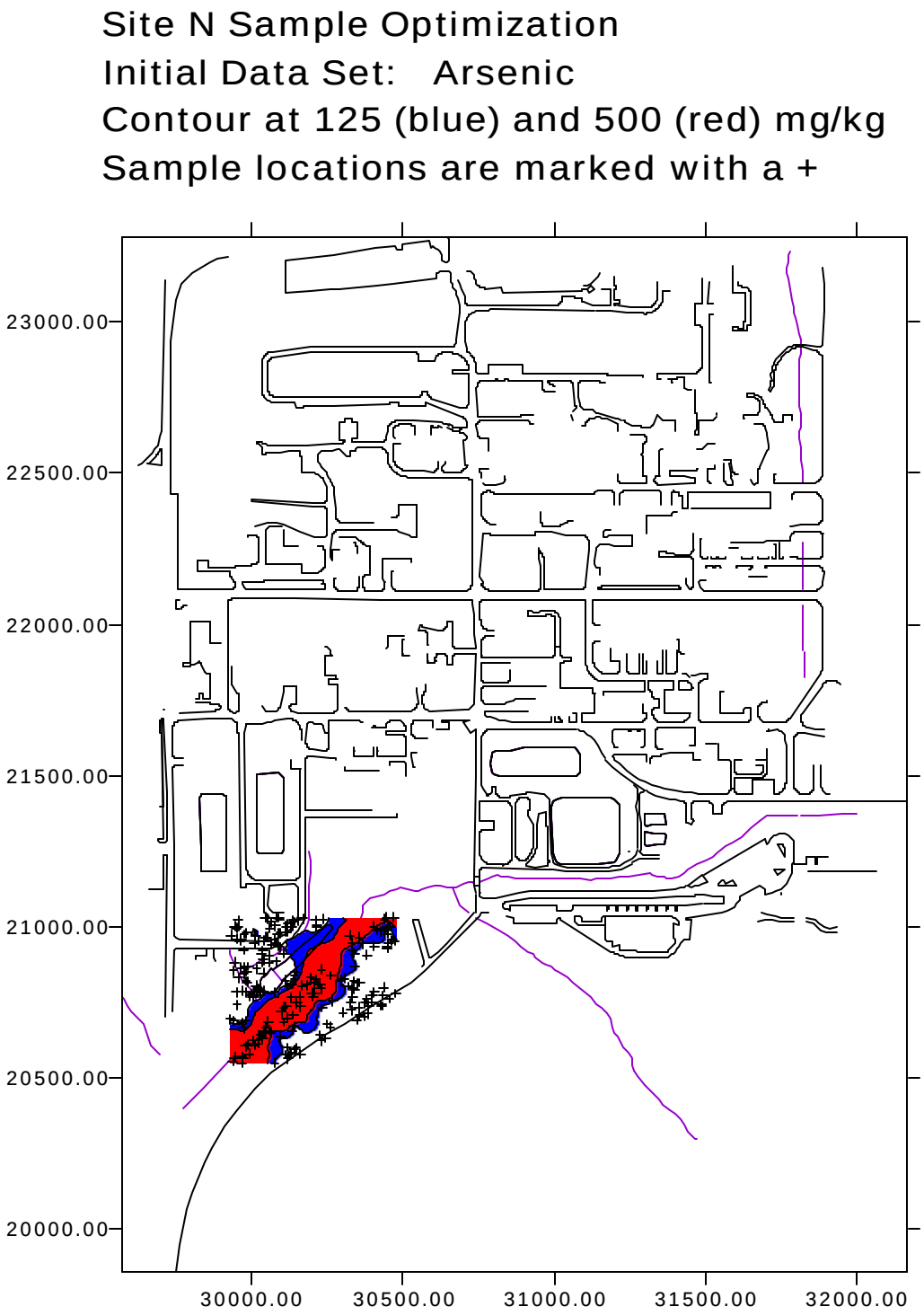

Figure 1. Site N initial sample locations provided to the analyst and arsenic contours for two threshold concentrations (125 and 500 mg/kg).

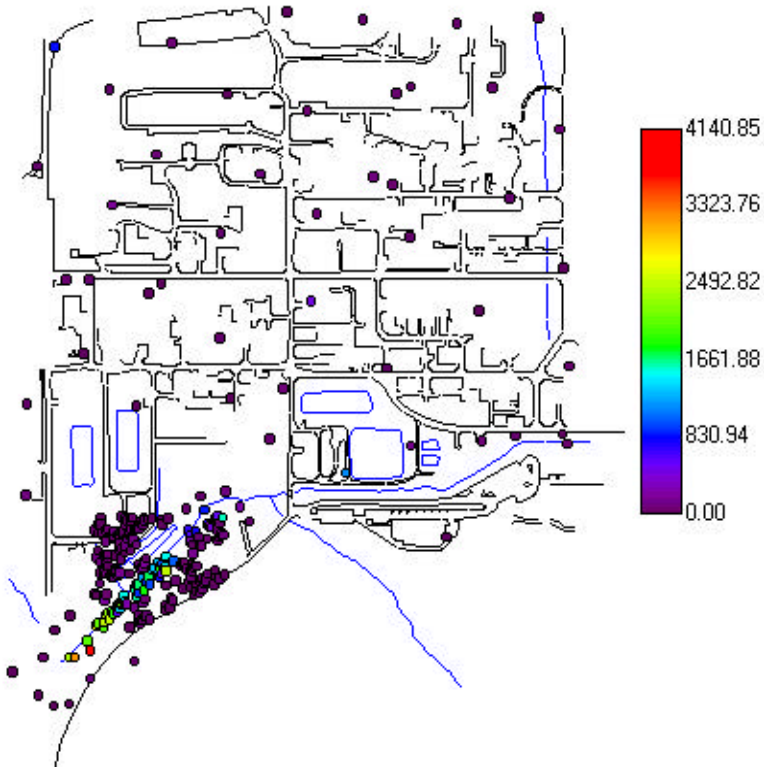

Figure 2. Site N final sample locations obtained using SADA. Sample locations are color-coded, with red indicating the highest arsenic concentrations and purple the lowest.

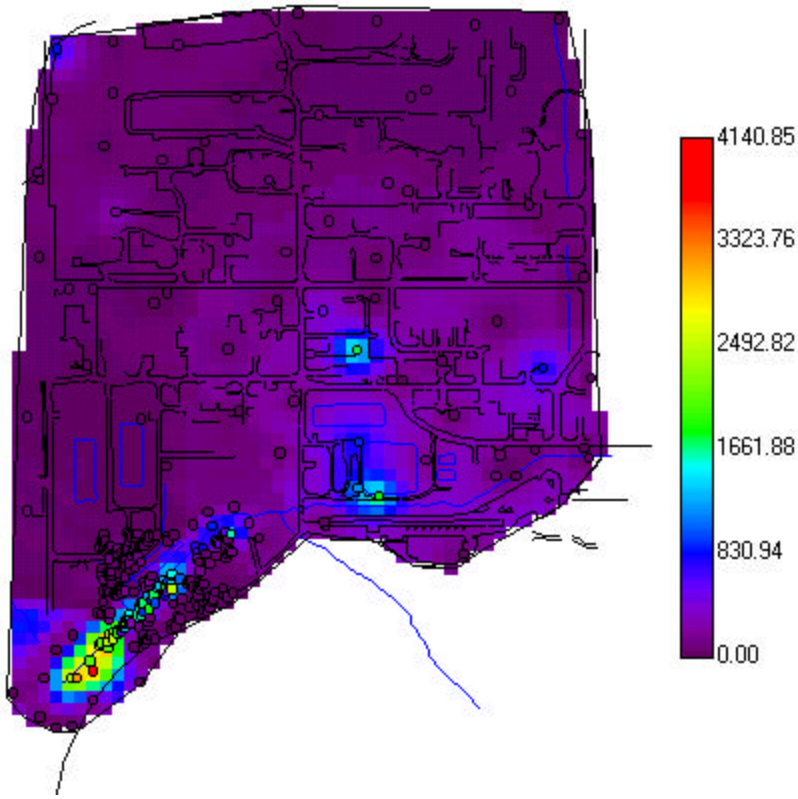

Figure 3. SADA contour map for Site N arsenic concentration after completion of the sample optimization.

Figure 3 shows several areas of the site to be above the arsenic threshold concentrations of 125 and 500 mg/kg. Areas colored blue, green, or red are above the 500 mg/kg threshold concentration. Areas in light purple may be above the 125 mg/kg threshold, but this is not clear. Areas in dark purple are below the minimum threshold concentration of 125 mg/kg.

For the baseline analysis of Site N using the entire data set (4,187 sample points), the technical team used two approaches to generate multiple lines of reasoning. The first approach consisted of evaluating the entire data set using the ordinary kriging interpolator in Surfer (Figure 4). In addition, the data set was evaluated using indicator kriging approach available in GSLIB Version 2.0, as shown in Figure 5. A comparison of these two figures indicates that the two approaches yielded similar results, thus providing a baseline for comparison to the SADA results. A comparison of SADA results (Figure 3) with the baseline results (Figures 4 and 5) indicates that SADA was able to define most, but not all, of the regions contaminated above the

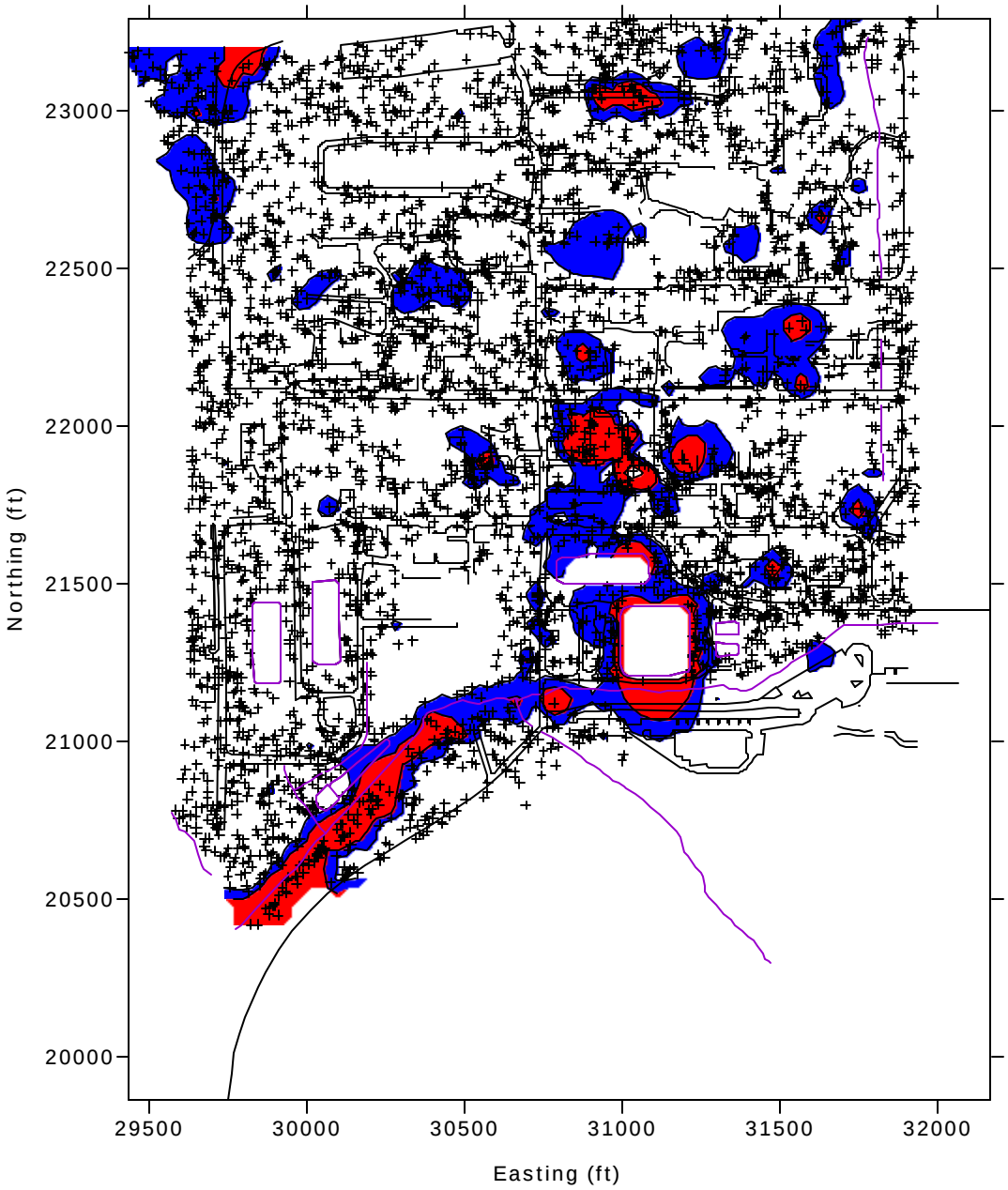

Figure 4. Baseline analysis generated by Surfer for the Site N sample optimization problem. Arsenic contours are shown at 125 mg/kg (blue) and 500 mg/kg (red). Sample locations are marked with a +.

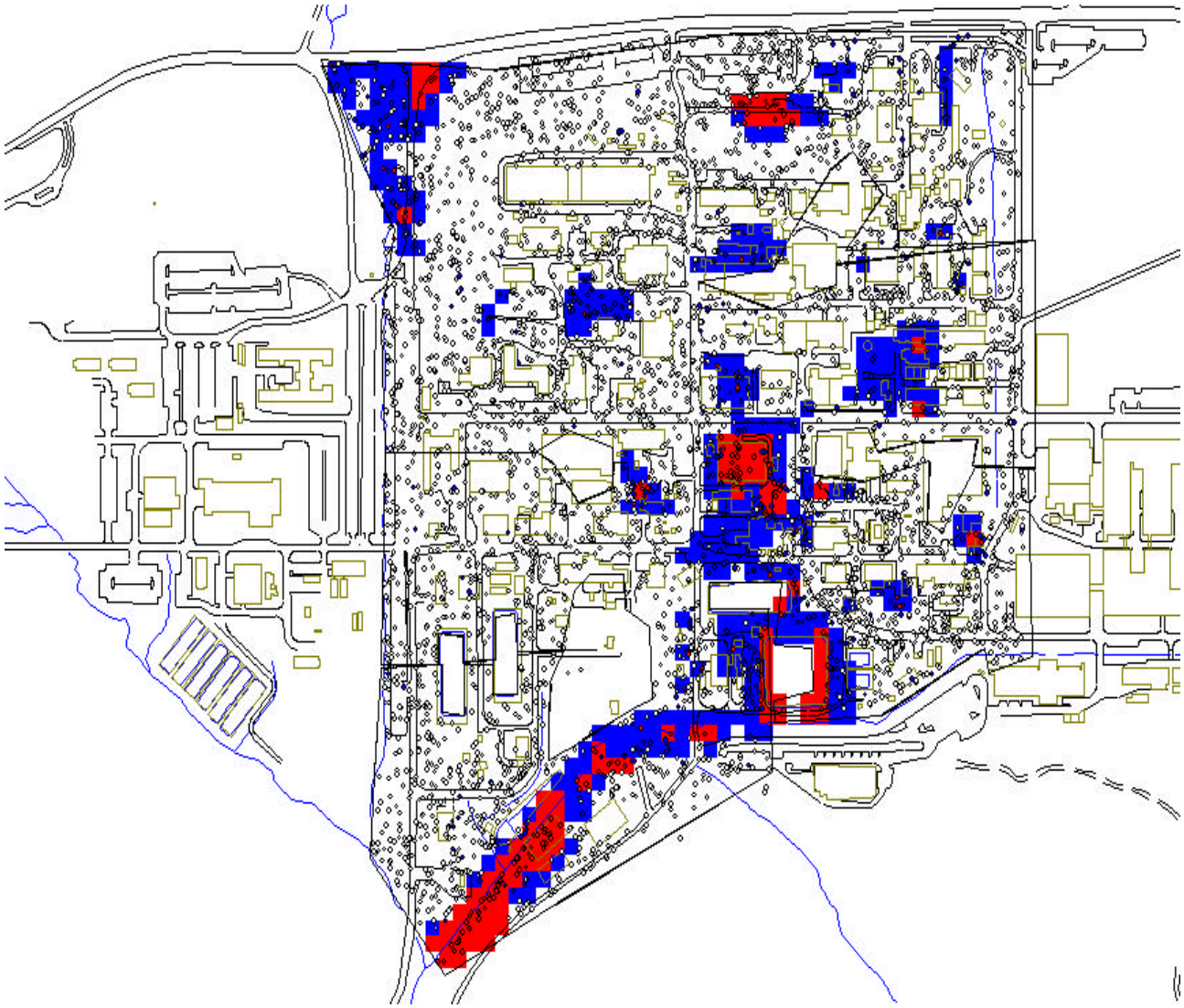

Figure 5. Baseline analysis generated by GSLIB for the Site N sample optimization problem. Arsenic contours are shown at 125 mg/kg (blue) and 500 mg/kg (red). Sample locations are marked with a 'o'.

arsenic threshold concentrations while using only 80 additional data points (2% of the complete data set). The data supplied to the analyst indicated that the southwest corner of the site was contaminated above the threshold levels (see Figure 1). The contours generated with SADA after sample optimization and data collection indicate that there are four newly identified areas of contamination that had arsenic concentrations in excess of 500 mg/kg (blue and green regions in Figure 3).

The baseline and SADA analyses predicted the areas in which the contaminant concentration exceeded the threshold concentration (Table 3). In addition to visual comparison of the results, the calculated areas were used as a basis for comparison. The baseline analysis estimated the area that exceeded the arsenic threshold concentration of 125 mg/kg to be 955,000 ft^2 and the area exceeding the arsenic threshold concentration of 500 mg/kg to be 247,500 ft^2. SADA estimated the area with arsenic concentrations greater than 125 mg/kg to be 714,500 ft^2 and the area greater than 500 mg/kg to be 186,605 ft^2. The SADA estimates were approximately 75% of the baseline analysis. The technical evaluation team concluded that this degree of accuracy was reasonable considering the constraint of 80 additional samples to characterize the entire 125-acre site.

UTRC used SADA to generate maps that estimated the probability of exceeding the 500 mg/kg arsenic threshold. Using these maps, the analyst prepared maps of the area requiring remediation for different

probability levels. Similar analyses were performed for the other two contaminants, cadmium and chromium.

Site N Cost-Benefit Problem

For the Site N cost-benefit test problem, the analyst was given contaminant data for soil on a region of the site that was well characterized. The goal of this test problem was to demonstrate the software's capability to conduct a cost-benefit analysis for soil contamination to support environmental decisions.

UTRC initiated the analysis by using SADA to plot the sample locations and contaminant data on a map with overlays of roads and water bodies (Figure 6). Next, UTRC performed statistical analyses of the data to determine the appropriate geospatial tool not only for interpolating contaminant concentrations between points but also for quantifying the uncertainty in these estimations. Selection of a geostatistical routine is the foundation for determining the area of remediation and for later cost-benefit analysis. Given a correlation structure, the distribution of data points dictates the choice of geostatistical routines. However, the ability to use a geostatistical method depends on the existence of a spatial correlation structure in the data. After examination of the data distributions, UTRC selected indicator kriging for interpolating As, Cd, and Cr concentration data. Use of geostatistical analysis allowed the UTRC analyst to provide results in terms of probability levels or other uncertainty qualifiers. During the geostatistical selection process, UTRC demonstrated the functionality of the multiple statistical and geostatistical routines in the SADA software, thereby providing multiple lines of reasoning. This functionality allows users of SADA software to conduct multiple evaluations; however, ultimately it is up to the analyst to optimize the treatment of the data.

After completion of the spatial correlation modeling, SADA was used to generate contaminant concentration contour maps and conduct cost-benefit analyses. The application and utilization of indicator kriging to produce these maps and conduct the cost-benefit analyses was demonstrated to be straightforward using SADA. Figure 7 is a plot of arsenic concentration contours generated by SADA. Figure 8 presents the test team's baseline analysis, obtained by interpolation of the data with Surfer. The lack of a direct correspondence between the threshold levels and the contour levels in the SADA analysis (Figure 7) makes comparison difficult. However, there is general agreement between the two analyses. Again, the choice of dark purple for

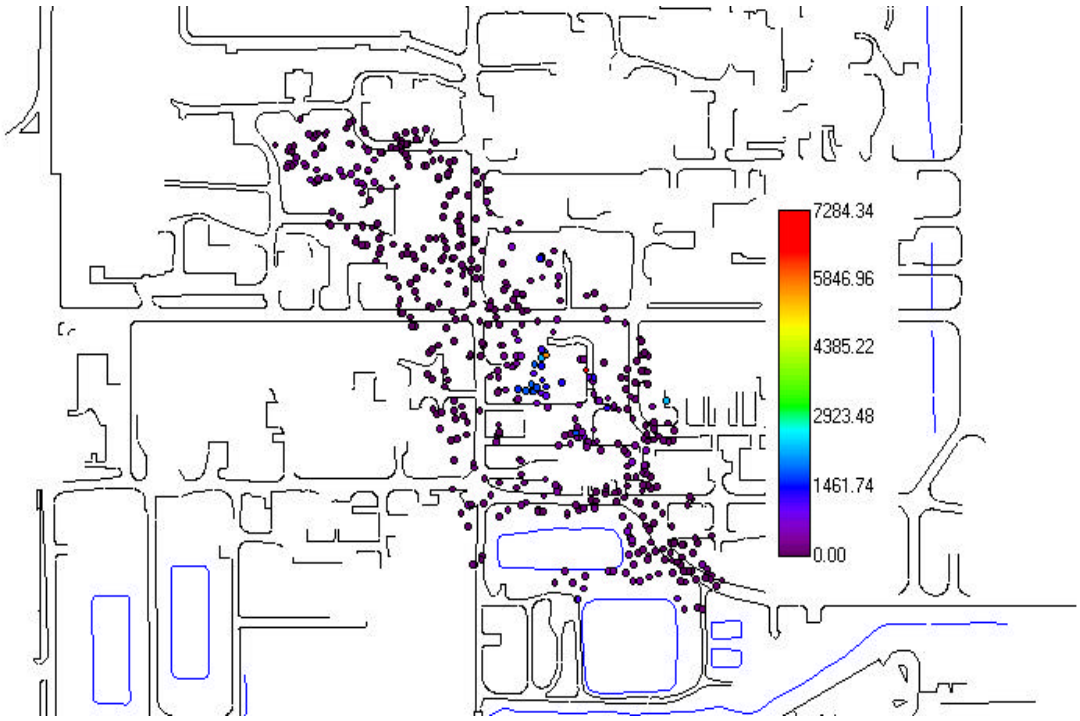

Figure 6. Sample locations and arsenic concentrations (mg/kg) generated by SADA for the Site N cost-benefit problem.

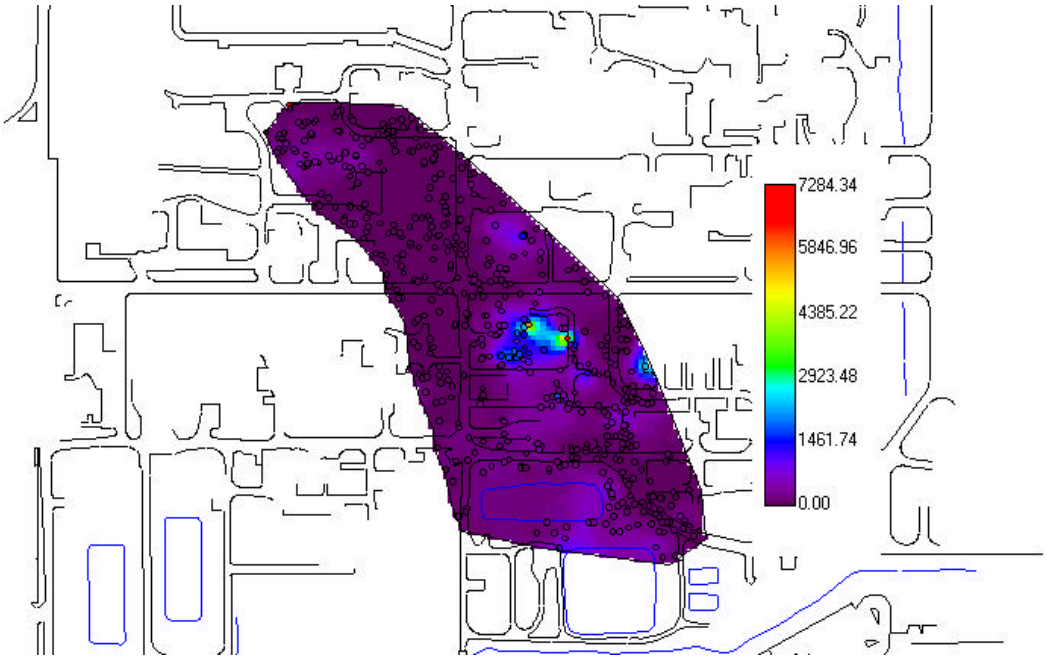

Figure 7. Arsenic contours (mg/kg) generated by SADA for the Site N cost-benefit problem.

the region of low concentration makes determination of exact locations on the site difficult. A transparent color would have been a better choice.

The test problem definition requested the analyst to estimate the area of contamination at three probability levels (10%, 50%, and 90%) for each threshold concentration. The probability level corresponds to the amount of uncertainty in the decision. The 10% probability level is the level at which the analyst believes that there is a 10% probability that the concentration of the contaminant at a specified location exceeds the threshold concentration. This leads to a maximum estimate of the contaminated region. Similarly, the 90% probability level corresponds to level at which the analyst believes that there is a 90% probability that the concentration of the contaminant at a specified location exceeds the threshold concentration. Based on the arsenic contours, SADA was used to define remediation zones for removing arsenic-contaminated soil at the 75 mg/kg threshold at the 50% probability level (Figure 9) and the 90% probability level (Figure 10). The gray highlighted regions in these figures represent the areas that exceed the threshold. The area exceeding the 75 mg/kg arsenic concentration is much smaller at the 90% probability level than at the 50% probability level, consistent with the higher probability of exceeding the threshold. Figure 9, depicting the 50% probability level, shows a very close agreement with the baseline analysis at the 75 mg/kg arsenic threshold, shown in Figure 8. The minor differences near the edges of the predicted contamination zone are caused by the different treatment of the data in the two analyses and the slightly differing selection of data boundaries.

For comparison, baseline area estimates were generated using Surfer to interpolate the data using kriging. Additional baseline analyses were conducted using kriging interpolants in GSLIB and Geo-EAS. Table 5 presents the area estimates of the baseline kriging analysis, baseline geostatistical analysis at the 50% probability level, and the SADA analysis at the 50% probability level. When comparing SADA results to the baseline geostatistical analysis, the area contaminated with arsenic estimated by SADA was 20% less than the baseline analysis. Likewise, the area contaminated with cadmium was 20% less than the baseline geostatistical analysis whereas the area contaminated with chromium was only 4% less than the baseline analysis. These slight differences between SADA results and the baseline geostatistical area estimates are due to different parameters selected by the analyst during data interpolations using kriging. However, it is concluded that the SADA area estimates at the 50% probability level are consistent with the baseline analysis.

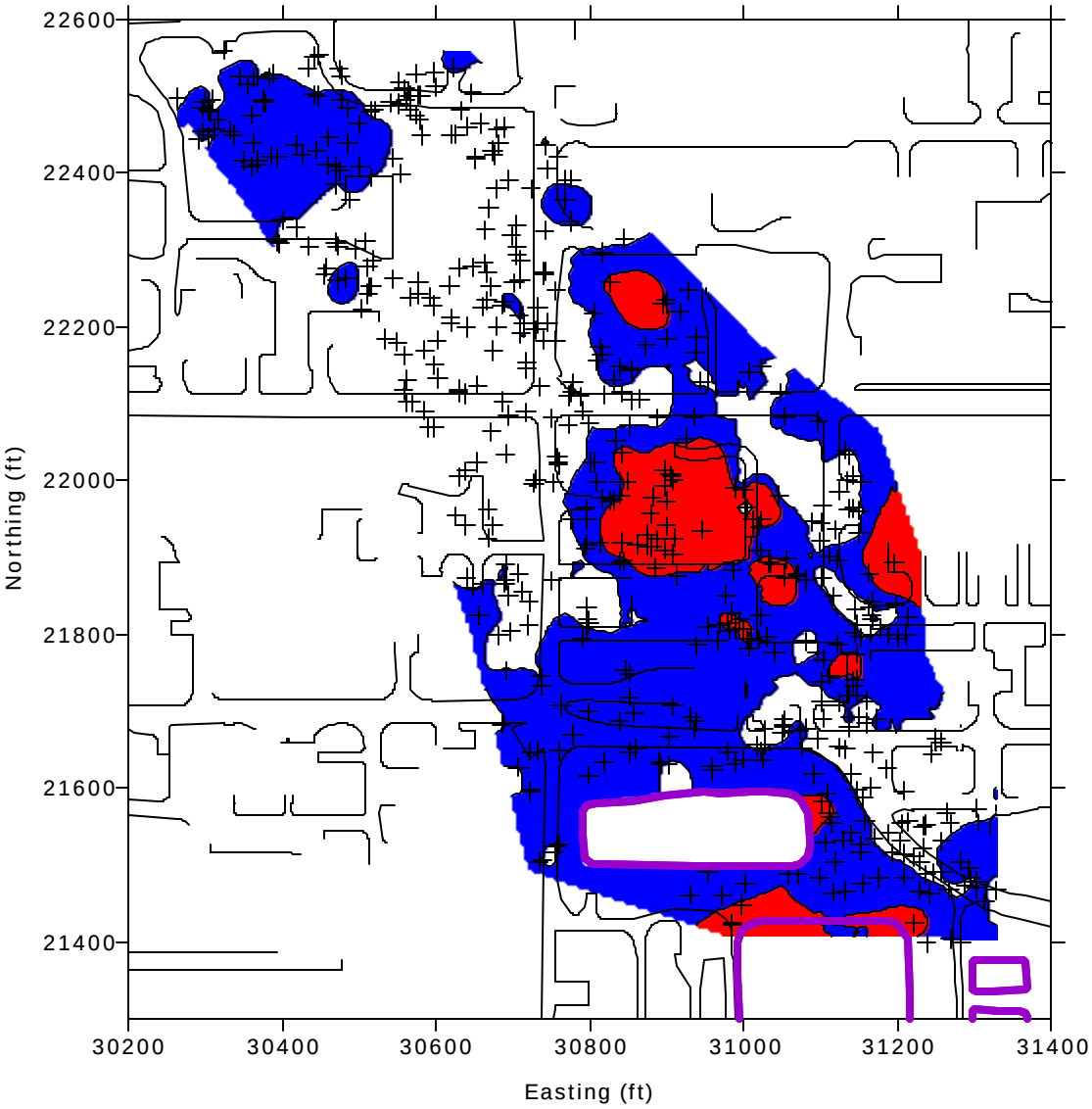

Figure 8. Baseline analysis performed by Surfer, with kriging interpolation of the data, for arsenic concentration contours in the Site N cost-benefit problem. Areas in blue correspond to regions above the arsenic 75 mg/kg threshold. Areas in red correspond to regions above the arsenic 500 mg/kg threshold.

A comparison between SADA results at the 90% probability level and the baseline analysis is presented in Table 6. The 90% probability level corresponds to the level at which the analyst believes that there is a 90% probability that the contamination concentration at a specified location exceeds the threshold concentration. The area estimates generated by SADA for As, Cd, and Cr are 12, 21, and 8%, respectively, less than the baseline analysis. As previously observed, the SADA area estimates are slightly less than the baseline analysis. The difference is due to the difference in the parameters selected for data interpolation by the SADA analyst and the technical team who performed the baseline analysis. However, the technical evaluation team concluded that the SADA generated area estimates at the 90% probability level are consistent with the baseline analysis.

Next, the UTRC analyst used SADA to estimate the cost for remediating the arsenic-contaminated soil. SADA generated cost curves based on the area of the site exceeding the arsenic threshold concentration of 75 mg/kg and an assumed unit cost of \$20/ft^3 for excavating and treating the contaminated soil (Figures 11 and 12). Figures 11 and 12 demonstrate one of the multiple lines of reasoning that SADA can perform to assist decision making. When using SADA, the operator can select any point on the curve to obtain an estimate of cost at a specified cleanup level. This is displayed in Figures 11 and 12 as the pair of numbers

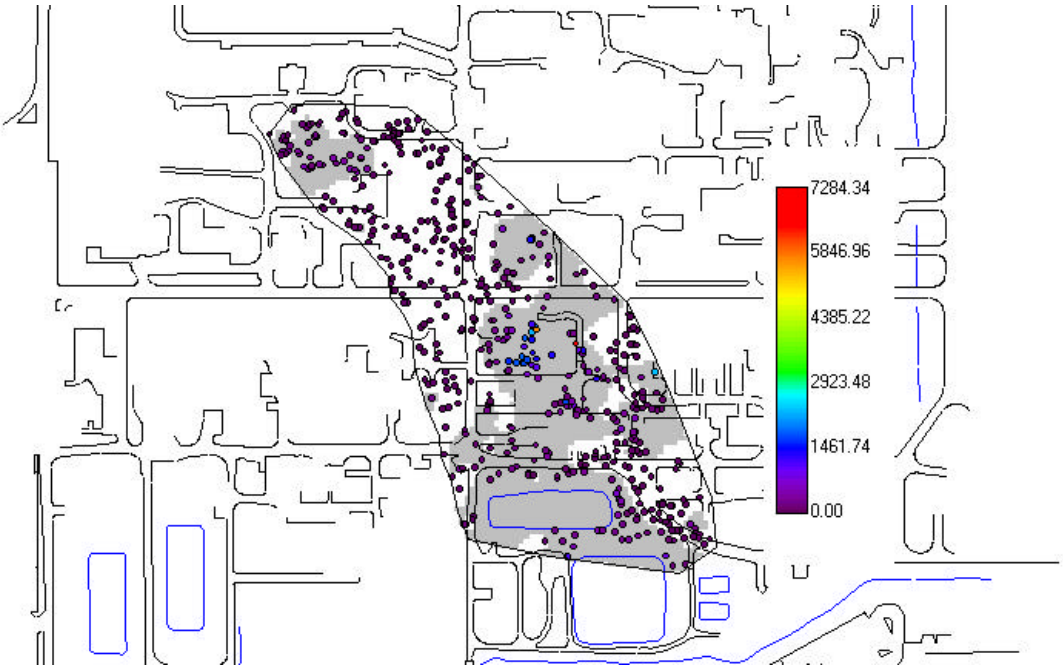

Figure 9. Cleanup zones (gray areas) for arsenic threshold concentration of 75 mg/kg with 50% probability level generated by SADA

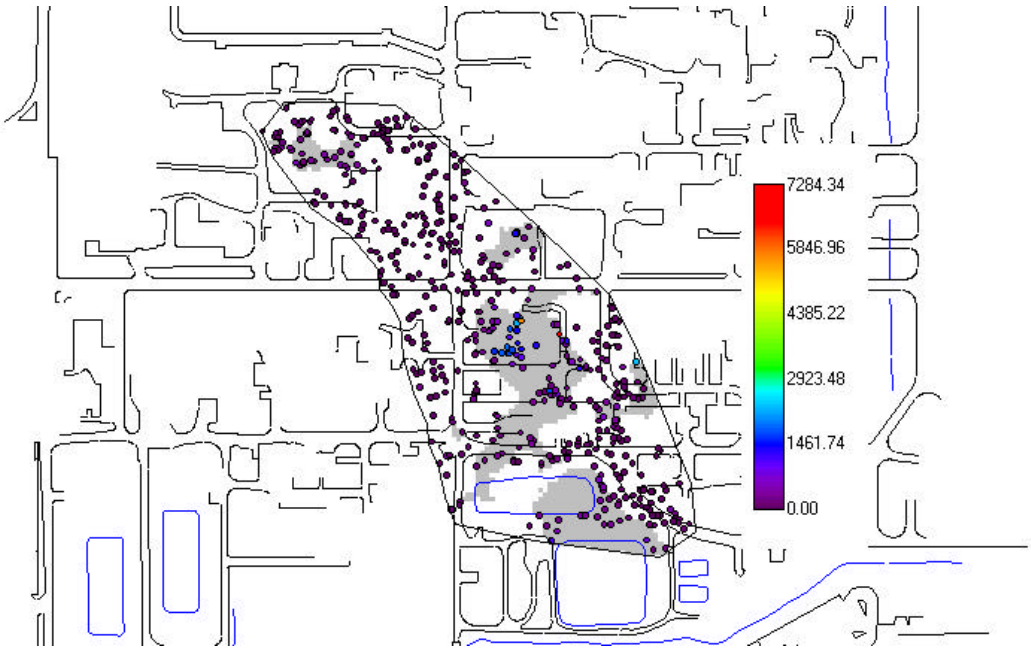

Figure 10. Cleanup zones (gray areas) for arsenic threshold of 75 mg/kg with 90% probability level generated by SADA.

Table 5. Comparison of baseline analyses and SADA area estimates for the Site N cost-benefit test problem at the 50% probability level

Constituent	Concentration threshold (ppm)	Area of contamination (ft^2)		
		Baseline kriging (Surfer)	Baseline kriging (geostatistics 50% probability)	SADA (50% probability)
Arsenic	75	330,000	389,000	312,048
Cadmium	70	285,000	325,000	258,336
Chromium	370	37,100	30,500	29,232

Table 6. Comparison of baseline analyses and SADA area estimates for the Site N cost-benefit test problem at the 90% probability level

Constituent	Concentration threshold (ppm)	Area of contamination (ft^2)	
		Baseline kriging (geostatistics 90% probability)	SADA (90% probability)
Arsenic	75	187,226	164,016
Cadmium	70	155,385	122,976
Chromium	370	12,190	11,232

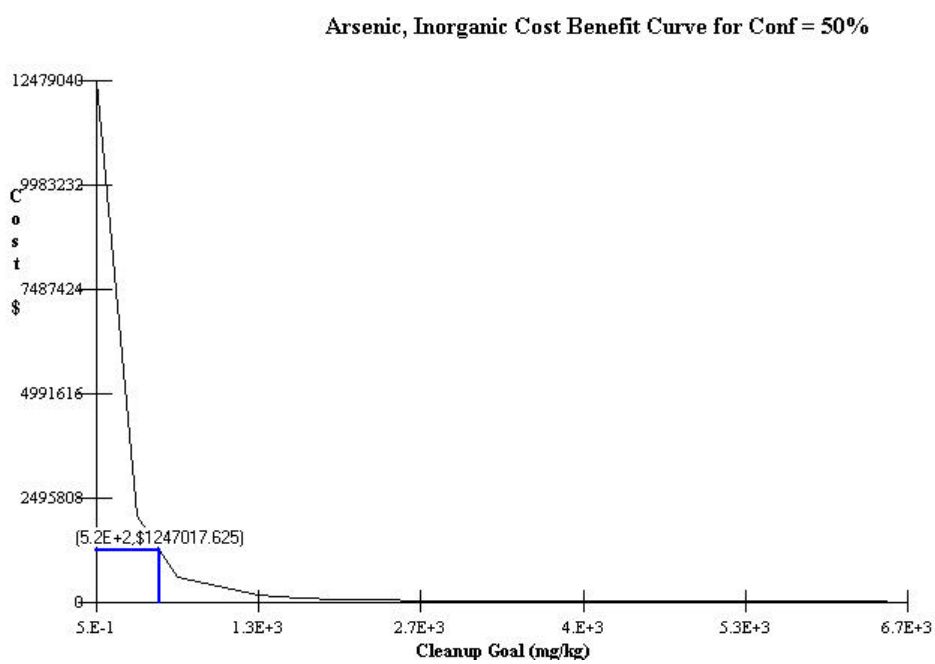

Figure 11. SADA-generated curve for arsenic cleanup costs as a function of concentration at the 50% probability level.

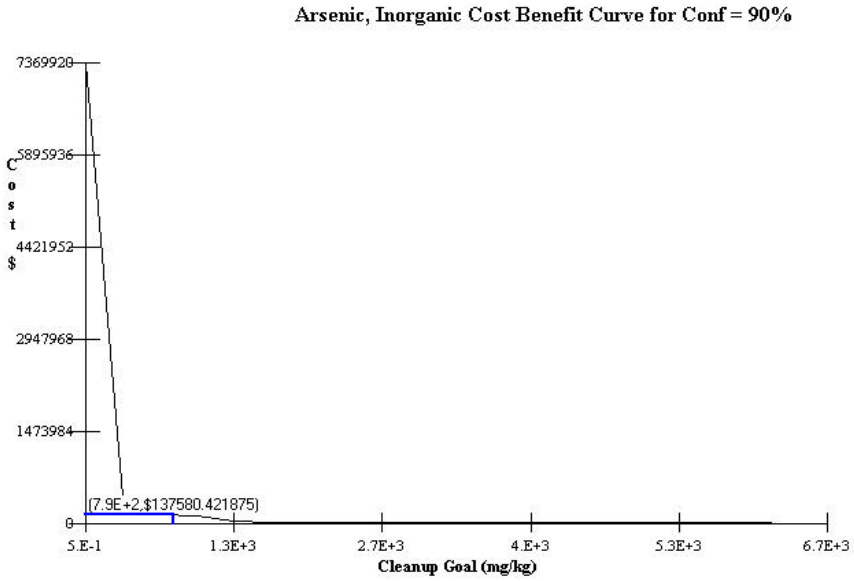

Figure 12. SADA-generated curve for arsenic cleanup costs as a function of concentration at the 90% probability level.

(concentration, cost) above the rectangle in the figures. In this example, for the 50% probability level, the cost to remediate soil contaminated above 520 mg/kg is \$1.25 10^6 (Figure 11), and at the 90% probability level the cost to remediate contaminated soil above 790 mg/kg is \$1.37 10^5 (Figure 12).

To demonstrate the human health risk assessment capabilities of SADA, UTRC calculated both the carcinogenic and noncarcinogenic risks from exposure to contaminated soil. As discussed in Section 2, SADA follows the Risk Assessment Guidance for Superfund Sites (EPA, 1989) and guidance for calculating risk-based preliminary remediation goals (EPA 1991). SADA has a complete data base of parameters to automate the human health risk calculations. The spatially distributed estimates of As, Cd, and Cr soil concentrations after completion of sample optimization were used as input concentrations for the human health risk modules in SADA to calculate risk and present the risk results spatially (Figure 13). SADA calculated risks associated with exposure to a single contaminant (arsenic; Figure 13) and also summed risk from exposure to the three contaminants (As, Cd, and Cr) identified in the test problem (Figure 14). The ability to sum risks is important when multiple contaminants are found at a site. The risk maps could have been improved by operator intervention to change the scale (logarithmic scale would be more appropriate for risk) and color scheme. The use of a linear scale does not allow much differentiation in risk to be seen.

The technical team evaluated the risk calculations in SADA by independently calculating the risks using contaminant concentrations from the baseline data and risk equations documented in EPA's Risk Assessment Guidance for Superfund (EPA 1989) and guidance for calculating risk-based preliminary remediation goals (EPA 1991). The technical team, using the same input parameters as the UTRC analyst and the same approach, independently reproduced the risks calculated by SADA for As, Cd, and Cr as well as the summed risk from exposure to all contaminants for Site N. This is the expected result and indicates that the EPA guidance on calculating human health risk is correctly implemented in SADA

Site S Cost-Benefit Problem

The Site S data set consisted of a series of wells with chlordane concentrations provided on a 5-ft vertical spacing. The test problem was developed to evaluate the software's capability to address a 3-D groundwater contamination problem from a cost-benefit perspective. UTRC used SADA to evaluate the chlordane groundwater data at 5-ft vertical intervals to create both 2-D and 3-D depictions of the contamination. The UTRC analyst began with a data exploration exercise to determine spatial correlation in the data and to define the boundaries of the chlordane contamination. The analyst concluded from the data exploration using SADA

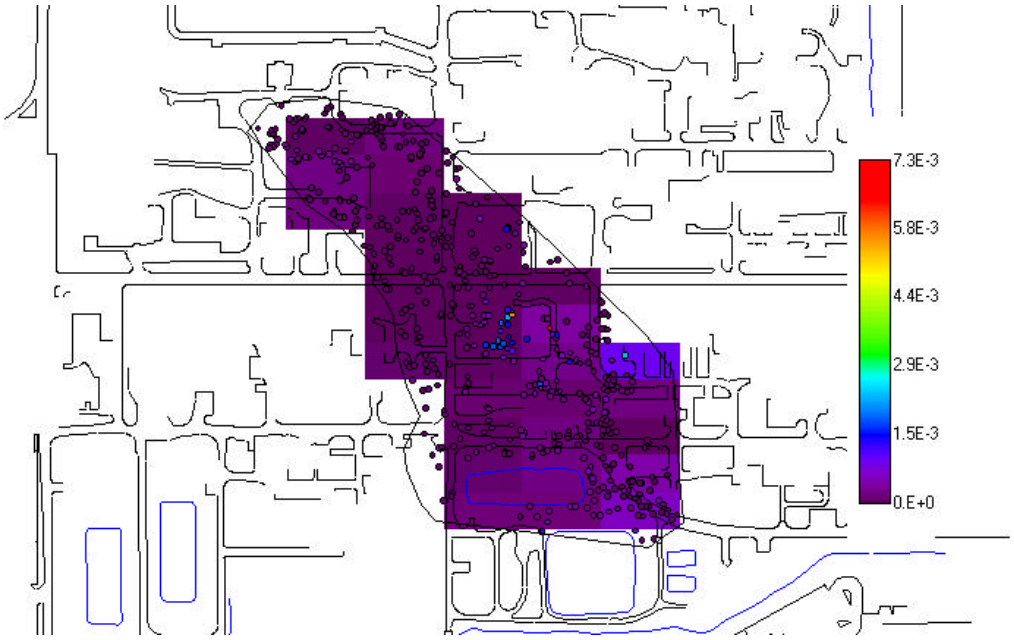

Figure 13. Carcinogenic risk for arsenic based on residential scenario produced using SADA.

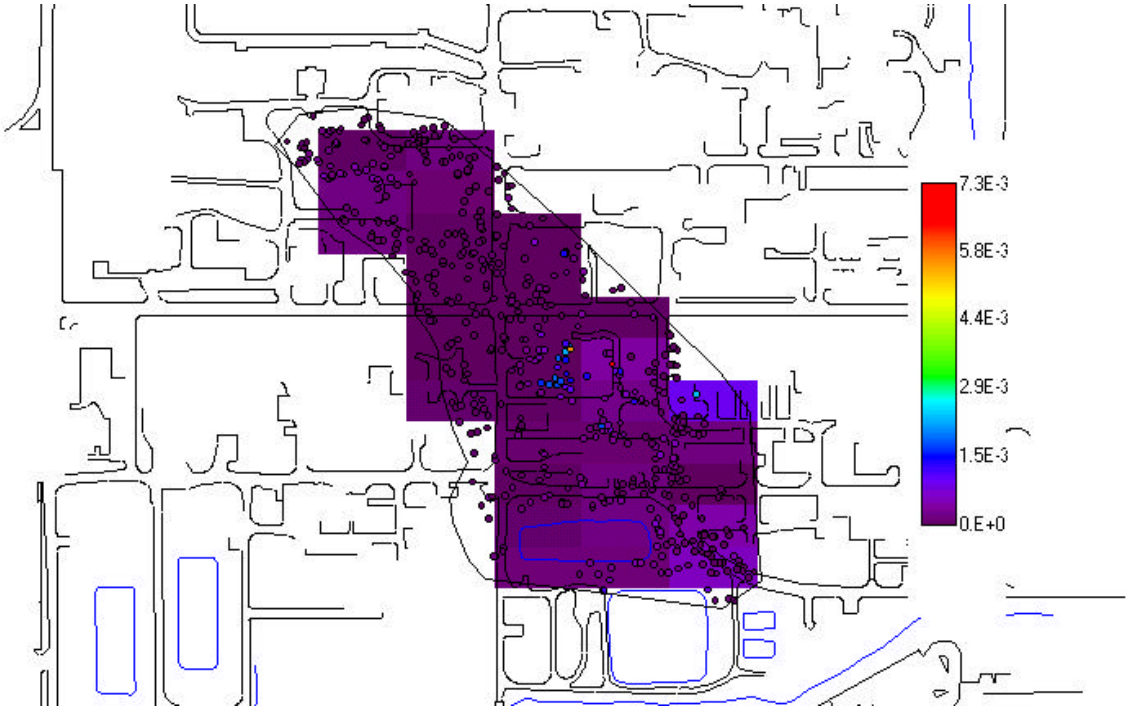

Figure 14. Summed carcinogenic risk for the three contaminants (arsenic + chromium + cadmium).

that the chlordane plume begins near the surface in the north and increases in depth as it travels south. Also, a significant anisotropy in the data was observed and confirmed in the spatial correlation analysis. The analyst also concluded that the data were neither lognormally nor normally distributed, and therefore indicator kriging was the interpolator of choice.

Next, UTRC used the indicator kriging function in SADA to generate 2-D contours of the chlordane data at 5-ft vertical intervals. The 2-D sections were combined to produce a 3-D depiction of the entire chlordane plume (Figure 15). The visualizations presented in Figure 15 could have been better. For the 2-D representation, the visualizations had the following problems:

- The color key did not match the threshold values of 5 and 500 µg/L, making comparison with the baseline analysis difficult.
- The implications of the blank areas near the edge of the plume are not clear. When SADA does not have enough data to obtain a reliable estimate for concentration, the region with inadequate information is depicted without color coding, as is seen in Figure 15.
- The sample locations are marked with a circle, but these are difficult to see.

For the 3-D representation, the lack of coordinates on the axes makes it difficult to interpret the figure. In addition, the fuzzy black region around the plume also makes data interpretation difficult. However, close examination of the 3-D map indicates a plume whose centerline decreases in depth as the distance from the source increases. This trend as depicted — a long, narrow plume that is moving deeper — is generally consistent with the data.

The chlordane data for Site S were generated by the technical team using a simulation model with a constant source of chlordane supplied to the aquifer. Hydrologic and chlordane transport parameters were obtained from field data at Site S and were taken to be constant over the problem domain. These assumptions permitted release and transport of chlordane through the aquifer to be represented by a partial differential equation that was solved analytically. This analytical solution provides an exact value for chlordane concentrations at each location to compare with the SADA results.

To evaluate the accuracy of the plume maps generated by SADA, the demonstration technical team compared the SADA results with the analytical solution as well as with the baseline analysis conducted by the technical team using the same data set as that supplied to UTRC. The baseline analysis was obtained by using Surfer to interpolate the data using ordinary kriging with an anisotropy ratio of 0.3. The concentration contour presented in Figure 16 represents the maximum concentration observed at the location (independent of depth) and provides a 2-D representation of the extent of the plume. Figure 16 shows contours based on the analytical solution and contours based on the baseline analysis. For the 500-µg/L contour, the analytical solution has a length of approximately 1000 ft and a maximum width of 100 ft. The analytical 500-µg/L contour reaches approximately 100 ft farther south than the transect defined by wells DP-122 through DP-125 (Figure 16). Because the Surfer-generated baseline analysis was based on the incomplete data set supplied to UTRC, it does not show the 500-µg/L contour extending as far south as the analytical solution does. Examining the data supplied for the baseline analysis, wells DP-123 and 124 are both below the 500-µg/L concentration limit. Thus, the baseline analysis indicates that the contour does not extend to these locations. The analytical solution, however, shows a region between these wells where the concentration exceeds the threshold, and therefore, the 500-µg/L contour does extend past these locations. The difference seen in the 5-µg/L contour also arises from incomplete data.

The baseline analysis tends to predict a larger area of contamination than does the analytical solution. These discrepancies illustrate the difficulty in obtaining precise plume boundaries without measuring data at every location.

The SADA-generated analysis of the 500-µg/L contour, based on the maximum measured value in each well (Figure 17), provided results (gray-shaded area) consistent with the Surfer baseline analysis depicted in Figure 16. There are minor differences between the SADA and baseline analyses at the leading edge of the 5- and 500-µg/L contours, with the baseline analysis predicting a slightly larger area of contamination. This is due to the different parameters and analysis techniques used in the two analyses.

Further comparison shows that the leading edge of the SADA-predicted 500-µg/L plume (Figure 17) extends to the south approximately 100 ft beyond the transect defined by wells DP-111 through DP-115, indicating a close match with the baseline analysis, in which the plume extended about 200 ft past the transect (Figure 16) The analytical solution indicates a larger area of contamination above the 500-µg/L level and a smaller area of contamination above the 5-µg/L level than either the baseline analysis or SADA analysis. This is expected because the analytical solution contours were based on more information about the plume location. The technical test team evaluated the maps produced by SADA at each vertical level by comparing these with a baseline analysis on the same data set. On the basis of these comparisons, the technical team concluded

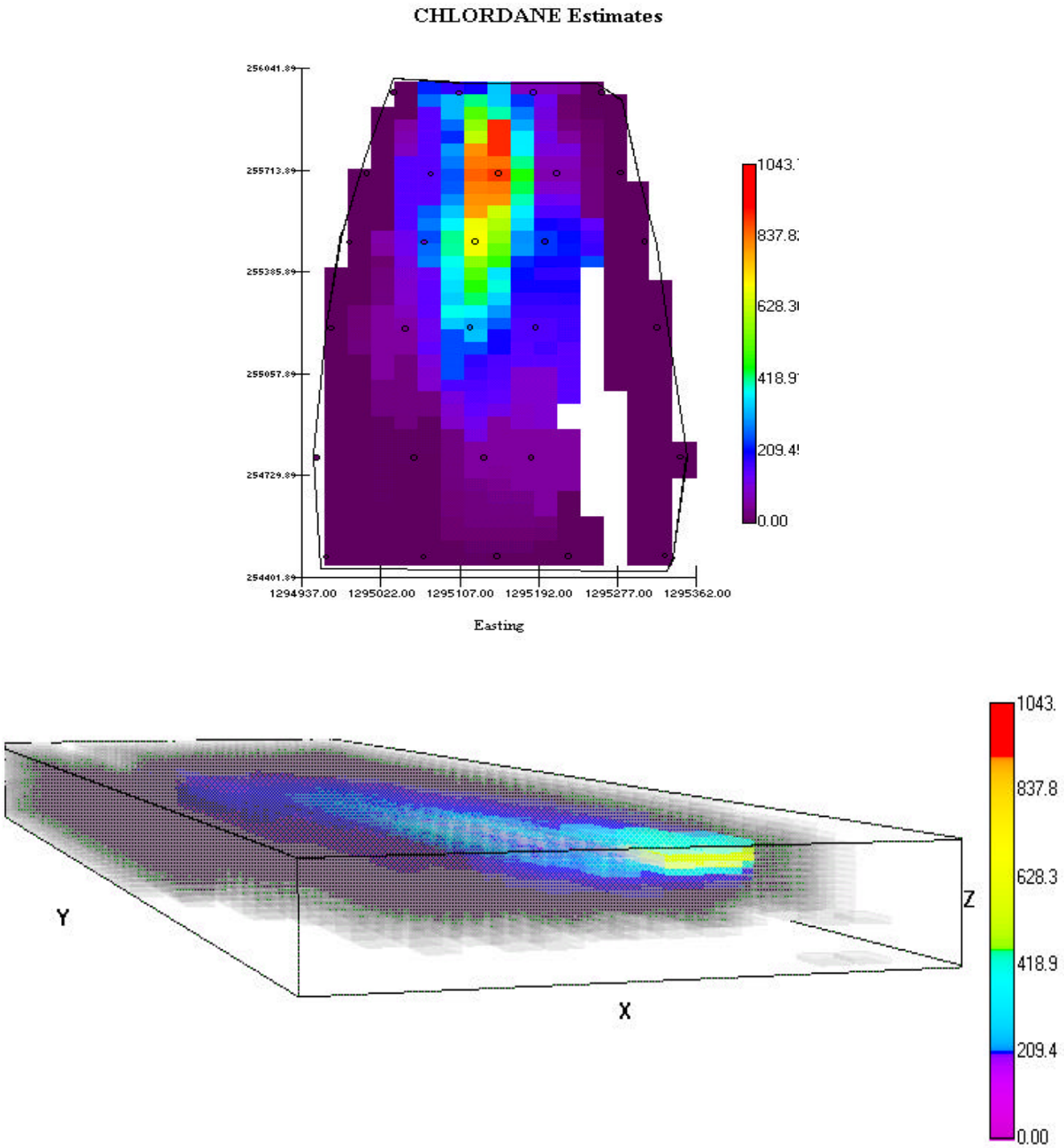

Figure 15. Two-dimensional depiction of chlordane concentrations for one 5-ft interval and 3-D depiction of entire plume generated by SADA for Site S.

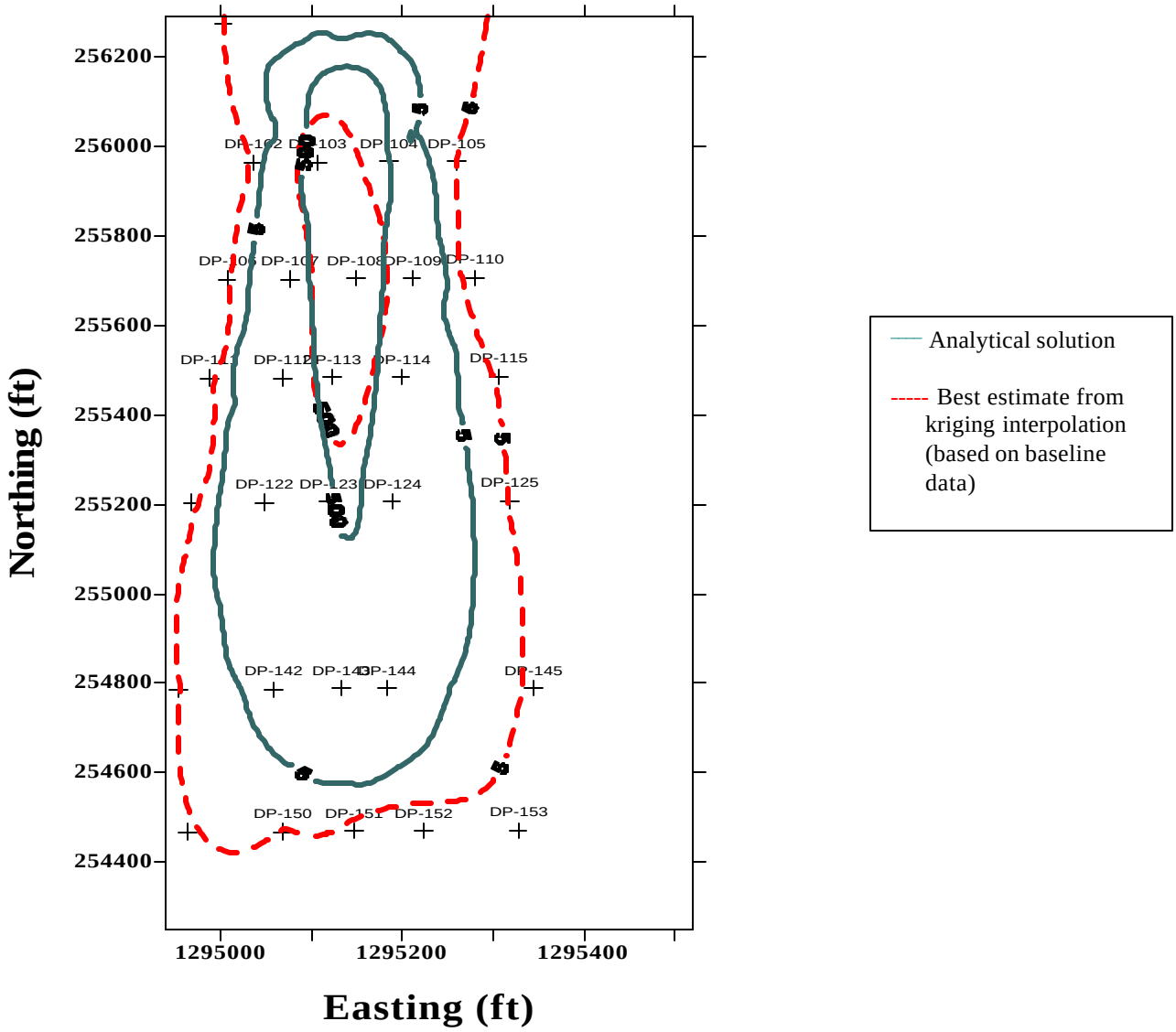

Figure 16. Site S chlordane 5- and 500-µg/L contours for the analytical solution (solid lines) and the baseline contour (dashed line) obtained using kriging with an anisotropy ratio of 0.3. Sample locations are posted (+) and labeled on the map.

that SADA produced an adequate match to the baseline analysis.

To complete the cost-benefit portions of the Site S test problem, UTRC used SADA to produce depictions of areas of chlordane-contaminated groundwater at the chlordane threshold concentrations of 5 and 500 µg/L with probability levels of 10 and 50%. The region enclosed by the 10% probability level contour represents the region in which there is at least a 10% chance that contamination exists above the threshold value and gives a larger estimate of area than the 50% probability level contour. Figure 18 provides an example of the SADA output depicting areas of contamination above the 5-µg/L threshold concentration at the 10% probability level. Figure 18 provides an example of one vertical level and the 3-D representation of the plume. The visualization problems noted for Figure 15 also apply to Figure 18.

For evaluation, the volume of groundwater with chlordane concentrations above the 5-µg/L and 500-µg/L thresholds at the 10 and 50% probability levels estimated by SADA were compared to the volume estimated by the technical team (Table 7). For the 50% probability level, there is good agreement between SADA, the baseline analysis using Surfer, and the baseline geostatistics. In fact, all three volume estimates are with 13% of each other, indicating agreement. For the 10% probability

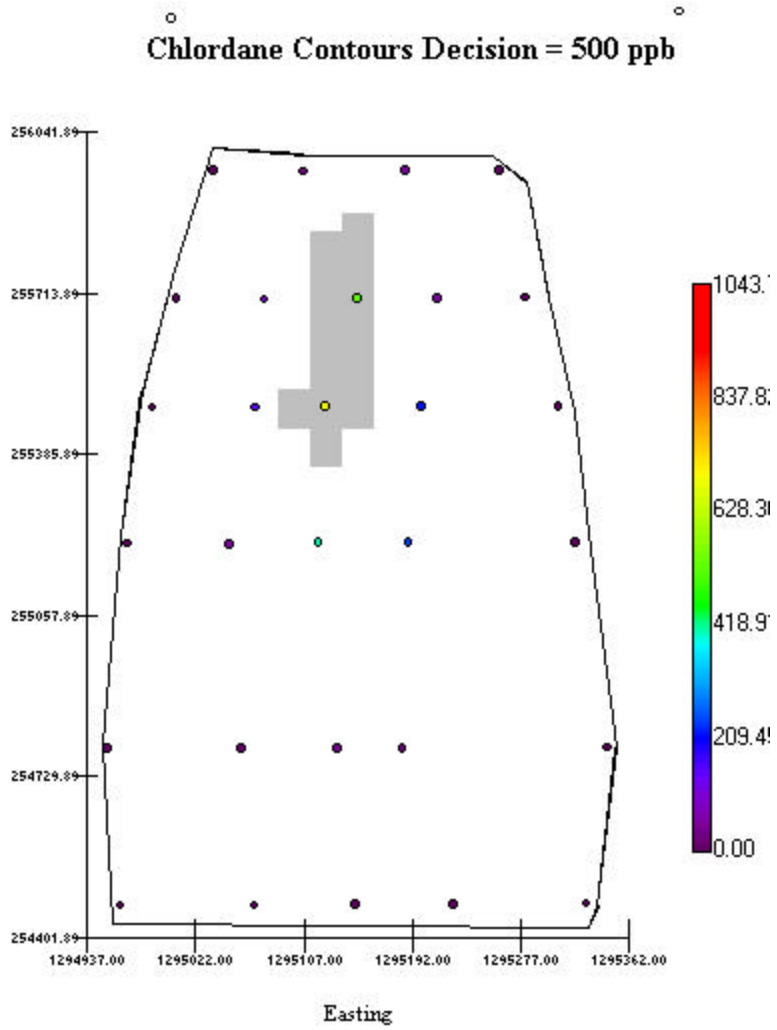

Figure 17. SADA-generated Site S chlordane contours at 500 µg/L produced using the maximum value in each well. Colored circles note sample locations.

level, the SADA volume estimates are 6% less at the 5-µg/L threshold and 9% less at 500 µg/L than the baseline area estimates. The difference between the SADA results and the baseline analysis is due to the slightly different kriging parameters selected for each analysis. Overall, the technical team concluded that there is close agreement among the volume estimates produced by SADA and the baseline geostatistical analysis.

The last analysis conducted by UTRC for Site S was to demonstrate the capabilities of SADA in assessing human health risk. UTRC calculated the carcinogenic risks from exposure to chlordane-contaminated groundwater following EPA guidance (EPA, 1989; EPA, 1991).

The chlordane concentrations were used as input concentrations for the risk modules in SADA to calculate and present the risk results in tabular form as well as spatially in risk maps. Figure 19 presents SADA carcinogenic risk outputs spatially in 2-D (one vertical level) and 3-D. The limitations to these visualizations are similar to those found in Figure 15. In addition, the risk map could have been improved by using a logarithmic scale to provide clearer definition of risk zones.

As in the Site N example, the technical team evaluated the risk calculations in SADA by independently calculating the risks using chlordane concentrations from the baseline data and the risk equations documented in EPA 1989 and in EPA's guidance for calculating preliminary remediation

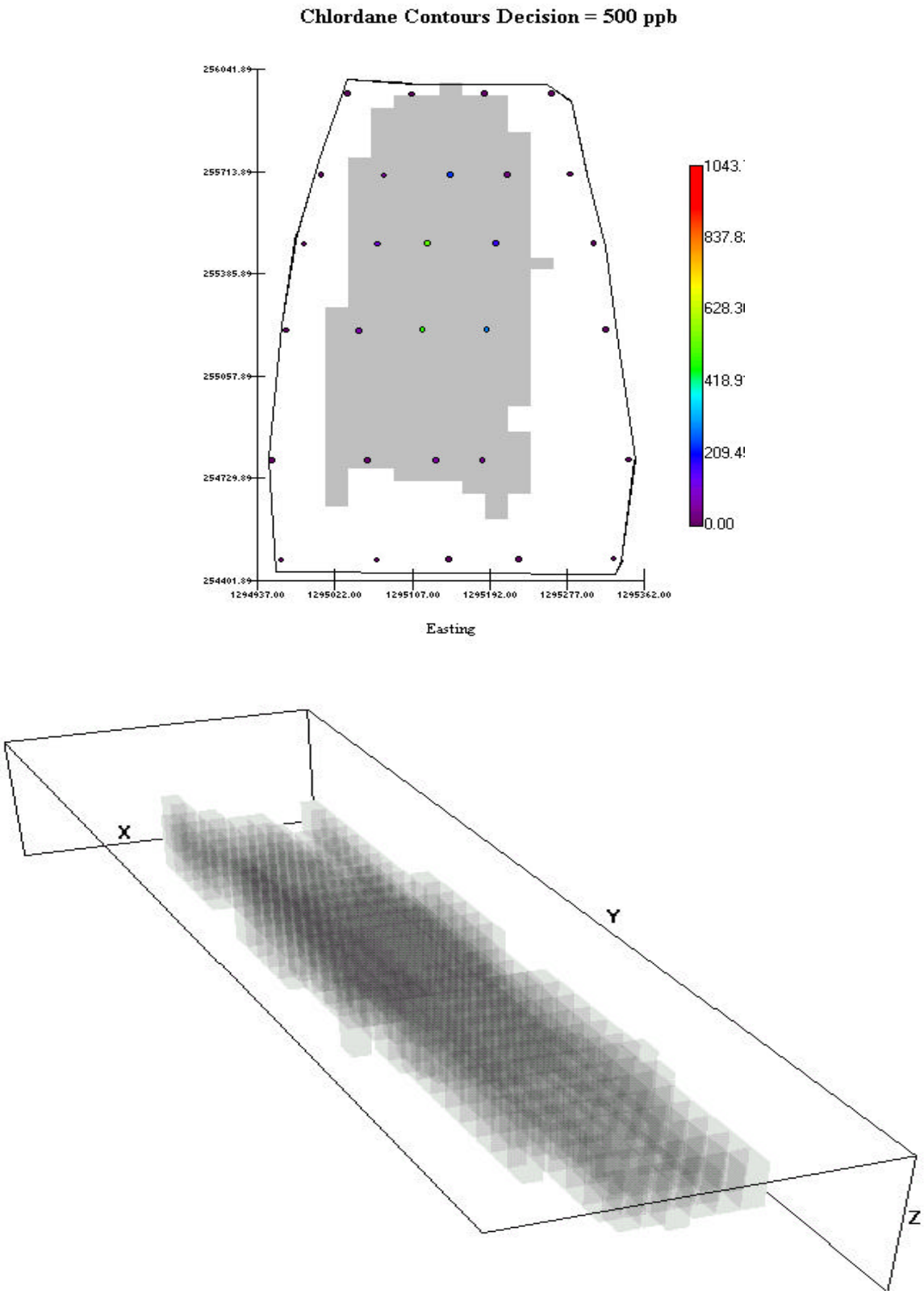

Figure 18. Site S areas where chlordane threshold of 5 µg/L is exceeded with 10% probability: 2-D depiction for one 5-ft interval and 3-D depiction of the entire plume generated by SADA.

goals (EPA 1991). Using the same technical approach and risk input parameters as the UTRC analyst, the technical team was able to independently reproduce the carcinogenic risks calculated by SADA for chlordane. This is the expected result and indicates that the EPA guidance on calculating human health risk is correctly implemented in SADA

Multiple Lines of Reasoning

The UTRC analyst conducted multiple data explorations and evaluations that were supported by the statistical and geostatistical functions in SADA. This information provided a quantitative measure of the probability that could be placed in the decision. Several data interpolation routines were considered on a problem-specific basis before selecting the best one for data analysis. Several sample optimization schemes are available for use. Selection of a particular scheme depends on the objectives of the analysis and the amount of data.

Secondary Evaluation Criteria

Ease of Use

The analysis team found that SADA was easy to use. It has a graphical user interface (GUI) with pull-down menus to permit use of the options in the software. SADA imports database files with comma-delimited format. It also imports .dxf image files and integrates them into the visualization of the problem.

The GUI provided a platform to address problems efficiently and to tailor the analysis to the problem under study (e.g., contours at certain threshold concentrations). The database structure permitted queries on any field (e.g., chemical name, date, concentration, and well identifiers) and also permitted filtering (e.g., to include only data within a range of elevations or to include selected data points).

SADA exhibited the capability to export text and graphics to standard word processing software directly. It also was able to generate project files. This allows the entire project to be moved to another machine with SADA software.

During the demonstration, several members of the technical team received a 4-hour introduction to SADA. The reviewers observed that SADA was a large, feature-rich software program that has on-line manual and case studies included in the software to guide the novice user through the system and applications. The reviewers felt that with one or two days of training, they would be able to use the fundamental features found in SADA. However, they all felt that regular use of the product would be needed to efficiently utilize all of the features found in the product, especially the geostatistical and human health risk features.

Efficiency and Range of Applicability

During the demonstration, UTRC provided one staff member for 4 days to perform the analysis of three problems. An additional 4 days were spent preparing the report that documented the models, assumptions, parameter choices, and results of the analysis. The demonstration showed that the software was capable of importing data and .dxf files to perform an evaluation. The software has a flexible structure that allows a wide range of environmental conditions (e.g., contaminant in groundwater, soil, multiple contaminants on a single site) to be represented.

Training and Technical Support

UTRC provides a number of options for SADA training and technical support. These include

- an extensive on-line help manual,
- tutorial case studies provided with the software,
- a 2-day training course, and
- technical support via internet.

The on-line user manual provides detailed instructions on how to operate SADA. The manual also gives recommendations on approaches to statistical/geostatistical modeling and other aspects of the code. The manual is organized in an orderly fashion and contains pictures of the pull-down menus the operator would see when using SADA. Screen captures demonstrating the type of output produced by SADA are also available in the on-line help.

Additional Information about the SADA Software

To use SADA efficiently, the operator should possess a basic understanding of the use of geospatial modeling in analyzing environmental problems and human health risk assessment. This includes an understanding of interpolation algorithms and geostatistics along with fundamental knowledge about database manipulations, sample optimization, and cost-benefit analysis.

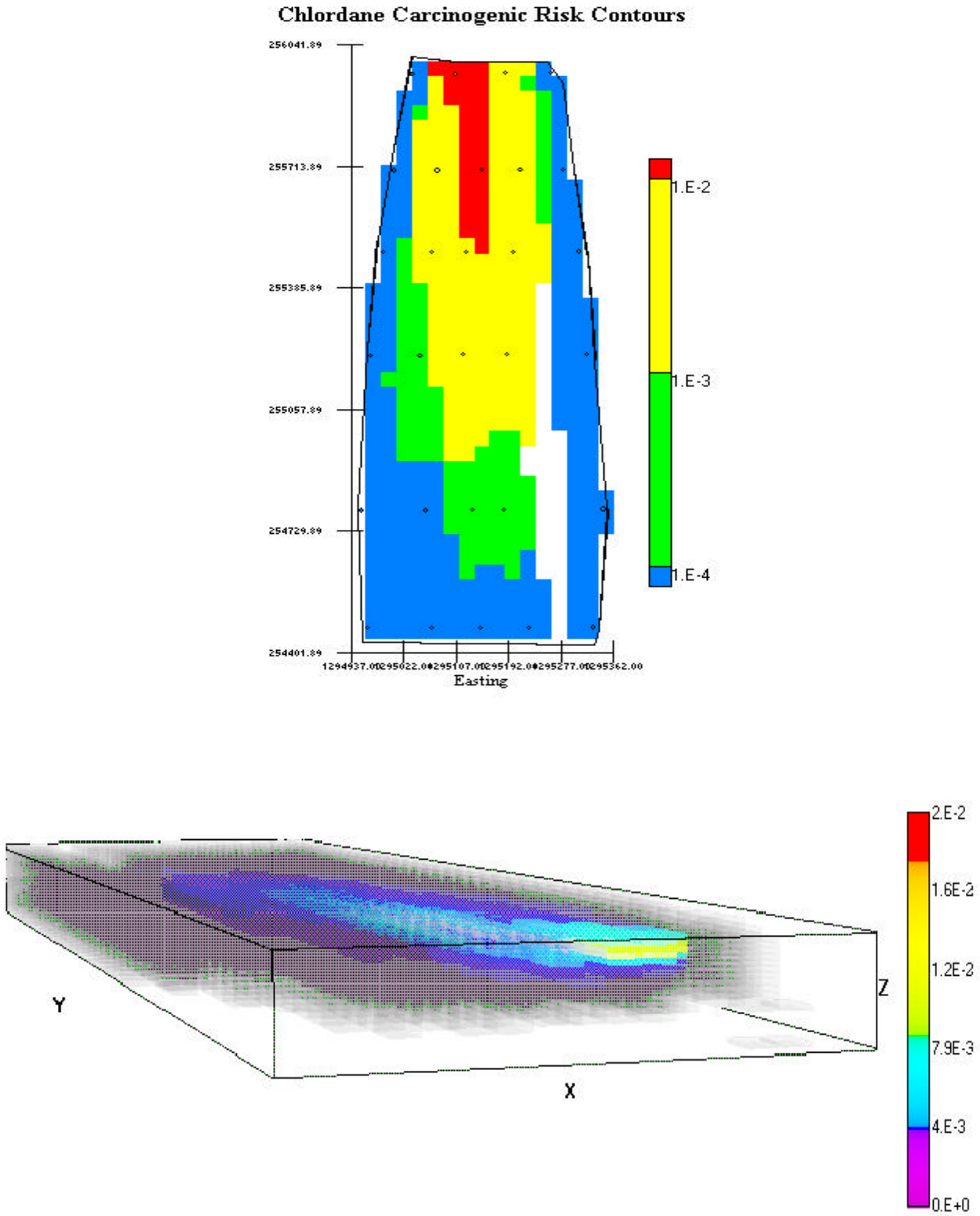

Figure 19. Site S chlordane carcinogenic risk contours based on ingestion of groundwater for a residential scenario: 2-D depiction of one 5-ft interval and 3-D depiction of the entire plume generated by SADA.

Table 7. Volume estimates for the Site S cost-benefit test problem by baseline analysis methods and SADA

Chlordane threshold concentrations and probability levels	Volume of chlordane-contaminated groundwater (ft^3)		
	Baseline Surfer kriging	Baseline geostatistics kriging	SADA
5 µg/L 50% probability level	15,783,000	17,423,070	16,250,000
5 µg/L 10% probability level	NA	22,458,800	20,990,000
500 µg/L 50% probability level	571,250	589,600	510,000
500 µg/L 10% probability level	NA	1,520,800	1,380,000

During the demonstration, SADA Beta Version 3.0 was operated on a Windows 95 platform using a laptop with a 266-MHz Pentium processor, 128 MB of RAM and 4 MB of video memory. SADA requires a minimum of 15 MB of disk space to load.

Summary of Performance

A summary of SADA's performance is presented in Table 8. Overall, the technical team observed that the main strength of SADA is its technical approach to assist environmental decision makers by defining areas of concern based on user-defined contaminant concentrations or human health risks. SADA's estimate of the degree of uncertainty in the prediction provides key information to assist in selection of future sample locations and in determining cost/risk tradeoffs. The incorporation of databases of risk parameters coupled with the pull-down menus make risk calculations easy to perform. The integration of geostatistical analysis, human health risk assessment, cost-benefit analysis, sampling design, and decision analysis into a single software product makes SADA a powerful tool for analyzing spatially correlated data. SADA demonstrated the ability to perform accurate sample optimization analysis, estimate areas and volumes of contamination for cost-benefit analysis, and estimate probability of exceeding thresholds based on contaminant concentrations or risk.

The technical team did not notice any major limitations in SADA. Several minor limitations were noted: the 3-D visualizations provided only a qualitative depiction of the plume because a frame of reference (axis scale or surface maps) was not provided; maps and drawings could be imported only as .dxf files; and data files could be imported only in comma-delimited format, which requires reformatting in another software product.

Table 8. SADA performance summary

Feature/parameter	Performance summary
Decision support	SADA integrated data, site maps, and surface features into 2-D and 3-D spatial representations of the problem. SADA is designed to automatically generate cost-benefit curves and human health risk maps. These maps can be based on the probability of exceeding threshold concentrations. SADA is also designed to assist the analyst in selecting sample optimization schemes based on geostatistical analysis of the existing data.
Documentation of analysis	Documentation of the process and parameters were provided and assumptions explained. Input data and parameters, outputs, and maps were exported to word processing files to document the analysis.
Comparison with baseline analysis and data	2-D and 3-D contaminant concentration contours consistent with measured data and baseline analysis. Accurately mapped sample locations and groundwater wells, buildings and surface features. Accurately posted data to sample locations. Quasi-3D layered maps of contaminant concentrations consistent with data. Estimates of area and/or volume of contaminated media for Site N (2-D) and S (3-D) were consistent with the baseline kriging analysis and baseline geostatistical analysis. Calculations of human health risk were consistent with EPA's *Risk Assessment Guidance for Superfund: Human Health Evaluation Manual* (EPA 1991).
Multiple lines of reasoning	SADA can calculate the probability of exceeding a threshold value (risk or concentration). This facilitates a better understanding of the uncertainty involved in the decision.
Ease of use	User-friendly, logical layout of menus on the graphical user interfaces. Performing risk calculations made easy through the extensive database of contaminants, exposure properties, and risk scenario parameters.
Efficiency	Three problems completed and documented with 8 person days of effort.
Range of applicability	SADA is designed to handle any form of spatially correlated data. Therefore, it can handle contamination in soils, groundwater, surface water, and air. It contains an extensive database of more than 1000 contaminant names and CAS numbers. Its extensive database on risk parameters, which follows EPA's *Risk Assessment Guidance for Superfund*, permits easy calculation of human health risk.
Training and technical support	On-line users' manual On-line help Examples provided with the software Two-day training course Technical support through internet
Operator skill base	Fundamental understanding of environmental contamination problems, geospatial analysis, cost-benefit analysis and human health risk assessment
Operating system	Windows 95, 98, NT
Cost	Free

Section 5 — SADA Update and Representative Applications

Objective

The purpose of this section is to allow UTRC to provide information regarding new developments with SADA since the demonstration activities. In addition, UTRC has provided a list of representative applications in which its technology has been or is currently being used.

Technology Update

SADA's initial full public release of version 1.0 was in November 1999. Version 1.0 of SADA has undergone additional development on a number of features since the beta version evaluated for this report. The major improvements include the following:

- Significant improvement of the computational speed and visual appearance in 3-D visualizations. Also, axis labels are included with the 3-D output in order to provide a frame of reference during visualization.
- SADA is now able to import Microsoft Access 97 files in addition to comma-delimited data files.
- Creation of an auto-documentation feature for SADA. In this feature, SADA generates a report that documents (at the user's requested level of detail) all sources, models, parameters, and assumptions used to produce the result being viewed in SADA. This report is in Hypertext Markup Language (HTML) format and can be read by many word processing programs (e.g., Microsoft Word or Corel WordPerfect) or network browsers (e.g., Netscape or Microsoft Internet Explorer).
- Expansion of the human health risk module to include a larger combination of media/land-use scenarios. Also, total risk and PRG values can explicitly include or exclude certain pathways. Inhalation pathway modifications have been made to comply with recent EPA guidance on this pathway.

Representative Applications

In applications to date, SADA has been found to significantly reduce the amount of startup time and modeling efforts associated with site characterization and risk assessment. In addition, the results have been found to process and produce information in a clear, transparent manner, directly supporting decision processes, and to serve as a communication tool between technical and non-technical audiences.

SADA has already been distributed worldwide via the internet. SADA users have applied SADA in a variety of situations ranging from environmental remediation to human health risk analysis at oil production sites. It is estimated that approximately 150 private-sector companies have been using the Beta version of SADA. In addition, a number of government agencies, including the Environmental Protection Agency, and various state offices have evaluated or implemented SADA. The following list provides some specific examples of how SADA has been used:

- determination of areas of concern in a harbor-dredging application in the northeast United States;
- geospatial modeling of human health risk in oil production sites in Australia;
- classical risk assessments at state facilities in Tennessee and Kentucky;
- secondary sampling design at Portsmouth Gaseous Diffusion Plant in Ohio;
- remedial design at a reactor facility in Oak Ridge, Tennessee.

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Appendix A — Summary of Test Problems

Site A: Sample Optimization Problem

Site A has been in operation since the late 1940s as an industrial machine plant that used solvents and degreasing agents. It overlies an important aquifer that supplies more than 2.7 million gal of water per day for industrial, commercial, and residential use. Site characterization and monitoring activities were initiated in the early 1980s, and it was determined that agricultural and industrial activities were sources of contamination. The industrial plant was shut down in 1985. The primary concern is volatile organic compounds (VOCs) in the aquifer and their potential migration to public water supplies. Source control is considered an important remediation objective to prevent further spreading of contamination.

The objective of this Site A problem was to challenge the software's capabilities as a sample optimization tool. The Site A test problem presents a three-dimensional (3-D) groundwater contamination scenario where two VOCs, dichloroethene (DCE) and trichloroethene (TCE), are present. The data that were supplied to the analysts included information on hydraulic head, subsurface geologic structure, and chemical concentrations from seven wells that covered an approximately 1000-ft square. Chemical analysis data were collected at 5-ft intervals from each well.

The design objective of this test problem was for the analyst to predict the optimum sample locations to define the depth and location of the plume at contamination levels exceeding the threshold concentration (either 10 or 100 μg/L). Because of the limited data set provided to the analysts and the variability found in natural systems, the analysts were asked to estimate the plume size and shape as well as the confidence in their prediction. A high level of confidence indicates that there is a high probability that the contaminant exceeds the threshold at that location. For example, at the 10-μg/L threshold, the 90% confidence level plume is defined as the region in which there is greater than a 90% chance that the contaminant concentration exceeds 10 μg/L. The analysts were asked to define the plume for three confidence levels — 10% (maximum plume, low certainty, and larger region), 50% (nominal plume), and 90% (minimum plume, high certainty, and smaller region). The initial data set provided to the analysts was a subset of the available baseline data and intended to be insufficient for fully defining the extent of contamination in any dimension. The analyst used the initial data set to make a preliminary estimate of the dimensions of the plume and the level of confidence in the prediction. In order to improve the confidence and better define the plume boundaries, the analyst needed to determine where the next sample should be collected. The analyst conveyed this information to the demonstration technical team, which then provided the analyst with the contamination data from the specified location or locations. This iterative process continued until the analyst reached the test problem design objective.

Site A: Cost-Benefit Problem

The objectives of the Site A cost-benefit problem were (1) to determine the accuracy with which the software predicts plume boundaries to define the extent of a 3-D groundwater contamination problem on a large scale (the problem domain is approximately 1 square mile) and (2) to evaluate human health risk estimates resulting from exposure to contaminated groundwater. The VOC contaminants of concern for the cost-benefit problem were perchloroethene (PCE) and trichloroethane (TCA).

In this test problem analysts were to define the location and depth of the PCE plume at concentrations of 100 and 500 μg/L and TCA concentrations of 5 and 50 μg/L at confidence levels of 10 (maximum plume), 50 (nominal plume), and 90% (minimum plume). This information could be used in a cost-benefit analysis of remediation goals versus cost of remediation. The analysts were provided with geological information, borehole logs, hydraulic data, and an extensive chemical analysis data set consisting of more than 80 wells. Chemical analysis data were collected at 5-ft intervals from each well. Data from a few wells were withheld from the analysts to provide a reference to check interpolation routines. Once the analysts defined the PCE and TCA plumes, they were asked to calculate the human health risks associated with drinking 2 L/d of

contaminated groundwater at two defined exposure points over the next 5 years. One exposure point was in the central region of the plume and one was at the outer edge. This information could be used in a cost-benefit analysis of reduction of human health risk as a function of remediation.

Site B: Sample Optimization and Cost-Benefit Problem

Site B is located in a sparsely populated area of the southern United States on a 1350-acre site about 3 miles south of a large river. The site is typical of many metal fabrication or industrial facilities because it has numerous potential sources of contamination (e.g., material storage areas, process activity areas, service facilities, and waste management areas). As with many large manufacturing facilities, accidental releases from laboratory activities and cleaning operations introduced solvents and other organic chemicals into the environment, contaminating soil, groundwater, and surface waters.

The objective of the Site B test problem was to challenge the software's capabilities as a sample optimization and cost-benefit tool. The test problem presents a two-dimensional (2-D) groundwater contamination scenario with three contaminants — vinyl chloride (VC), TCE, and technetium-99 (Tc-99). Chemical analysis data were collected at a series of groundwater monitoring wells on quarterly basis for more than 10 years along the direction of flow near the centerline of the plume. The analysts were supplied with data from one sampling period.

There were two design objectives for this test problem. First, the analyst was to predict the optimum sample location to define the depth and location of the plume at specified contaminant threshold concentrations with confidence levels of 50, 75, and 90%. The initial data set provided to the analyst was a subset of the available baseline data and was intended to be insufficient for fully defining the extent of contamination in two dimensions. The analyst used the initial data set to make a preliminary estimate of the dimensions of the plume and the level of confidence in the prediction. In order to improve the confidence in defining the plume boundaries, the analyst needed to determine the location for collecting the next sample. The analyst conveyed this information to the demonstration technical team, who then provided the analyst with the contamination data from the specified location or locations. This iterative process continued until the analyst reached the design objective.

Once the location and depth of the plume was defined, the second design objective was addressed. The second design objective was to estimate the volume of contamination at the specified threshold concentrations at confidence levels of 50, 75, and 90%. This information could be used in a cost-benefit analysis of remediation goals versus cost of remediation. Also, if possible, the analyst was asked to calculate health risks associated with drinking 2 L/d of contaminated groundwater from two exposure points in the plume. One exposure point was near the centerline of the plume, while the other was on the edge of the plume. This information could be used in a cost-benefit analysis of reduction of human health risk as a function of remediation.

Site D: Sample Optimization and Cost-Benefit Problem

Site D is located in the western United States and consists of about 3000 acres of land bounded by municipal areas on the west and southwest and unincorporated areas on northwest and east. The site has been an active industrial facility since it began operation in 1936. Operations have included maintenance and repair of aircraft and, recently, the maintenance and repair of communications equipment and electronics. The aquifer beneath the site is several hundred feet thick and consists of three or four different layers of sand or silty sand. The primary concern is VOC contamination of soil and groundwater as well as contamination of soil with metals.

The objective of the Site D problem was to test the software's capability as a tool for sample optimization and cost-benefit problems. This test problem was a 3-D groundwater sample optimization problem for four VOC contaminants — PCE, DCE, TCE, and trichloroethane (TCA). The test problem required the developer to predict the optimum sample locations to define the region of the contamination that exceeded threshold concentrations for each contaminant. Contaminant data were supplied for a series of wells screened at different depths for four quarters in a 1-year time frame. This initial data set was insufficient to fully define the extent of contamination. The analyst used the initial data set to make a preliminary estimate of the

dimensions of the plume and the level of confidence in the prediction. In order to improve the confidence in the prediction of the plume boundaries, the analyst needed to determine the location for collecting the next sample. The analyst conveyed this information to the demonstration technical team, who then provided the analyst with the contamination data from the specified location or locations. This iterative process was continued until the analyst determined that the data could support definition of the location and depth of the plume exceeding the threshold concentrations with confidence levels of 10, 50, and 90% for each contaminant.

After the analyst was satisfied that the sample optimization problem was complete and the plume was defined, he or she was given the option to continue and perform a cost-benefit analysis. At Site D, the cost-benefit problem required estimation of the volume of contamination at specified threshold concentrations with confidence levels of 10, 50, and 90%. This information could then be used in a cost-benefit analysis of remediation goals versus cost of remediation.

Site N: Sample Optimization Problem

Site N is located in a sparsely populated area of the southern United States and is typical of many metal fabrication or industrial facilities in that it has numerous potential sources of contamination (e.g., material storage areas, process activity areas, service facilities, and waste management areas). Industrial operations include feed and withdrawal of material from the primary process; recovery of heavy metals from various waste materials and treatment of industrial wastes. The primary concern is contamination of the surface soils by heavy metals.

The objective of the Site N sample optimization problem was to challenge the software's capability as a sample optimization tool to define the areal extent of contamination. The Site N data set contains the most extensive and reliable data for evaluating the accuracy of the analysis for a soil contamination problem. To focus only on the accuracy of the soil sample optimization analysis, the problem was simplified by removing information regarding groundwater contamination at this site, and it was limited to three contaminants. The Site N test problem involves surface soil contamination (a 2-D problem) for three contaminants — arsenic (As), cadmium (Cd), and chromium (Cr). Initial sampling indicated a small contaminated region on the site; however, the initial sampling was limited to only a small area (less than 5% of the site area).

The design objective of this test problem was for the analyst to develop a sampling plan that defines the extent of contamination on the 150-acre site based on exceedence of the specified threshold concentrations with confidence levels of 10, 50% and 90%. Budgetary constraints limited the total expenditure for sampling to $96,000. Sample costs were $1200 per sample, which included collecting and analyzing the surface soil sample for all three contaminants. Therefore, the number of additional samples had to be less than 80. The analyst used the initial data to define the areas of contamination and predict the location of additional samples. The analyst was then provided with additional data at these locations and could perform the sample optimization process again until the areal extent of contamination was defined or the maximum number of samples (80) was attained. If the analyst determined that 80 samples was insufficient to adequately characterize the entire 150-acre site, the analyst was asked to use the software to select the regions with the highest probability of containing contaminated soil.

Site N: Cost-Benefit Problem

The objective of the Site N cost-benefit problem was to challenge the software's ability to perform cost-benefit analysis as defined in terms of area of contaminated soil above threshold concentrations and/or estimates of human health risk from exposure to contaminated soil. This test problem considers surface soil contamination (2-D) for three contaminants — As, Cd, and Cr. The analysts were given an extensive data set for a small region of the site and asked to conduct a cost-benefit analysis to evaluate the cost for remediation to achieve specified threshold concentrations. If possible, an estimate of the confidence in the projected remediation areas was provided at the 50 and 90% confidence limits. For human health risk analysis, two scenarios were considered. The first was the case of an on-site worker who was assumed to have consumed 500 mg/d of soil for one year during excavation activities. The worker would have worked in all areas of the site during the excavation process. The second scenario considered a resident who was assumed to live on a

200- by 100-ft area at a specified location on the site and to have consumed 100 mg/d of soil for 30 years. This information could be used in a cost-benefit (i.e., reduction of human health risk) analysis as a function of remediation.

Site S: Sample Optimization Problem

Site S has been in operation since 1966. It was an industrial fertilizer plant producing pesticides and fertilizer and used industrial solvents such as carbon tetrachloride (CTC) to clean equipment. Recently, it was determined that routine process operations were causing a release of CTC onto the ground; the CTC was then leaching into the subsurface. Measurements of the CTC concentration in groundwater have been as high as 80 ppm a few hundred feet down-gradient from the source area. The site boundary is approximately 5000 ft from the facility where the release occurred. Sentinel wells at the boundary are not contaminated with CTC.

The objective of the Site S sample optimization problem was to challenge the software's capability as a sample optimization tool. The test problem involved a 3-D groundwater contamination scenario for a single contaminant, CTC. To focus only on the accuracy of the analysis, the problem was simplified. Information regarding surface structures (e.g., buildings and roads) was not supplied to the analysts. In addition, the data set was modified such that the contaminant concentrations were known exactly at each point (i.e., release and transport parameters were specified, and concentrations could be determined from an analytical solution). This analytical solution permitted a reliable benchmark for evaluating the accuracy of the software's predictions.

The design objective of this test problem was for the analyst to define the location and depth of the plume at CTC concentrations exceeding 5 and 500 μg/L with confidence levels of 10, 50, and 90%. The initial data set provided to the analysts was insufficient to define the plume accurately. The analyst used the initial data to make a preliminary estimate of the dimensions of the plume and the level of confidence in the prediction. In order to improve the confidence in the predicted plume boundaries, the analyst needed to determine where the next sample should be collected. The analyst conveyed this information to the demonstration technical team, who then provided the analyst with the contamination data from the specified location or locations. This iterative process continued until the analyst reached the design objective.

Site S: Cost-Benefit Problem

The objective of the Site S cost-benefit problem was to challenge the software's capability as a cost-benefit tool. The test problem involved a 3-D groundwater cost-benefit problem for a single contaminant, chlordane. Analysts were given an extensive data set consisting of data from 34 wells over an area that was 2000 ft long and 1000 ft wide. Vertical chlordane contamination concentrations were provided at 5-ft intervals from the water table to beneath the deepest observed contamination.

This test problem had three design objectives. The first was to define the region, mass, and volume of the plume at chlordane concentrations of 5 and 500 μg/L. The second objective was to extend the analysis to define the plume volumes as a function of three confidence levels — 10, 50, and 90%. This information could be used in a cost-benefit analysis of remediation goals versus cost of remediation. The third objective was to evaluate the human health risk at three drinking-water wells near the site, assuming that a resident drinks 2 L/d of water from a well screened over a 10-ft interval across the maximum chlordane concentration in the plume. The analysts were asked to estimate the health risks at two locations at times of 1, 5, and 10 years in the future. For the health risk analysis, the analysts were told to assume source control preventing further release of chlordane to the aquifer. This information could be used in a cost-benefit analysis of reduction of human health risk as a function of remediation.

Site T: Sample Optimization Problem

Site T was developed in the 1950s as an area to store agricultural equipment as well as fertilizers, pesticides, herbicides, and insecticides. The site consists of 18 acres in an undeveloped area of the western United States, with the nearest residence being approximately 0.5 mile north of the site. Mixing operations (fertilizers and

pesticides or herbicides and insecticides) were discontinued or replaced in the 1980s when concentrations of pesticides and herbicides in soil and wastewater were determined to be of concern.

The objective of the Site T sample optimization problem was to challenge the software's capability as a sample optimization tool. The test problem presents a surface and subsurface soil contamination scenario for four VOCs: ethylene dibromide (EDB), dichloropropane (DCP), dibromochloropropane (DBCP), and CTC. This sample optimization problem had two stages. In the first stage, the analysts were asked to prepare a sampling strategy to define the areal extent of surface soil contamination that exceeded the threshold concentrations listed in Table A-1 with confidence levels of 10, 50, and 90% on a 50- by 50-ft grid. This was done in an iterative fashion in which the analysts would request data at additional locations and repeat the analysis until they could determine, with the aid of their software, that the plume was adequately defined.

The stage two design objective addressed subsurface contamination. After defining the region of surface contamination, the analysts were asked to define subsurface contamination in the regions found to have surface contamination above the 90% confidence limit. In stage two, the analysts were asked to suggest subsurface sampling locations on a 10-ft vertical scale to fully characterize the soil contamination at depths from 0 to 30 ft below ground surface (the approximate location of the aquifer).

Site T: Cost-Benefit Problem

The objective of the Site T cost-benefit problem was to challenge the software's capability as a cost-benefit tool. The test problem involved a 3-D groundwater contamination scenario with four VOCs (EDB, DCB, DBCP, and CTC). The analysts were given an extensive data set and asked to estimate the volume, mass, and location of the plumes at specified threshold concentrations for each VOC. If possible, the analysts were asked to estimate the 50 and 90% confidence plumes at the specified concentrations. This information could be used in a cost-benefit analysis of various remediation goals versus the cost of remediation. For health risk cost-benefit analysis, the analysts were asked to evaluate the risks to a residential receptor (with location and well screen depth specified) and an on-site receptor over the next 10 years. For the residential receptor, consumption of 2 L/d of groundwater was the exposure pathway. For the on-site receptor, groundwater consumption of 1 L/d was the exposure pathway. For both human health risk estimates, the analysts were told to assume removal of any and all future sources that may impact the groundwater. This information could be used in a cost-benefit analysis of various remediation goals versus the cost of remediation.

Table A-1. Site T soil contamination threshold concentrations

Contaminant	Threshold concentration (μg/kg)
Ethylene dibromide (EDB)	21
Dichloropropane (DCP)	500
Dibromochloropropane (DBCP)	50
Carbon tetrachloride (CTC)	5

Appendix B — Description of Interpolation Methods

A major component of the analysis of environmental data sets involves predicting physical or chemical properties (contaminant concentrations, hydraulic head, thickness of a geologic layer, etc.) at locations between measured data. This process, called interpolation, is often critical in developing an understanding of the nature and extent of the environmental problem. The premise of interpolation is that the estimated value of a parameter is a weighted average of measured values around it. Different interpolation routines use different criteria to select the weights. Because of the importance of obtaining estimates of data between measured data points in many fields of science, a wide number of interpolation routines exist.

Three classes of interpolation routines commonly used in environmental analysis are nearest neighbor, inverse distance, and kriging. These three classes cover the range found in the software used in the demonstration and use increasingly complex models to select their weighting functions.

Nearest neighbor is the simplest interpolation routine. In this approach, the estimated value of a parameter is set to the value of the spatially nearest neighbor. This routine is most useful when the analyst has a lot of data and is estimating parameters at only a few locations. Another simple interpolation scheme is averaging of nearby data points. This scheme is an extension of the nearest neighbor approach and interpolates parameter values as an average of the measured values within the neighborhood (specified distance). The weights for averaging interpolation are all equal to $1/n$, where n is the number of data points used in the average. The nearest neighbor and averaging interpolation routines do not use any information about the location of the data values.

Inverse distance weighting (IDW) interpolation is another simple interpolation routine that is widely used. It does account for the spatial distance between data values and the interpolation location. Estimates of the parameter are obtained from a weighted average of neighboring measured values. The weights of IDW interpolation are proportional to the inverse of these distances raised to a power. The assigned weights are fractions that are normalized such that the sum of all the weights is equal to 1.0. In environmental problems, contaminant concentrations typically vary by several orders of magnitude. For example, the concentration may be a few thousand micrograms per liter near the source and tens of micrograms per liter away from the source. With IDW, the extremely high concentrations tend to have influence over large distances, causing smearing of the estimated area of contamination. For example, for a location that is 100 m from a measured value of 5 μg/L and 1000 m from a measured value of 5000μg/L, using a distance weighting factor of 1 in IDW yields a weight of 5000/1000 for the high-concentration data point and 5/100 for the low-concentration data point. Thus, the predicted value is much more heavily influenced by the large measured value that is physically farther from the location at which an estimate is desired. To minimize this problem, the inverted distance weight can be increased to further reduce the effect of data points located farther away. IDW does not directly account for spatial correlation that often exists in the data. The choice of the power used to obtain the interpolation weights is dependent on the skills of the analyst and is often obtained through trial and error.

The third class of interpolation schemes is kriging. Kriging attempts to develop an estimate of the spatial correlation in the data to assist in interpolation. Spatial correlation represents the correlation between two measurements as a function of the distance and direction between their locations. Ordinary kriging interpolation methods assume that the spatial correlation function is based on the assumption that the measured data points are normally distributed. This kriging method is often used in environmental contamination problems and was used by some DSS products in the demonstration and in the baseline analysis. If the data are neither lognormal nor normally distributed, interpolations can be handled with indicator kriging. Some of the DSS products in this demonstration used this approach. Indicator kriging differs from ordinary kriging in that it makes no assumption on the distribution of data and is essentially a nonparametric counterpart to ordinary kriging.

Both kriging approaches involve two steps. In the first step, the measured data are examined to determine the spatial correlation structure that exists in the data. The parameters that describe the correlation structure are calculated as a variogram. The variogram merely describes the spatial relationship between data points. Fitting a model to the variogram is the most important and technically challenging step. In the second step, the kriging process interpolates data values at unsampled locations by a moving-average technique that uses the results from the variogram to calculate the weighting factors. In kriging, the spatial correlation structure is quantitatively evaluated and used to calculate the interpolation weights.

Although geostatistical-based interpolation approaches are more mathematically rigorous than the simple interpolation approaches using nearest neighbor or IDW, they are not necessarily better representations of the data. Statistical and geostatistical approaches attempt to minimize a mathematical constraint, similar to a least squares minimization used in curve-fitting of data. While the solution provided is the "best" answer within the mathematical constraints applied to the problem, it is not necessarily the best fit of the data. There are two reasons for this.

First, in most environmental problems, the data are insufficient to determine the optimum model to use to assess the data. Typically, there are several different models that can provide a defensible assessment of the spatial correlation in the data. Each of these models has its own strengths and limitations, and the model choice is subjective. In principle, selection of a geostatistical model is equivalent to picking the functional form of the equation when curve-fitting. For example, given three pairs of data points, (1,1), (2,4) and (3,9), the analyst may choose to determine the best-fit line. Doing so gives the expression $y = 4x - 3.33$, where y is the dependent variable and x is the independent variable. This has a goodness of fit correlation of 0.97, which most would consider to be a good fit of the data. This equation is the "best" linear fit of the data constrained to minimization of the sum of the squares of the residuals (difference between measured value and predicted value at the locations of measured values). Other functional forms (e.g., exponential, trigonometric, and polynomial) could be used to assess the data. Each of these would give a different "best" estimate for interpolation of the data. In this example, the data match exactly with $y = x^2$, and this is the best match of this data. However, that this is the best match cannot be known with any high degree of confidence.

This conundrum leads to the second reason for the difficulty, if not impossibility, of finding the most appropriate model to use for interpolation — which is that unless the analyst is extremely fortunate, the measured data will not conform to the mathematical model used to represent the data. This difficulty is often attributed to the variability found in natural systems, but is in fact a measure of the difference between the model and the real-world data. To continue with the previous example, assume that another data point is collected at $x = 2.5$ and the value is $y = 6.67$. This latest value falls on the previous linear best-fit line, and the correlation coefficient increases to 0.98. Further, it does not fall on the curve $y = x^2$. The best-fit 2nd-order polynomial now changes from $y = x^2$ to become $y = 0.85x^2 + 0.67x - 0.55$. The one data point dramatically changed the "best"-fit parameters for the polynomial and therefore the estimated value at locations that do not have measured values.

Lack of any clear basis for choosing one mathematical model over another and the fact that the data are not distributed in a manner consistent with the simple mathematical functions in the model also apply to the statistical and geostatistical approaches, albeit in a more complicated manner. In natural systems, the complexity increases over the above example because of the multidimensional spatial characteristics of environmental problems. This example highlighted the difficulty in concluding that one data representation is better than another. At best, the interpolation can be reviewed to determine if it is consistent with the data. The example also highlights the need for multiple lines of reasoning when assessing environmental data sets. Examining the data through use of different contouring algorithms and model parameters often helps lead to a more consistent understanding of the data and helps eliminate poor choices for interpolation parameters.