Prepared in cooperation with the U.S. Department of Energy

Visualization and Time-Series Analysis of Ground-Water Data for C-Area, Savannah River Site, South Carolina, 1984–2004

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U.S. Department of the Interior
U.S. Geological Survey

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By Paul A. Conrads, Edwin A. Roehl, Jr., Ruby C. Daamen, Francis H. Chapelle,
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Contents

Abstract 1
Introduction 1
  Purpose and Scope 4
  Description of Study Area 5
  Approach 5
Data Used in the Study 6
  Data Processing, Gridding, and Time-Series Synthesis 6
Time-Series Analysis 12
  Time Series of Volatile Organic Compound Degradation Products 13
  Analysis of Inferential Analytes 20
  Three-Dimensional Visualization 20
Summary and Conclusions 20
Acknowledgments 24
References Cited 24
Appendix 1: User’s manual for the Ground-Water Data Viewer 27

Figures

1–4. Maps showing:

  1. Location of Savannah River Site in South Carolina 1
  2. Designated areas at the Savannah River Site, South Carolina 2
  3. C-Area at the Savannah River Site, South Carolina 3
  4. C-Area trichloroethylene (TCE) plume 4
5. Generalized cross section showing the hydrogeology in the vicinity of Castor Creek, the C-Area Reactor, and the C-Area Seepage Basin 5
6. Upper Three Runs aquifer grid showing the number of wells aggregated in each 0.1- x 0.1-km cell 8
7. Gordon aquifer grid showing the number of wells aggregated in each 0.1- x 0.1-km cell 8
8. Graph showing number of measurements for each Upper Three Runs and Gordon aquifers cell having measurements 13
9. Analyte “degradation map” from parent to end product for four classes of volatile organic compounds 13

10–21. Graphs showing:

  10. Chloride concentrations measured in the Upper Three Runs aquifer for the four cells for which time series were analyzed 14
  11. Depth to water measured in the Upper Three Runs aquifer for the four cells for which time series were analyzed 15
  12. Cell 1307 average and maximum Class A analyte concentrations 15
  13. Cell 1206 average and maximum Class A analyte concentrations 16
  14. Cell 1208 average and maximum Class A analyte concentrations 16
  15. Cell 1509 average and maximum Class A analyte concentrations 17
  16. Cell 1307 average and maximum Class B analyte concentrations 17

17. Cell 1206 average and maximum Class B analyte concentrations 18
18. Cell 1208 average and maximum Class B analyte concentrations 18
19. Cell 1509 average and maximum Class B analyte concentrations 19
20. Average and maximum Class C analyte (carbon tetrachloride) concentrations for cells 1206, 1208, 1307, and1509 19
21. Average and maximum Class D analyte concentrations for cells 1206, 1208, 1307, and 1509 20
22. Sceenshot of the Ground-Water Data Viewer showing maximum *cis*-1,2-dichloroethylene concentration for the Upper Three Runs aquifer for 2000, 2002, and 2004 22
23. Graphs showing maximum Class B analyte concentrations for the Upper Three Runs aquifer from 1999 to 2004 23

Tables

1. Analyte codes for analytes measured in the Upper Three Runs and Gordon aquifers, South Carolina 7
2. Cell assignments of Upper Three Runs and Gordon aquifer wells, South Carolina 9
3. Statistics for cells used in time-series analysis 14
4. Pearson correlation coefficients and coefficients of determination for cell 1208 chlorinated hydrocarbons and candidate predictor analytes 21

Conversion Factors

SI to Inch/Pound

Multiply	By	To obtain
	Length	
meter (m)	3.281	foot (ft)
meter (m)	1.094	yard (yd)
	Area	
square meter (m^2)	0.0002471	acre
square meter (m^2)	10.76	square foot (ft^2)
square kilometer (km^2)	0.3861	square mile (mi^2)
	Volume	
cubic meter (m^3)	6.290	barrel (petroleum, 1 barrel = 42 gal)
liter (L)	33.82	ounce, fluid (fl. oz)
liter (L)	2.113	pint (pt)
liter (L)	1.057	quart (qt)
liter (L)	0.2642	gallon (gal)
	Mass	
gram (g)	0.03527	ounce, avoirdupois (oz)
	Hydraulic conductivity	
meter per day (m/d)	3.281	foot per day
	Transmissivity*	
meter squared per day (m^2/d)	10.76	foot squared per day (ft^2/d)

*Transmissivity: The standard unit for transmissivity is cubic meter per day per square meter times meter of aquifer thickness [(m^3/d)/m^2]m. In this report, the mathematically reduced form, meter squared per day (m^2/d), is used for convenience.

Vertical coordinate information is referenced to North American Vertical Datum of 1988 (NAVD 88). Horizontal coordinate information is referenced to the North American Datum of 1983 (NAD 83).

Specific conductance is given in microsiemens per centimeter at 25 degrees Celsius (µS/cm at 25 °C).

Concentrations of chemical constituents in water are given either in milligrams per liter (mg/L) or micrograms per liter (µg/L).

Acronyms used in this report

ADMi	Advanced Data Mining, LLC
ANN	artificial neural networks
CBRP	C-Area Burning/Rubble Pit
CRSB	C-Reactor Seepage Basin
CRADA	Cooperative Research and Development Agreement
CPT	cone penetrometer technology
DSS	Decision Support System
GDV	Ground-Water Data Viewer
GIS	geographic information system
PCE	tetrachloroethylene
R	correlation coefficient
R^2	coefficient of determination
SRS	Savannah River Site
TCE	trichloroethylene
TDS	total dissolved solids
TIN	triangulated irregular network
3D	three dimensional
USDOE	U.S. Department of Energy
USGS	U.S. Geological Survey
UTM	Universal Transverse Mercator
UTR	Upper Three Runs
VBA	Visual Basic for Applications™
VOC	volatile organic compounds

Visualization and Time-Series Analysis of Ground-Water Data for C-Area, Savannah River Site, South Carolina, 1984–2004

By Paul A. Conrads[1], Edwin A. Roehl, Jr.[2], Ruby C. Daamen[2], Francis H. Chapelle[1], Mark A. Lowery[1], and Uwe H. Mundry[2]

Abstract

In 2004, the U.S. Geological Survey, in cooperation with the U.S. Department of Energy, initiated a study of historical ground-water data of C-Area on the Savannah River Site in South Carolina. The soils and ground water at C-Area are contaminated with high concentrations of trichloroethylene and lesser amounts of tetrachloroethylene. The objectives of the investigation were (1) to analyze the historical data to determine if data-mining techniques could be applied to the historical database to ascertain whether natural attenuation of recalcitrant contaminants, such as volatile organic compounds, is occurring and (2) to determine whether inferential (surrogate) analytes could be used for more cost-effective monitoring. Twenty-one years of data (1984–2004) were collected from 396 wells in the study area and converted from record data to time-series data for analysis. A Ground-Water Data Viewer was developed to allow users to spatially and temporally visualize the analyte data. Overall, because the data were temporally and spatially sparse, data analysis was limited to only qualitative descriptions.

Introduction

In 1951, the U.S. Department of Energy (USDOE), formerly the Atomic Energy Commission, created the Savannah River Site (SRS) to produce nuclear materials for national defense. The SRS is located in parts of Aiken, Barnwell, and Allendale Counties, South Carolina (fig. 1). The operation of the first nuclear production reactor, R, began in 1953 (fig. 2). In addition, there are four other nuclear reactors at the SRS, which are located in Areas C, K, L, and P. Reactors R and P were permanently deactivated in 1964 and 1991, respectively, and except for the

Figure 1. Location of Savannah River Site in South Carolina.

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[1] U.S. Geological Survey, South Carolina Water Science Center, Columbia, South Carolina.

[2] Advanced Data Mining International, LLC, Greenville, South Carolina.

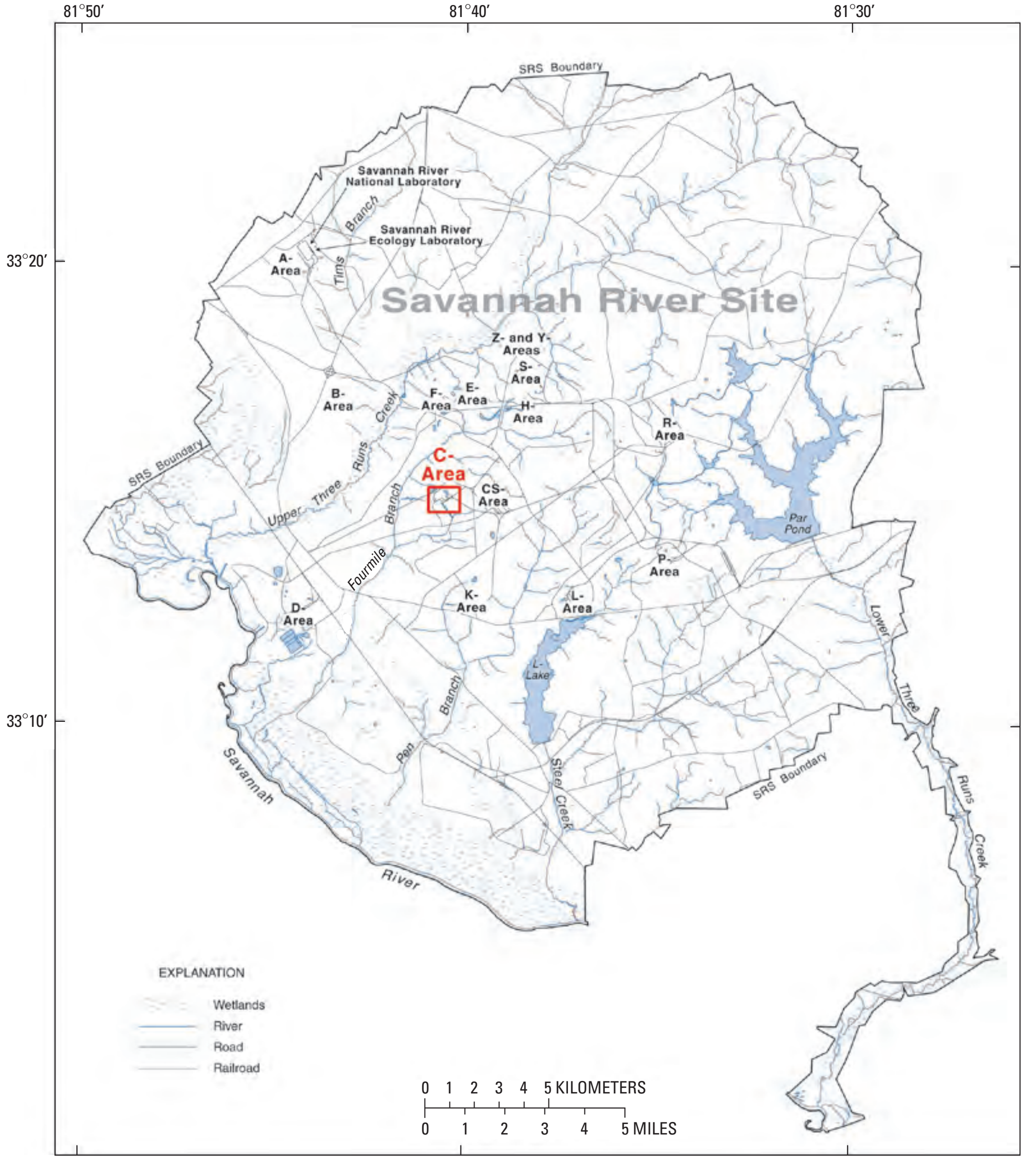


Figure 2. Designated areas at the Savannah River Site, South Carolina.

restart testing of the K Reactor in 1991, all of the remaining reactors have been placed on standby since the late 1980s. Other areas on the SRS include Areas F and H (reactor materials, separation), Areas E, F, H, S, Y, and Z (water management), Area D (heavy water processing), Areas A, B, and CS (administration), the Savannah River Ecology Laboratory, and the Savannah River National Laboratory (fig. 2; Arnett and others, 1992).

In 2004, the U.S. Geological Survey (USGS), in cooperation with the USDOE, initiated a study of historical ground-water data of C-Area at the SRS (figs. 2, 3). The C-Area Burning/Rubble Pit (CBRP) was constructed near the C Reactor in 1951 and used for the disposal of organic solvents and waste oil until 1973. The soils and ground water at C-Area are contaminated with high concentrations of volatile organic compounds (VOCs), including trichloroethylene (TCE) and lesser amounts of tetrachloroethylene (PCE; Gary Mills, Savannah River Ecology Laboratory, written commun., 2001). Cone penetrometer technology sampling in 1999 showed high concentrations of TCE beneath and downgradient from the CBRP (Flach and others, 1999). The extent and concentration of two distinct TCE plumes are

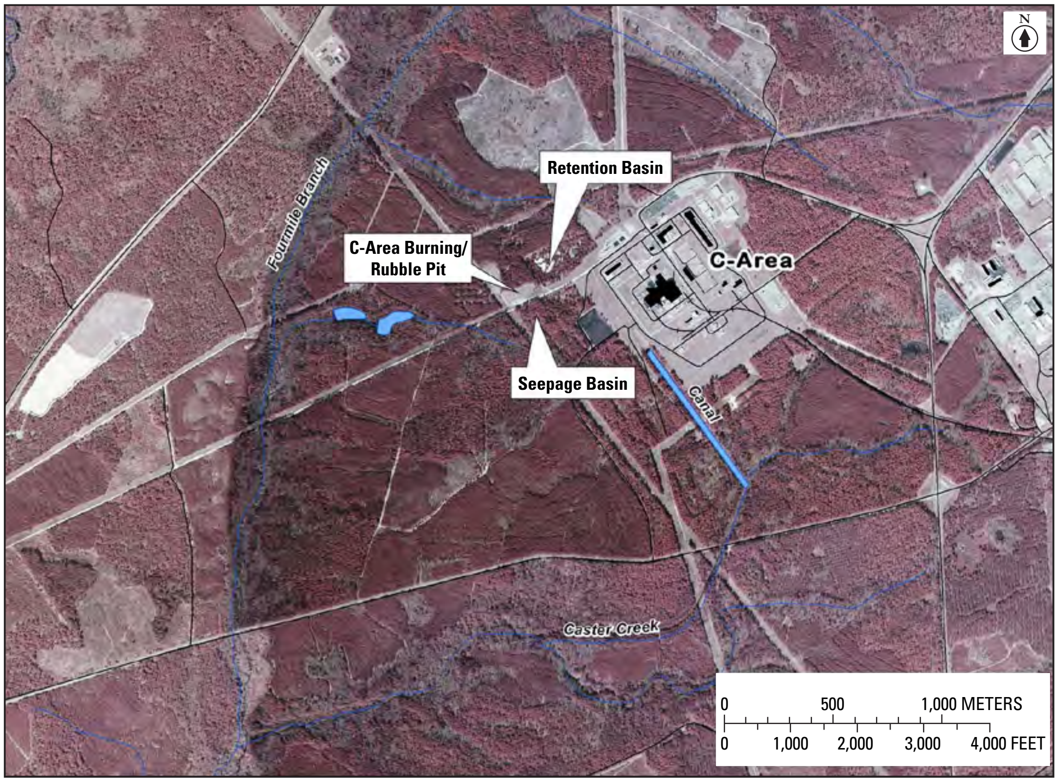


Figure 3. C-Area at the Savannah River Site, South Carolina.

shown in figure 4 (Karen Vangelas, Savannah River Ecology Laboratory, written commun., 2004). The northern plume is associated with the CBRP. The source of the southern plume is inside the C-Reactor fence and associated with the C-Reactor Seepage Basin (CRSB) that was in use from 1959 to 1970 (Bills and others, 2000).

The soil, surface water, and ground water in the vicinity of the C-Area have been monitored extensively for years. Because of the large number of sites that USDOE is responsible for, both at SRS and on a national level, sampling costs, especially the analytical costs, are a great concern. The objectives of this study were (1) to analyze the historical data to determine if data-mining techniques could be applied to the historical database to ascertain whether natural attenuation of recalcitrant contaminants, such as VOCs, is occurring and (2) to determine whether inferential analytes could be used for more cost-effective monitoring.

The USGS entered into a Cooperative Research and Development Agreement (CRADA) with Advanced Data Mining, LLC (ADMi) in 2002 to collaborate on applying data-mining techniques and artificial neural network (ANN) models to water-resources investigations. The emerging field of data mining addresses the issue of extracting information from large databases (Weiss and Indurkhya, 1998). Data mining is a powerful tool for converting large databases into knowledge to solve problems that are otherwise imponderable because of the large numbers of explanatory variables or poorly understood process physics. Data mining integrates methods from different fields, such as signal processing, statistics, artificial intelligence, and multidimensional visualization. Data mining uses methods for maximizing the information content of data, determining which variables have the strongest correlations to the problems of interest, and developing models that predict the consequences of alternative courses of action and(or) future outcomes. Data mining is used extensively in financial services, banking, advertising, manufacturing, and e-commerce to classify the behaviors of organizations and individuals and to predict future outcomes.

Collaborative data-mining and ANN studies between the USGS and ADMi have included predicting the location of the saltwater-freshwater interface, modulated by discharges from a dam and tidal forcing, on the Cooper River (Roehl and others, 2000) and the Pee Dee and Waccamaw Rivers and Atlantic Intracoastal Waterway (Conrads and Roehl, 2007); predicting water levels and salinity responses in a tidal marsh due to variable flow conditions and alternative channel geometries in the Savannah Harbor Estuary (Conrads and others, 2006a); integrating hydrologic databases and hindcasting water depths to support ecological studies in the Everglades (Conrads and others, 2006b); estimating water depths at ungaged areas in the Everglades (Conrads and Roehl, 2006b); simulating point-source effluent and rainfall impacts on dissolved oxygen for two estuarine systems, the Cooper and Beaufort Rivers (Conrads, Roehl, and Cook, 2002; Conrads, Roehl,

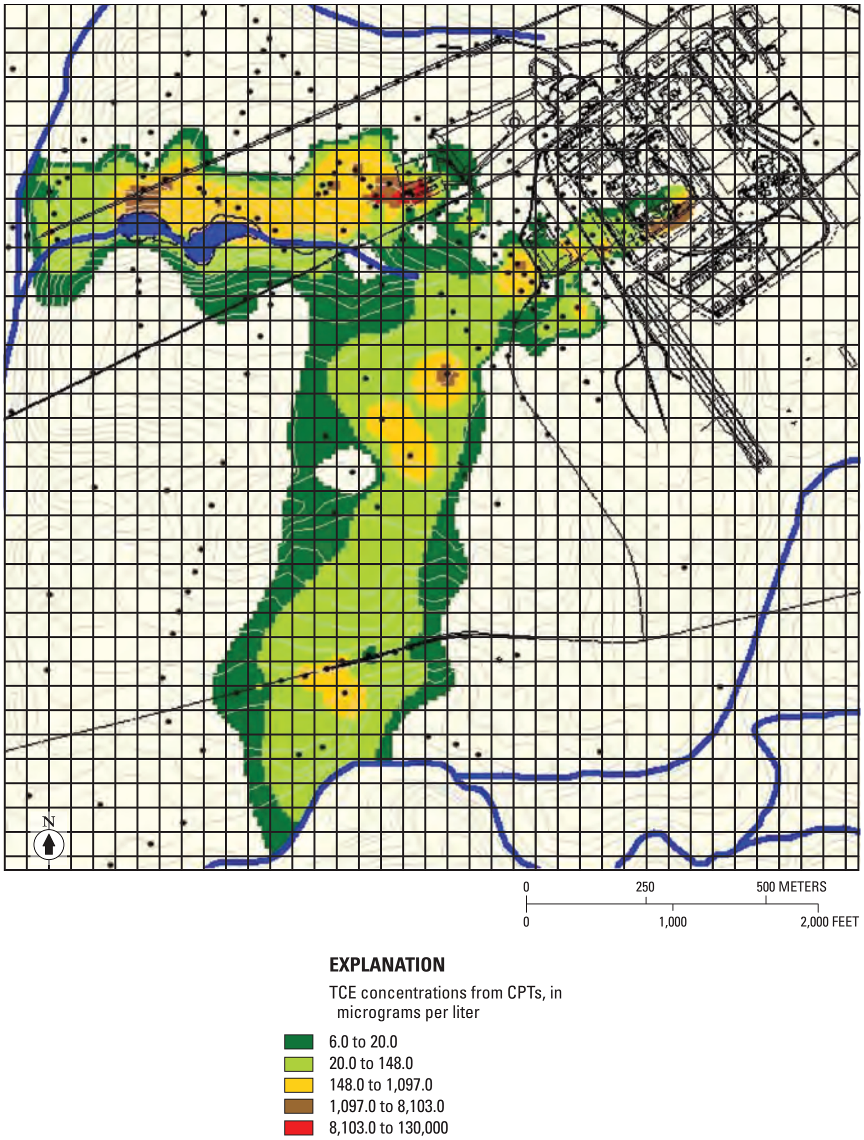


Figure 4. C-Area trichloroethylene (TCE) plume (figure supplied by U.S. Department of Energy). Dots represent cone penetrometer technology (CPT) sampling locations.

and Martello, 2002; Conrads and others, 2003; Conrads, Roehl, Martello, and Saxon, 2006); and predicting “natural” water temperatures for small streams in western Oregon and Wisconsin (Risley and others, 2003; Roehl and others, 2006; Stewart and others, 2006).

Purpose and Scope

This report presents the results of compiling and analyzing 21 years (1984–2004) of historical ground-water-quality monitoring data measured in the Upper Three Runs and Gordon aquifers at C-Area at the SRS. This report also describes development and application of a custom visualization program, the Ground-Water Data Viewer (GDV).

An important part of the USGS mission is to provide scientific information for the effective management of the Nation’s water resources. Often, ground-water and surface-water systems of concern, such as the C-Area system, have large historical databases that are underutilized and not well interpreted for addressing contemporary water-quality issues. The techniques presented in this report demonstrate how valuable information can be extracted from existing databases to assist local, State, and Federal agencies in making water-management decisions. The application of data-mining techniques to the ground-water data for C-Area at the SRS demonstrates how disparate historical monitoring networks can be integrated using a Decision Support System (DSS) to interrogate and visualize historical data and assist water-resource managers in evaluating future monitoring approaches.

The techniques are readily applicable to other systems for evaluation of historical data and for alternative monitoring strategies.

Description of Study Area

The SRS is located in the Atlantic Coastal Plain physiographic province of South Carolina and occupies more than 777 square kilometers (km^2) along the Georgia-South Carolina border. The southwestern boundary of the SRS is formed by the Savannah River. The five major streams that drain from SRS into the Savannah River are Upper Three Runs Creek, Fourmile Branch, Pen Branch, Steel Creek, and Lower Three Runs Creek (fig. 2). The general topography of the Coastal Plain consists of rounded hills with gradual slopes; however, some areas of highly irregular terrain exist in the province, and some elevations exceed 213 meters (m; North American Vertical Datum, NAVD 88). The highest elevation on the SRS is approximately 128 m NAVD 88 near Tims Branch and the northwest boundary of SRS (fig. 2). The land-surface elevation at the boundary of the upper and lower Coastal Plains, located southeast of the SRS, is generally less than 62 m NAVD 88 (Lanier, 1996).

Aadland and others (1992) and Falls and others (1997) described the major geologic and hydrogeologic units of east-central Georgia and west-central South Carolina in the vicinity of the SRS. At the SRS, the downdipping carbonate strata of Eocene and post-Eocene age constitute the Floridan aquifer system. Updip clastic equivalents of the Floridan aquifer system include the Upper Three Runs and Gordon aquifers and the intervening Gordon confining unit. Where the Gordon confining unit is absent in the updip localities, the combined Upper Three Runs and Gordon aquifers are known as the Steed Pond aquifer (Aadland and others, 1992).

The dominant porosity type of the Upper Three Runs aquifer is intergranular in the sands and intergranular and moldic in the sandy carbonates and limestones. The Upper Three Runs aquifer has a reported transmissivity of 78 meters squared per day (m^2/d) and hydraulic conductivity of 2.4 meters per day (m/d; Kidd, 1996; Snipes and others, 1996; Falls and others, 1997).

C-Area, the location of the study area for this report, covers approximately 1 square kilometer (km^2) in central SRS (fig. 2). The CBRP is located approximately 61 m southwest from the C-Reactor Retention Basin (fig. 3). The elevation of the CBRP is approximately 82 m NAVD 88, and surface water generally flows toward Fourmile Branch to the northwest and Caster Creek to the southeast (fig. 3). Surface-water flows have been altered in the area as a result of the construction of a canal extending from the C-Area to Caster Creek, road building, and silvaculture activities (Science Applications International Corporation, 1997). A schematic of the hydrogeology of the C-Area is shown in figure 5. The upper five units—Upper Aquifer Zone, Tan Clay Confining Unit, Middle Aquifer Zone, Lower Confining Unit, and Lower Aquifer Zone—are associated with the Upper Three Runs aquifer (Flach and others, 1999; Bills and others, 2000).

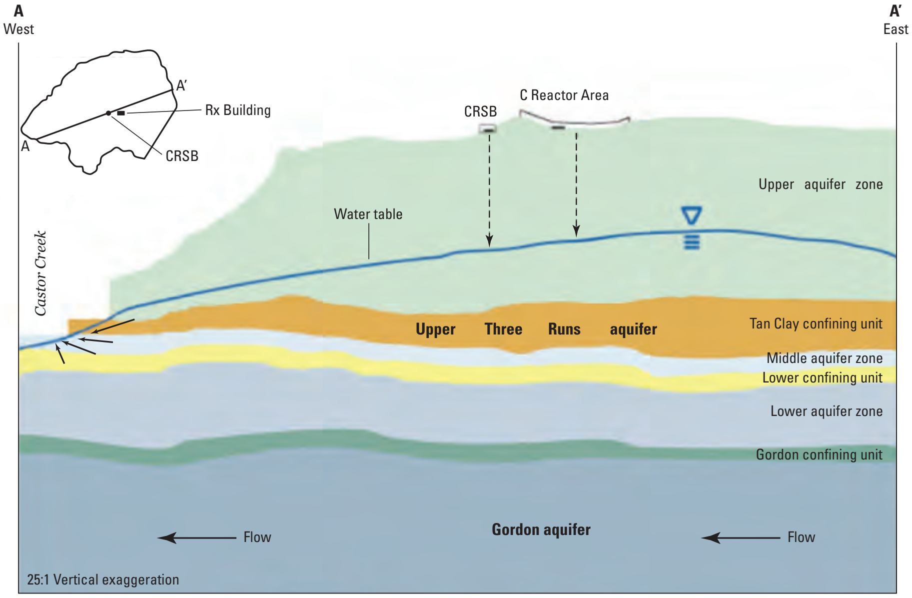


Figure 5. Generalized cross section showing the hydrogeology in the vicinity of Castor Creek, the C-Area Reactor (Rx Bldg), and the C-Reactor Seepage Basin (CRSB; modified from Bills and others, 2000). The upper five units—Upper Aquifer Zone, Tan Clay Confining Unit, Middle Aquifer Zone, Lower Confining Unit, and Lower Aquifer Zone—are associated with the Upper Three Runs aquifer.

Approach

To meet the objectives of the study, approximately 51,000 individual historical records of ground-water analyte measurements were compiled and converted into time series to support data visualization and empirical analyses to ascertain the fate and transport of analytes of interest. To accomplish this, the study was undertaken in several tasks.

1. Available historical records were obtained from the USDOE. The study was limited to data and documents that were digitally available from various databases.
2. The data were compiled into a Microsoft Access™ relational database.
3. A geographic information system (GIS) application was developed to ascertain which measurement locations, hereafter called "wells," were located in the Upper Three Runs and Gordon aquifers.
4. The two aquifers were gridded into cells, and wells were assigned to grid cells on the basis of their location.
5. Data from each aquifer were aggregated by analyte type into cells and time steps (intervals) to create time series for analysis.
6. A three-dimensional (3D) GDV was developed to visualize the analyte behaviors over time and by location. The GDV provides an integrated, interactive environment for exploring and analyzing the data.
7. Cross correlation and other analyses were performed on the time series to determine whether natural attenuation of contaminants is occurring and whether inferential (surrogate) analytes could be used for more cost-effective monitoring.

Data Used in the Study

C-Area well data retrieved from the USDOE databases included location names, Universal Transverse Mercator (UTM) coordinates, installation dates, ground elevation, total depth, screen intervals, water quality, and field data for specified dates. In addition, the USDOE provided geophysical logs and cone penetrometer technology (CPT) logs for wells and borings, and monitoring and modeling reports for the C-Area. As with most historical databases, there may be inconsistent entries for well identification and well location. When creating relational databases, these inconsistencies often result in "lost" records, or wells in this case, if they are not reconciled. Often, reconciling historical database issues can be time consuming and resource intensive. Many inconsistencies were found in the data records. In order to make the best use of limited resources to address the study objectives, the decision was made to limit the dataset to electronically available data that are consistent with respect to site identification and location. The datasets used in the analysis of the C-Area for this report are spatially and temporally sparse.

Data Processing, Gridding, and Time-Series Synthesis

The data of interest for the study were measurements that characterized change in the system over the period of record from 1984 to 2004. Due to the sparseness of the data, it was necessary to aggregate the data in space and time to create time series for analysis. The data used in this study did not include aquifer assignments; therefore, GIS software was used to determine the aquifers in which the wells were screened. Triangulated irregular network (TIN) surfaces of the Upper Three Runs aquifer, Gordon confining unit, and Gordon aquifer (Falls and others, 1997) were created to accomplish this task. The wells were then plotted on the TIN surfaces, and elevations of the top and bottom of the well screens were used to determine in which aquifer the wells were screened.

In the C-Area, there were 51 ground-water analytes that had codes listed in the original database metadata (table 1). Records were found for 46 of the 91 analytes among the 43,291 Upper Three Runs aquifer-related records from 336 wells. Among the 6,339 records for the Gordon aquifer, records were found for 28 analytes for 60 wells. It should be noted that TCE was not one of the analytes included in the datasets.

It was necessary to convert the ground-water records into time series for analysis and inclusion in the database for the GDV. The general approach involved overlaying a rectangular grid on the study area, bounded by the most distant wells in C-Area, and aggregating well data for all wells in each grid cell. Measurements from wells within each cell were then aggregated into time steps. Two sets of time series were generated: the average values and the maximum values within a cell at each time step. Thus, for each analyte measured in each cell of each aquifer, measurements were spatially aggregated (horizontally and vertically) and temporally aggregated to create time series. Note that "non-detects" were set to one-half the detection limit in the time series, so the actual lowest measured values are possibly censored by the detection limits. Despite the apparently large number of records, relative to the a temporal scale of 21 years and spatial scale of approximately 9 km^2, the temporal and spatial densities of the records were found to be sparse.

The spatial density of the records was evaluated at cell sizes of 25 × 25, 50 × 50, and 100 × 100 square meters (m^2). With consideration for representing all of the C-Area wells and for comparing the behavior of the Upper Three Run and Gordon aquifers, a 0.1- × 0.1-km cell size was selected, which

Table 1. Analyte codes for analytes measured in the Upper Three Runs (UTR) and Gordon aquifers, South Carolina.

[“1” indicates the analyte was measured]

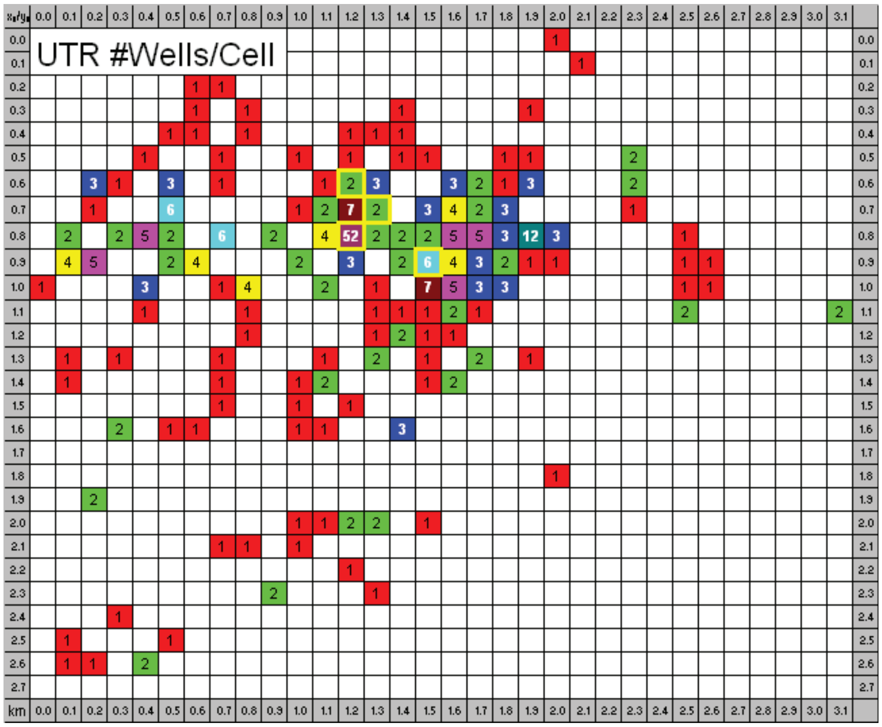
Analyte	Analyte code	UTR included	Gordon included
1,1,1,2-Tetrachloroethane	1	0	0
1,1,1-Trichloroethane	2	1	1
1,1,2,2-Tetrachloroethane	3	1	1
1,1,2-Trichloroethane	4	1	1
1,1-Dichloroethane	5	1	1
1,1-Dichloroethylene	6	1	1
1,2-Dichloroethane (EDC)	7	1	1
1,2-Dichloroethylene	8	1	1
Air temperature	9	1	1
Alkalinity (as $CaCO_3$)	10	1	1
Calcium	11	1	1
Carbon tetrachloride	12	1	1
Chloride	13	1	1
Chloroethane (ethyl chloride)	14	1	1
Chloroethene (vinyl chloride)	15	1	1
Chloromethane (methyl chloride)	16	1	1
cis-1,2-Dichloroethylene	17	1	1
Depth to water	19	1	1
Dichloromethane (methylene chloride)	20	1	1
Dissolved organic carbon	21	1	0
Iron	23	1	1
Magnesium	24	1	1
Nitrate	25	1	1
Nitrate-nitrite as nitrogen	26	1	0
Nitrites	27	1	0
pH	28	1	1
Phosphate	29	0	0
Phosphorus	30	1	0
Silica	31	1	0
Specific conductance	32	1	1
Sulfate	33	1	1
Sulfide	34	1	1
Temperature	35	0	0
Tetrachloroethylene (PCE)	36	1	1
Total dissolved solids	37	1	0
Total organic carbon	38	1	0
Total organic halogens	39	1	0
Trans-1,2-Dichloroethylene	40	1	1
Trichloroethylene (TCE)	41	0	0
Carbon dioxide	100	1	0
Ethane	101	1	0
Ethylene	102	1	0
Ferric iron	103	1	0
Ferrous iron	104	1	0
Hydrogen	105	1	0
Hydrogen sulfide	106	1	0
Methane	107	1	0
Nitrogen	108	1	0
Oxygen	109	1	0
Phenolphthalein alkalinity	110	1	1
Total suspended solids	111	0	0
Totals		46	28

averaged the 336 wells in the Upper Three Runs aquifer and 60 wells in the Gordon aquifer into 146 and 54 cells, respectively (figs. 6 and 7). The wells assigned to each cell by grid cell coordinates are listed in table 2.

The 0.1- × 0.1-km cell size provides low spatial resolution in the immediate vicinity around the contaminant sources but adequate resolution for the entire C-Area and allows questions related to the larger spatial scale to be addressed. Smaller grid cells could be applied over a smaller portion of C-Area where the data density is greater to address finer scale questions and issues.

Temporal measurement densities were evaluated at 3- and 12-month intervals. With consideration for maximizing the number of grid cells with concurrent measurements, the 12-month interval was selected for the averaging time interval. It should be noted that (1) far fewer data were collected in the Gordon aquifer and (2) much of the water-level recording equipment was operated only briefly or intermittently, so a lack of concurrency in measurements is an important issue.

The GDV was developed to provide a means to better understand the evolution



UTR #Wells/Cell

x_0/y_0	0.0	0.1	0.2	0.3	0.4	0.5	0.6	0.7	0.8	0.9	1.0	1.1	1.2	1.3	1.4	1.5	1.6	1.7	1.8	1.9	2.0	2.1	2.2	2.3	2.4	2.5	2.6	2.7	2.8	2.9	3.0	3.1	
0.0																					1												0.0
0.1																						1											0.1
0.2							1	1																									0.2
0.3							1		1						1					1													0.3
0.4						1	1		1				1	1	1																		0.4
0.5					1			1			1		1		1	1			1	1				2									0.5
0.6			3	1		3		1				1	2	3			3	2	1	3				2									0.6
0.7			1			6					1	2	7	2		3	4	2	3					1									0.7
0.8		2		2	5	2		6		2		4	52	2	2	2	5	5	3	12	3					1							0.8
0.9		4	5			2	4				2		3		2	6	4	3	2	1	1					1	1						0.9
1.0	1				3			1	4			2		1		7	5	3	3							1	1						1.0
1.1					1				1					1	1	1	2	1								2						2	1.1
1.2									1					1	2	1	1																1.2
1.3		1		1				1				1		2		1		2		1													1.3
1.4		1						1			1	2				1	2																1.4
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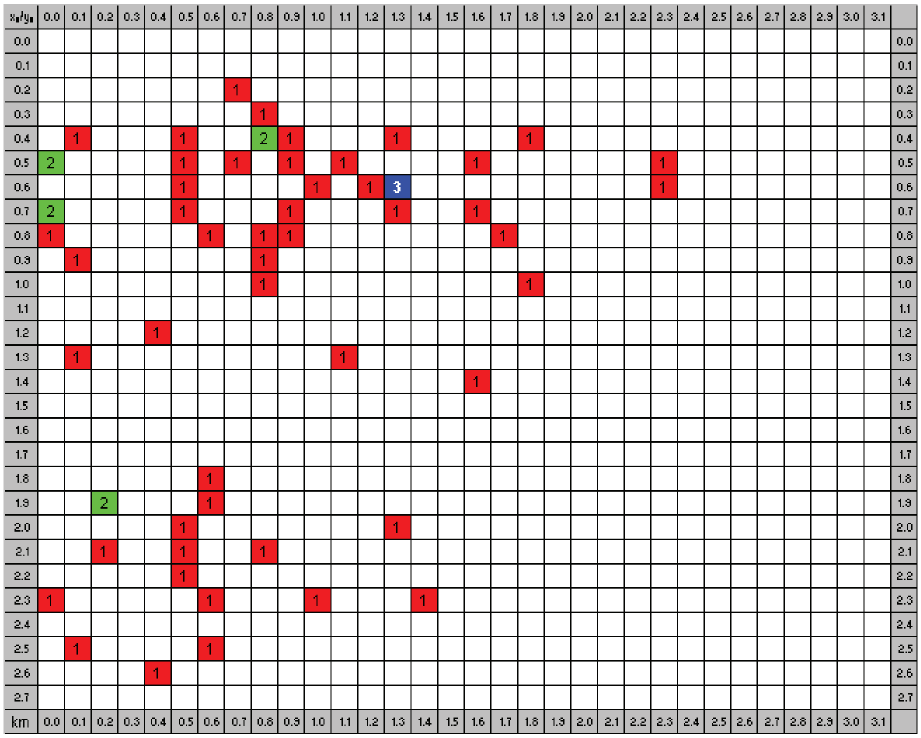
2.6		1	1		2																												2.6
2.7																																	2.7
km	0.0	0.1	0.2	0.3	0.4	0.5	0.6	0.7	0.8	0.9	1.0	1.1	1.2	1.3	1.4	1.5	1.6	1.7	1.8	1.9	2.0	2.1	2.2	2.3	2.4	2.5	2.6	2.7	2.8	2.9	3.0	3.1	

Figure 6. Upper Three Runs (UTR) aquifer grid showing the number of wells aggregated in each 0.1 x 0.1 km cell. The Universal Transverse Mecator (UTM) coordinates of the center of the origin cell at upper left is x0 = 435073, y0 = 3679743. The four cells with the yellow border, at x, y = (1.2, 0.6), (1.3, 0.7), (1.2, 0.8), and (1.5, 0.9), are those used in the time-series analysis. Numbers in the cells represent the number of wells. Cells with the same color have the same number of wells.



x_0/y_0	0.0	0.1	0.2	0.3	0.4	0.5	0.6	0.7	0.8	0.9	1.0	1.1	1.2	1.3	1.4	1.5	1.6	1.7	1.8	1.9	2.0	2.1	2.2	2.3	2.4	2.5	2.6	2.7	2.8	2.9	3.0	3.1	
0.0																																	0.0
0.1																																	0.1
0.2								1																									0.2
0.3									1																								0.3
0.4		1				1			2	1				1					1														0.4
0.5	2					1		1		1		1					1							1									0.5
0.6						1					1		1	3										1									0.6
0.7	2					1				1				1			1																0.7
0.8	1						1		1	1								1															0.8
0.9		1							1																								0.9
1.0									1										1														1.0
1.1																																	1.1
1.2					1																												1.2
1.3		1										1																					1.3
1.4																	1																1.4
1.5																																	1.5
1.6																																	1.6
1.7																																	1.7
1.8							1																										1.8
1.9			2				1																										1.9
2.0						1								1																			2.0
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2.4																																	2.4
2.5		1					1																										2.5
2.6					1																												2.6
2.7																																	2.7
km	0.0	0.1	0.2	0.3	0.4	0.5	0.6	0.7	0.8	0.9	1.0	1.1	1.2	1.3	1.4	1.5	1.6	1.7	1.8	1.9	2.0	2.1	2.2	2.3	2.4	2.5	2.6	2.7	2.8	2.9	3.0	3.1	

Figure 7. Gordon aquifer grid showing the number of wells aggregated in each 0.1 x 0.1 km cell. The Universal Transverse Mecator (UTM) coordinates of the center of the origin cell at upper left is x0 = 435073, y0 = 3679743. Numbers in the cells represent the number of wells. Cells with the same color have the same number of wells.

Table 2. Cell assignments of Upper Three Runs and Gordon aquifer wells, South Carolina.

[x and y coordinates are shown in figures 6 and 7, respectively. x, x-grid coordinate; y, y-grid coordinate; UTR, Upper Three Runs]

x	y	UTR wells	Gordon wells
2	0	CGW-49	
2.1	0.1	CGW-48	
0.6	0.2	CGW-51	
0.7	0.2	CGW-06	CGW-07
0.6	0.3	CGW-52	
0.8	0.3	CGW-04	CGW-05
1.4	0.3	CGW-16	
1.9	0.3	CGW-29	
0.1	0.4		CGW-99
0.5	0.4	CRW 8D	CRW 8A
0.6	0.4	CGW-54	
0.8	0.4	CGW-65	CGW-03; CGW-64
0.9	0.4		CGW-02
1.2	0.4	CGW-12	
1.3	0.4	CGW-14	CGW-13
1.4	0.4	CGW-15	
1.8	0.4		CGW-28
0	0.5		CGW-101; CRW 18T
0.4	0.5	131C-114	
0.5	0.5		CGW-56
0.7	0.5	CGW-62	CGW-63
0.9	0.5		CGW-01
1	0.5	CGW-09	
1.1	0.5		CGW-10
1.2	0.5	CGW-11	
1.4	0.5	CGW-47	
1.5	0.5	CGW-44	
1.6	0.5		CGW-27
1.8	0.5	CGW-35	
1.9	0.5	CGW-92	
2.3	0.5	CGW-33; CRW 1D	CRW 1A
0.2	0.6	131C-116; CRP 52A; CRP 52B	
0.3	0.6	131C-113	
0.5	0.6	131C-86; CRW 12C; CRW 12D	CRW 12A
0.7	0.6	CGW-61	
1	0.6		CGW-17
1.1	0.6	CRP 7D	
1.2	0.6	CRP 2; CRP 9D	CRSB-100
1.3	0.6	CRW 6C; CGW-46; CRSB-99	CGW-45; CRSB-98; CRW 6A
1.6	0.6	CGW-24; CGW-25; CGW-85	
1.7	0.6	CGW-86; CGW-87	
1.8	0.6	CRG-04	
1.9	0.6	CGW-91; CGW-97; CRG-03	
2.3	0.6	CGW-32; CRW 2D	CRW 2A
0	0.7		CGW-100; CRW 19T
0.2	0.7	131C-117	
0.5	0.7	131C-81; 131C-82; 131C-83; 131C-84; CRP 20CL; CRP 20CU	CGW-79
0.9	0.7		CRSB-48

Table 2. Cell assignments of Upper Three Runs and Gordon aquifer wells, South Carolina. — Continued

[x and y coordinates are shown in figures 6 and 7, respectively. x, x-grid coordinate; y, y-grid coordinate; UTR, Upper Three Runs]

x	y	UTR wells	Gordon wells
1	0.7	CGW-81	
1.1	0.7	CRP 16DL; CRP 16DU	
1.2	0.7	SVE 16A; AS 11; AS 17; CRP 11D; SVE 3A; SVE 8A; SVE 9A	
1.3	0.7	CRP 1; CRP 5D	CRSB-97
1.5	0.7	CRSB-94; CRSB-95; CRSB-96	
1.6	0.7	CRW 3C; CRW 3D; CGW-26; CGW-93	CRW 3A
1.7	0.7	CGW-84; CGW-96	
1.8	0.7	CGW-98; CRG-11A; CRG-13A	
2.3	0.7	CCP 1D	
0	0.8		CGW-102
0.1	0.8	CRP 51A; CRP 51B	
0.3	0.8	CRP 22CL; CRP 22CU	
0.4	0.8	131C-80; CRP 43A; CRP 43B; CRP 48A; CRP 48B	
0.5	0.8	CRP 42A; CRP 42B	
0.6	0.8		CGW-78
0.7	0.8	CRP 19C; CRP 19D; CRP 40A; CRP 40B; CRP 45A; CRP 45B	
0.8	0.8		CRSB-86
0.9	0.8	CRP 18C; CRP 18D	CRSB-50
1.1	0.8	CRP 8D; CRP 10D; CRP 17DL; CRP 17DU	
1.2	0.8	AS 3; AS 4; CRP 28DU; SVE 1A; SVE 2A; SVE 4A; SVE 5A; SVE 6A; SVE 7A; SVE 12A; SVE 13A; SVE 15A; SVE 17A; SVE 18A; SVE 20A; SVE 22A; SVE 23A; AS 1; AS 2; AS 5; AS 6; AS 7; AS 8; AS 9; AS 10; AS 12; AS 13; AS 14; AS 15; AS 16; CRP 3; CRP 3C; CRP 3D; CRP 4; CRP 23C; CRP 23DU; CRP 24DL; CRP 24DU; CRP 25DL; CRP 25DM; CRP 25DU; CRP 26DL; CRP 26DU; CRP 27DL; CRP 27DU; CRP 28C; CRSB-56; SVE 10A; SVE 11A; SVE 14A; SVE 19A; SVE 21A	
1.3	0.8	CRSB-90; CRSB-91	
1.4	0.8	CRSB-18; CRSB-25	
1.5	0.8	CSB 6A; CRSB-24	
1.6	0.8	CRSB-26; CRSB-7; CRSB-8; CRSB-92; CRSB-93	
1.7	0.8	CRW 4D; CRG-12A; CRSB-27; CRSB-28; CRW 4C	CRW 4A
1.8	0.8	CDB 1; CDB 2; CGW-95	
1.9	0.8	CGW-94; CRG-05; CRG-07; CRG-08; CRGW-10; CRGW-11; CRGW-3; CRGW-4; CRGW-5; CRGW-6; CRGW-7; CRGW-9	
2	0.8	CRGW-1; CRGW-12; CRGW-2	
2.5	0.8	CGW-31	
0.1	0.9	131C-118; 131C-119; CRP 50A; CRP 50B	CGW-80
0.2	0.9	CRP 21; CRP 44A; CRP 44B; CRP 49A; CRP 49B	
0.5	0.9	CRP 47A; CRP 47B	
0.6	0.9	CRP 41A; CRP 41B; CRP 46A; CRP 46B	
0.8	0.9		CRSB-82
1	0.9	CRSB-40; CRSB-52	
1.2	0.9	CRP 6DR; CRSB-88; CRSB-89	
1.4	0.9	CRSB-19; CRSB-20	
1.5	0.9	CSB 4A; CSB 5A; CRSB-10; CRSB-17; CRSB-9; CSB 3C	
1.6	0.9	CSB 1A; CRSB-5; CRSB-6; CSB 2C	
1.7	0.9	CRSB-29; CRSB-30; CRSB-4	
1.8	0.9	CRG-10A; CRSB-31	
1.9	0.9	CGW-89	
2	0.9	CGW-88	
2.5	0.9	CGW-30	

Table 2. Cell assignments of Upper Three Runs and Gordon aquifer wells, South Carolina. — Continued

[x and y coordinates are shown in figures 6 and 7, respectively. x, x-grid coordinate; y, y-grid coordinate; UTR, Upper Three Runs]

x	y	UTR wells	Gordon wells
2.6	0.9	CGW-34	
0	1	131C-120	
0.4	1	131C-90; 131C-91; 131C-92	
0.7	1	CGW-75	
0.8	1	131C-96; 131C-97; CRSB-96A; CRW 10C	CRW 10A
1.1	1	CRSB-41; CRSB-42	
1.3	1	CRSB-35	
1.5	1	CRSB-11; CRSB-12; CRSB-13; CRSB-21; CRSB-22; CSB 8D; CSB 9D	
1.6	1	CSB 2A; CSB 3A; CRSB-14; CRSB-15; CRSB-16	
1.7	1	CRSB-1; CRSB-2; CRSB-3	
1.8	1	CRW 5D; CSB 7D; CSB 1C	CRW 5A
2.5	1	CCB 1	
2.6	1	CCB 4	
0.4	1.1	131C-95	
0.8	1.1	131C-98	
1.3	1.1	CRSB-36	
1.4	1.1	CRSB-37	
1.5	1.1	CRSB-23	
1.6	1.1	CGW-58; CRSB-32	
1.7	1.1	CGW-57	
2.5	1.1	CCB 2; CCB 3	
3.1	1.1	RGW 17C; RGW 17D	
0.4	1.2		CGW-83
0.8	1.2	CGW-22	
1.3	1.2	CRSB-47A	
1.4	1.2	CRSB-38; CRSB-39	
1.5	1.2	CGW-18	
1.6	1.2	CGW-60	
0.1	1.3	CSB 12D	CRW 14A
0.3	1.3	CRSB-115	
0.7	1.3	CGW-23	
1.1	1.3	CRSB-116	CRW 9A
1.3	1.3	CSB 10D; CRSB-47	
1.5	1.3	CGW-36	
1.7	1.3	CGW-50; CGW-59	
1.9	1.3	CRSB-101	
0.1	1.4	CRSB-66	
0.7	1.4	CRSB-58	
1	1.4	CRSB-119	
1.1	1.4	CSB 11D; CRSB-117	
1.5	1.4	CGW-37	
1.6	1.4	CGW-39; CRW 7D	CRW 7A
0.7	1.5	CRSB-59	
1	1.5	CRSB-120	
1.2	1.5	CRSB-118	
0.3	1.6	CSB 13D; CRSB-114	
0.5	1.6	CGW-74	
0.6	1.6	CRSB-60	
1	1.6	CGW-73	

Table 2. Cell assignments of Upper Three Runs and Gordon aquifer wells, South Carolina. — Continued

[x and y coordinates are shown in figures 6 and 7, respectively. x, x-grid coordinate; y, y-grid coordinate; UTR, Upper Three Runs]

x	y	UTR wells	Gordon wells
1.1	1.6	CRSB-121	
1.4	1.6	RGW 16C; RGW 16D; CRSB-102	
0.6	1.8		CRSB-62
2	1.8	CRSB-103	
0.2	1.9	CRW 15D; CRW 15C	CRSB-113; CRW 15A
0.6	1.9		CRSB-62A
0.5	2		CRSB-63
1	2	CRSB-122	
1.1	2	CRSB-123	
1.2	2	CGW-41; CGW-42	
1.3	2	CGW-40; CRW 11D	CRW 11A
1.5	2	CRSB-107	
0.2	2.1		CRSB-112
0.5	2.1		CRSB-64
0.7	2.1	CGW-82	
0.8	2.1	CGW-20	CGW-19
1	2.1	CGW-43	
0.5	2.2		CRSB-65
1.2	2.2	CGW-76	
0	2.3		CRSB-111
0.6	2.3		CRSB-66A
0.9	2.3	CSB 15D; CGW-71	
1	2.3		CRW 13A
1.3	2.3	CGW-77	
1.4	2.3		CRSB-106
0.3	2.4	CGW-69	
0.1	2.5	CSB 14D	CRW 17A
0.5	2.5	CGW-70	
0.6	2.5		CRSB-109
0.1	2.6	CGW-66	
0.2	2.6	CGW-67	
0.4	2.6	CGW-68; CRW 16D	CRW 16A

of the data-collection process and interactions among the monitored analytes. The GDV is a Decision Support System developed in Excel™ and Visual Basic for Applications™ (VBA). Dutta and others (1997) describe Decision Support Systems as "computer-based systems helping decision-makers to solve various semi-structured and unstructured problems involving multiple attributes, objectives, and goals." The GDV allows users to spatially visualize C-Area ground-water analyte data measured in the Upper Three Runs and Gordon aquifers between 1984 and 2004. The data were processed to convert the large, but nonetheless temporally and spatially sparse, monitoring well- and record-oriented databases into time series of yearly average and maximum values that were then mapped onto a spatial grid of 0.1- × 0.1-km cells. The GDV provides features for statistically evaluating transport and degradation behavior. The GDV can help users answer "What, where, when, and how much?" about all of the analytes represented in C-Area's historical database. The GDV also provides analysis tools that temporally and spatially smooth, interpolate, and shift the time series to expand the possibilities for ascertaining behavioral trends in analyte degradation and transport. A user's manual for the GDV is provided in the Appendix and describes the installation, operation, and removal of the application.

Time-Series Analysis

The time series of yearly averaged and maximum measurements described previously and hereafter referred to as "measurements" were created to organize the raw data into a form that could be used to analyze and perhaps model the fate and transport of conservative and non-conservative constituents in ground-water systems using advanced data-mining techniques. The necessity of using a 1-year (12-month) time step for the C-Area measurements indicates that each analyte time series will have at most 21 measurements, which would be a satisfactory number if the measurements were to accurately represent the system's physical processes.

For each cell to have an associated time series, a fully populated time-series database would be composed of the number of analytes multiplied by 21 measurements per analyte. With 46 and 28 analytes measured in the Upper Three Runs and Gordon aquifers, respectively, full populations would have 966 and 588 measurements per cell, respectively. Figure 8 shows the number of measurements per cell in each aquifer. In the Upper Three Runs aquifer, 4 of the 146 cells have 300 or more measurements, and 97 have less than 30 measurements. In the Gordon aquifer, 37 of the 54 cells have less than 50 measurements, and none have more that 100. The total numbers of measurements for the Upper Three Runs and Gordon aquifers are 10,798 and 1,621, respectively, compared with theoretical full populations of 141,036 measurements for the Upper Three Runs aquifer and 31,752 measurements for the Gordon aquifer. Therefore, the percent of full population for the Upper Three Runs and Gordon aquifers is 7.7 and 5.1, respectively. These statistics suggest spatial and(or) temporal sparseness in and among the time series, even after there has been considerable spatial and temporal aggregation of the raw records.

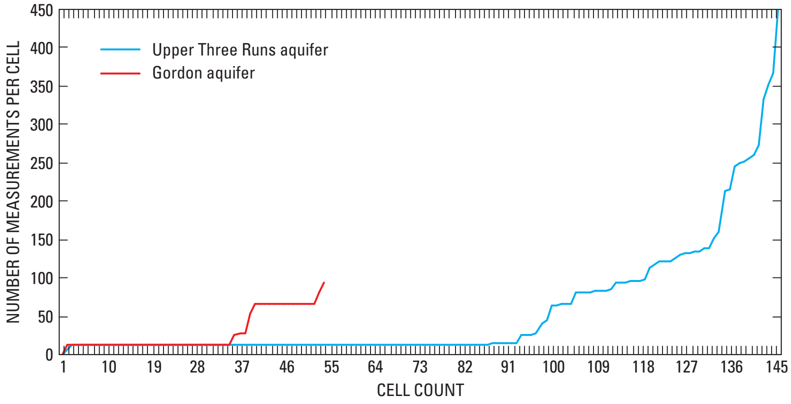
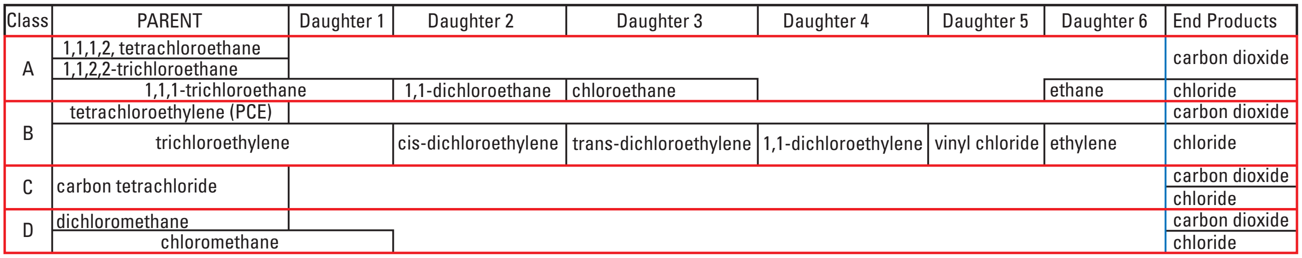


Figure 8. Graph showing number of measurements for each Upper Three Runs and Gordon aquifers cell having measurements. Cell counts have been sorted from lowest to highest.

Time Series of Volatile Organic Compound Degradation Products

The degradation of volatile organic compounds (VOCs) to end products can be characterized by the transformation from "parent" to "daughter" products and to the eventual end products. Analyte degradation maps from parent to daughter end products are charted for four VOCs—organic carbon, nitrate, sulfate, and iron,—under reducing conditions and are labeled as Class A through D (fig. 9). From left to right, each class is composed of one or more "parent" analyte, intermediate "daughter" analytes that are formed by the degradation of parent or preceding daughter analytes, and carbon dioxide and(or) chloride end products. Chloride and carbon dioxide are degradation end products of chlorinated VOCs in Classes A to D (fig. 9). Additionally, degradation occurs only in anaerobic environments, so oxygen concentration is also an important indicator of the potential for degradation; however, there were few carbon dioxide and dissolved-oxygen measurements made in the four cells. Parent analytes in all four VOC degradation classes are chlorinated VOCs and ultimately are reduced to end products of carbon dioxide and chlorides. Note that a class can begin with multiple starting parents. Three of the four VOC degradation classes have intermediate daughter products and can result from more than one parent. For example, in Class A, 1,1-dichloroethane is a degradation product of 1,1,1-trichloroethane, which can act as a parent analyte or can be a degradation product of 1,1,2,2-trichloroethane and 1,1,1,2-tetrachlorethane.

Flow velocities at C-Area are believed to be less than 30 m per year (Siple, 1967), making the flow velocities slow relative to the grid's 0.1- × 0.1-km cell size. Temporal changes in analyte concentrations can be due to advection, dispersion (diffusion), biochemical reactions, and occurrences of new sources. Inspection of the time series in the GDV shows little large-scale spatial movement (advection) of contaminants



Class	PARENT	Daughter 1	Daughter 2	Daughter 3	Daughter 4	Daughter 5	Daughter 6	End Products
A	1,1,1,2, tetrachloroethane							carbon dioxide
	1,1,2,2-trichloroethane							
	1,1,1-trichloroethane		1,1-dichloroethane	chloroethane			ethane	chloride
B	tetrachloroethylene (PCE)							carbon dioxide
	trichloroethylene		cis-dichloroethylene	trans-dichloroethylene	1,1-dichloroethylene	vinyl chloride	ethylene	chloride
C	carbon tetrachloride							carbon dioxide chloride
D	dichloromethane							carbon dioxide
	chloromethane							chloride

Figure 9. Analyte "degradation map" from parent to end product for four classes of volatile organic compounds.

across the grid, suggesting that analyte behaviors could be compared reasonably using time series from cells having higher data densities. Therefore, four Upper Three Runs aquifer cells having the highest numbers of measurements were selected for time-series analysis. The four cells were those located at grid x, y = (1.2, 0.6), (1.3, 0.7), (1.2, 0.8), and (1.5, 0.9) (fig. 6) and are hereafter referred to as cells 1206, 1307, 1208, and 1509, respectively. Three of the cells are near the contaminant source at CBRP: cell 1208 is downgradient in the plume and near the source area, cell 1307 is upgradient with less contamination, and cell 1206 is to the side of the plume with the lowest VOC concentrations. Cell 1509 is downgradient from the contaminated source area associated with the CRSB. The properties of the four cells are listed in table 3 and show that while cell 1208 has more measurements than the other cells, the cell 1208 measurements were taken from 52 different wells in the cell as compared to 2 wells in cells 1206 and 1307 and 6 wells in cell 1509.

Table 3. Statistics for cells used in time-series analysis.

[CBRP, C-Area Burning/Rubble Pit; CRSB, C-Reactor Seepage Basin]

Facility	Cell	Number of wells	Number of measurements
CBRP	1206	2	366
CBRP	1307	2	332
CBRP	1208	52	450
CRSB	1509	6	352

The average and maximum values for chloride concentrations and depth to water in the four cells are shown in figures 10 and 11, respectively. The chloride and depth-to-water averages were computed from all measurements of an analyte from within a cell for a given time stamp (date and time). The maximums are the highest measured value of an analyte from within a cell for a given time stamp. Comparing average and maximum values gives an indication of spatial and temporal variability within a cell for a given time stamp. A small difference between an average and maximum indicates little variability and no difference indicates that they are the same measurement.

The chlorides appear to remain essentially constant at low levels with the exception of a single spike concentration in 1996. The depths generally track together with apparent peaks during 2002. The higher variability in cell 1208 might be due to measurements taken at a relatively large number of wells (52).

Figures 12 through 15 show the Class A ethane time series for the four cells. All concentrations are at or below 1 mg/L and exhibit little temporal variability, which is consistent with the negligible chlorides concentrations shown in figure 10. For each cell and time stamp, concentrations frequently are identical. This could be the result of censored data and the detection limit being reported. Earlier concentrations could have been measured using analytical chemistry methods that had difficulty discriminating between chemically similar analytes. It is possible that the same values were entered into the database for multiple chlorinated ethanes.

The Class B ethylene time series for the four cells are shown in figures 16 through 19. In recent years (1999–2004), appreciable variability has occurred in maximum concentration in cell 1208 (fig. 18) which may coincide with the advent of more accurate gas chromatograph measurement technology. Similarly, figures 20 and 21 present Class C and D time series, respectively, like Class B, show variability in the concentration of other analytes in recent years in cell 1208.

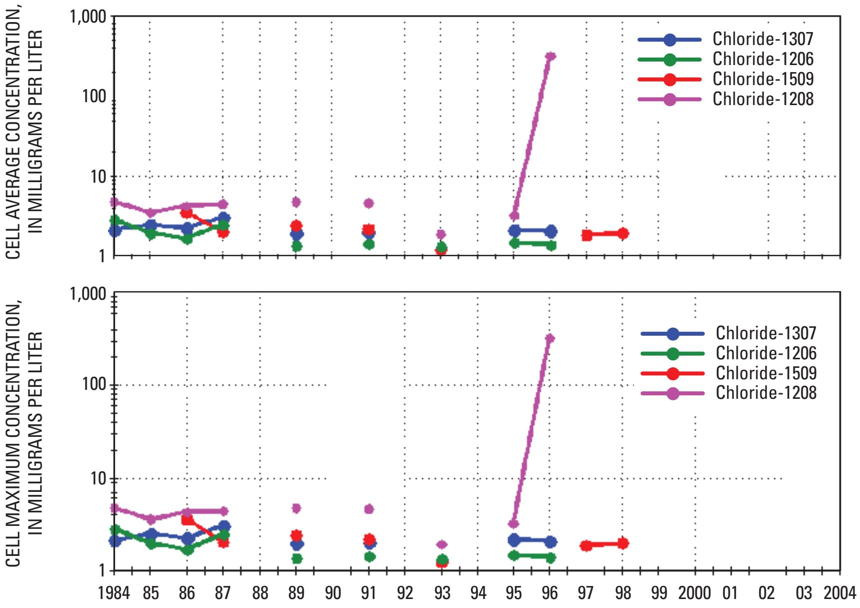


Figure 10. Chlorides concentrations measured in the Upper Three Runs aquifer for the four cells for which time series were analyzed.

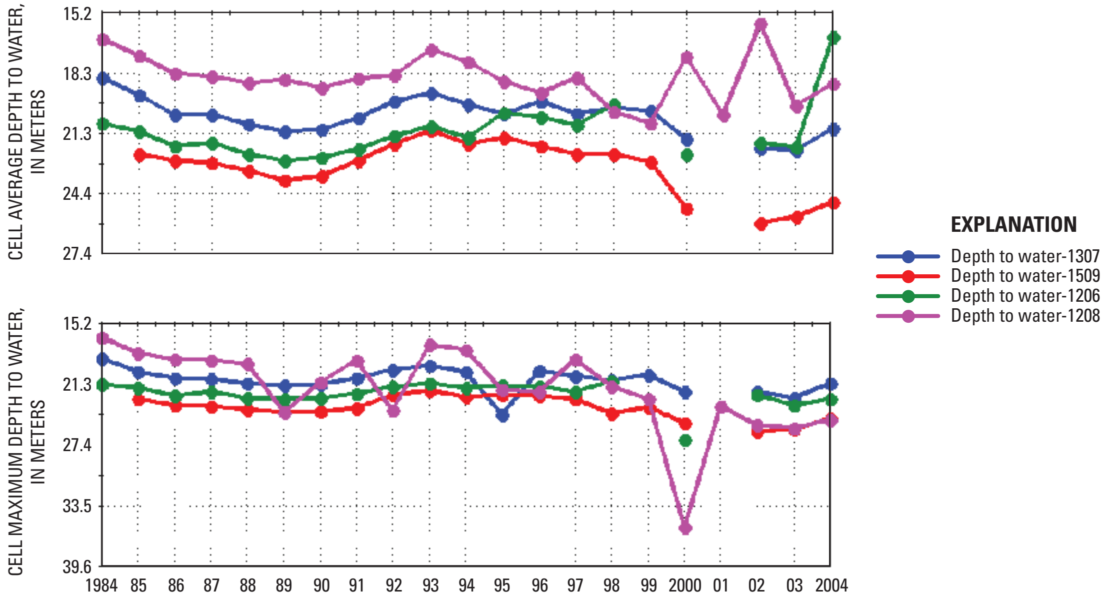


Figure 11. Depth to water measured in the Upper Three Runs aquifer for the four cells for which time series were analyzed.

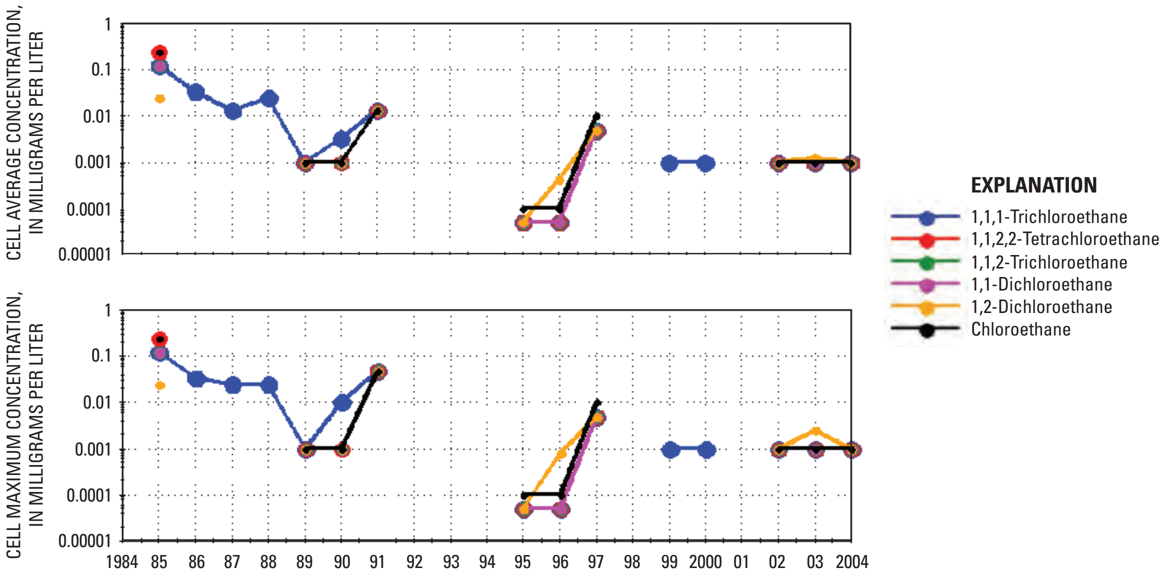


Figure 12. Cell 1307 average and maximum Class A analyte concentrations.

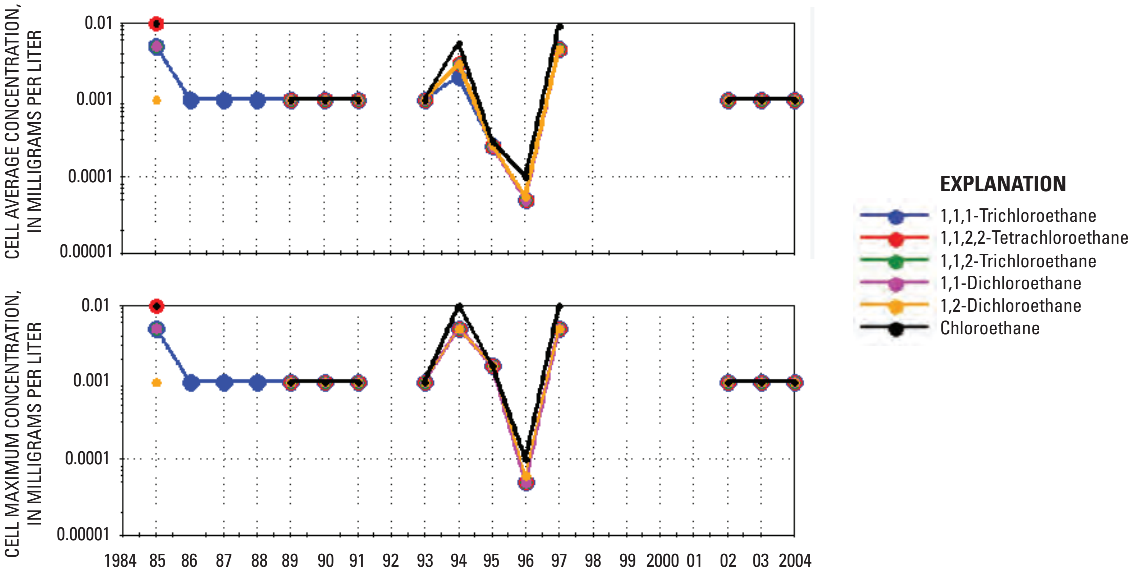


Figure 13. Cell 1206 average and maximum Class A analyte concentrations.

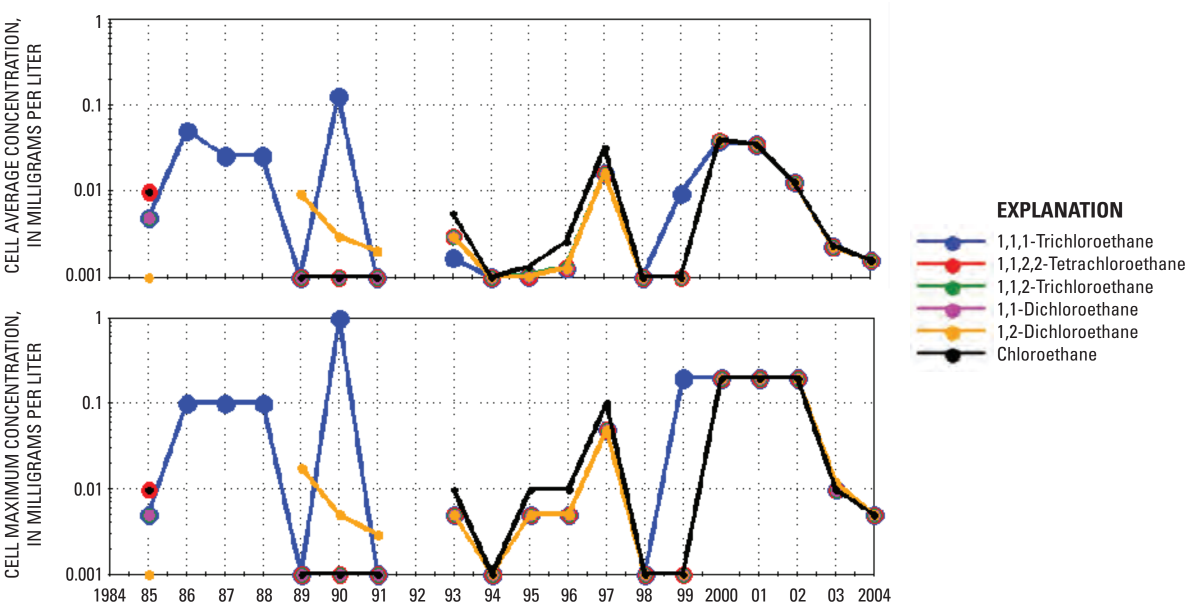


Figure 14. Cell 1208 average and maximum Class A analyte concentrations.

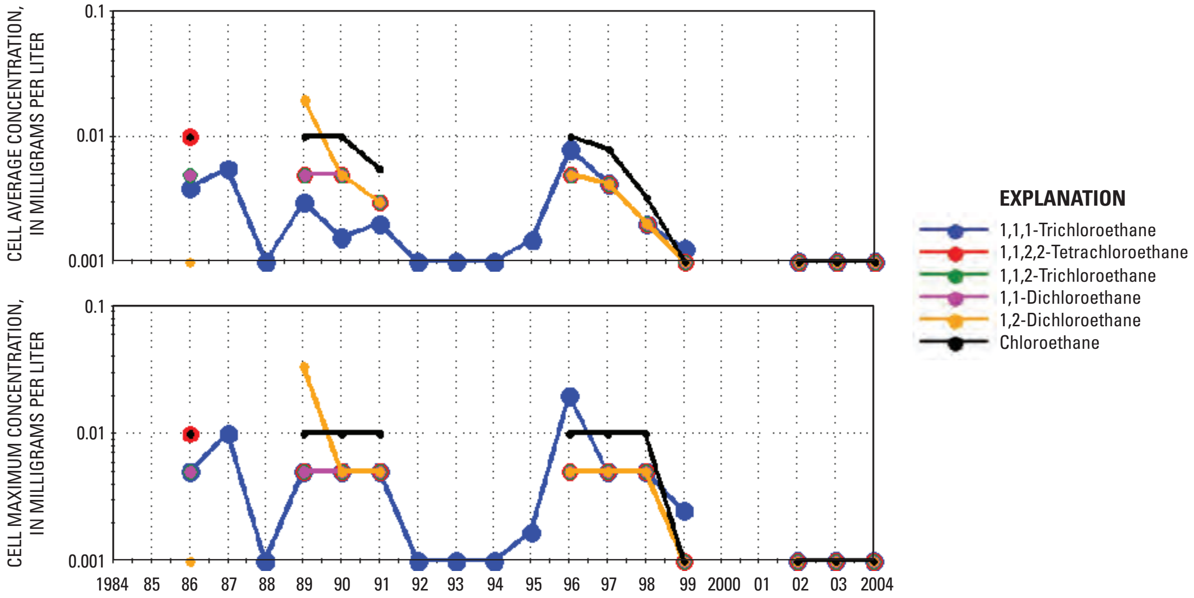


Figure 15. Cell 1509 average and maximum Class A analyte concentrations.

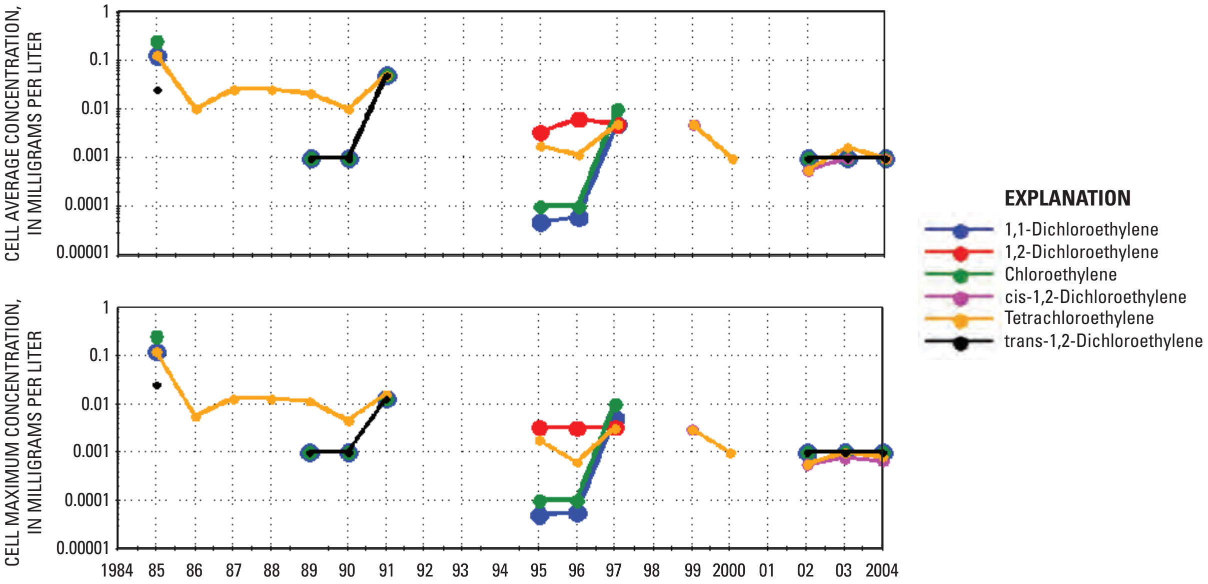


Figure 16. Cell 1307 average and maximum Class B analyte concentrations.

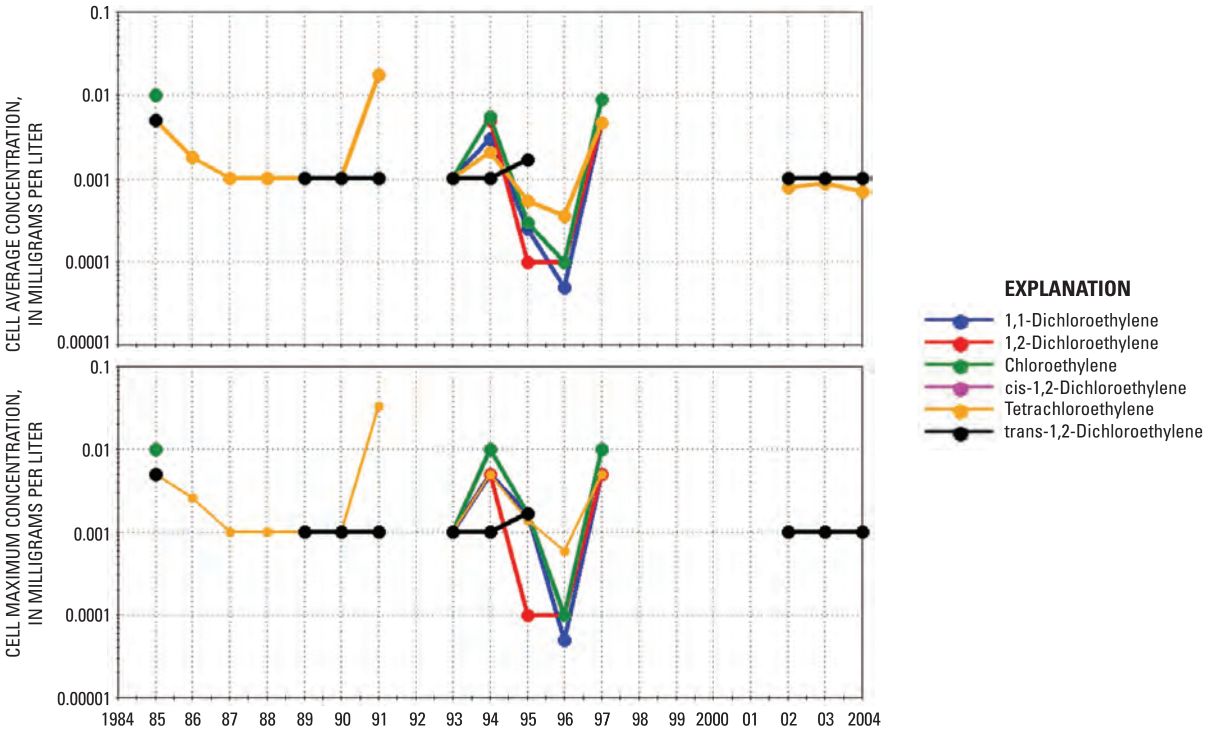


Figure 17. Cell 1206 average and maximum Class B analyte concentrations.

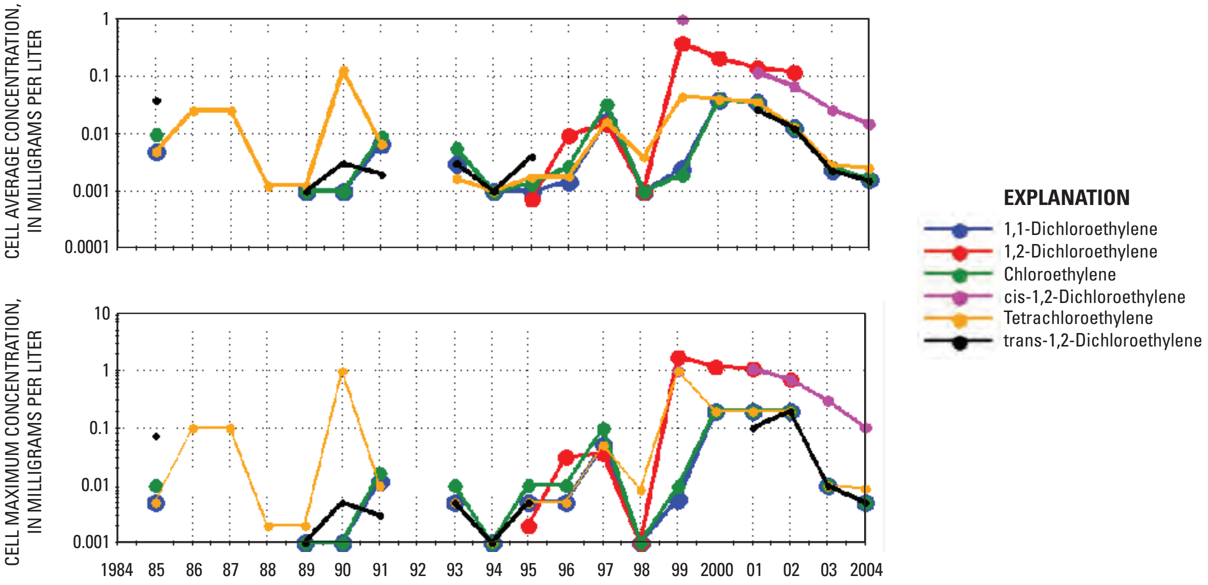


Figure 18. Cell 1208 average and maximum Class B analyte concentrations.

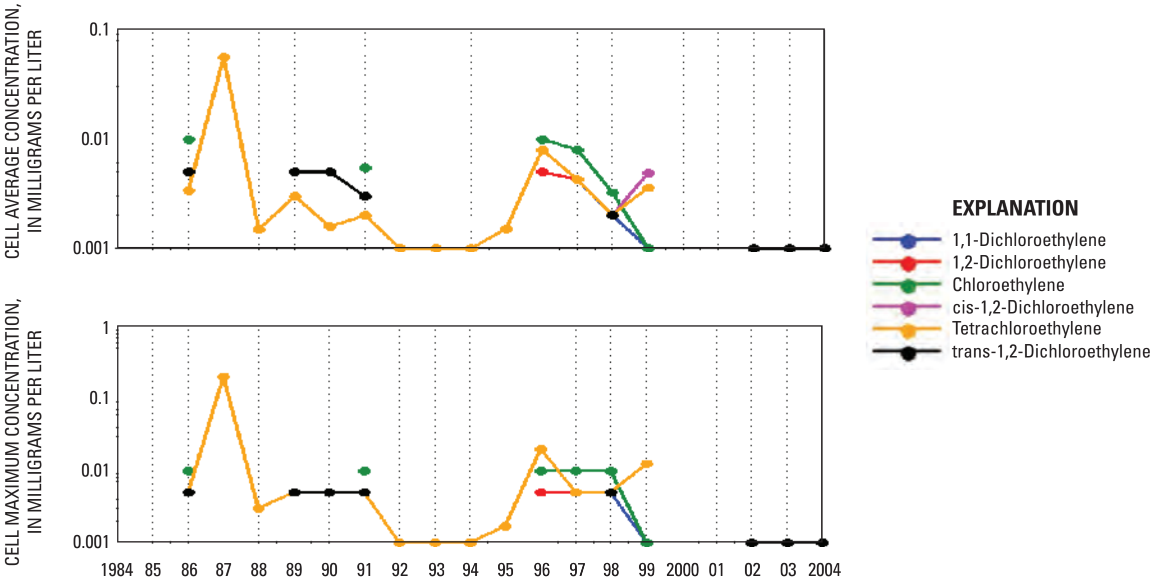


Figure 19. Cell 1509 average and maximum Class B analyte concentrations.

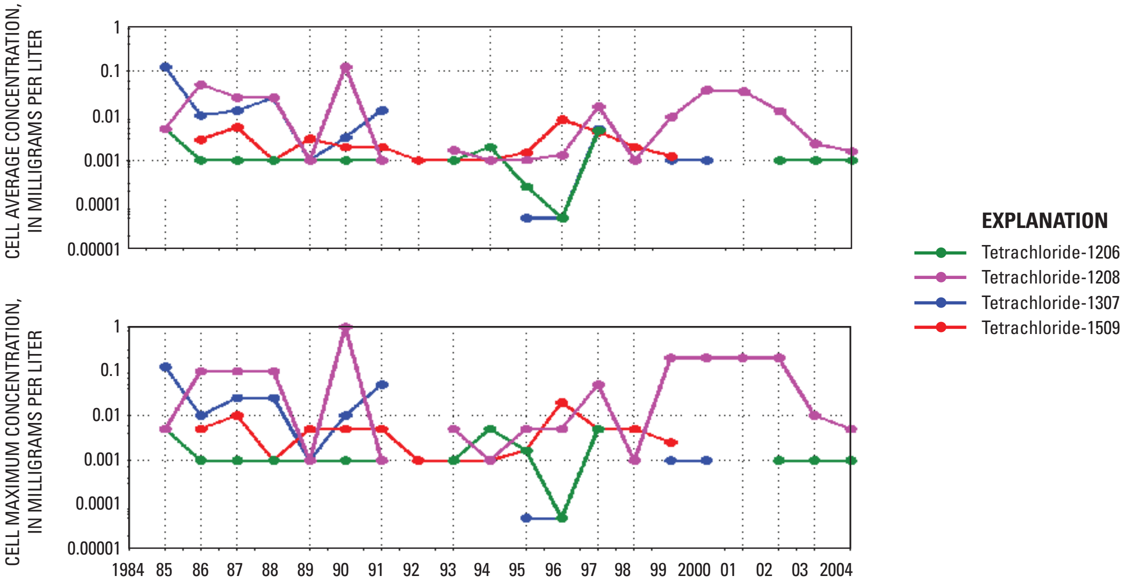


Figure 20. Average and maximum Class C analyte (carbon tetrachloride) concentrations for cells 1206, 1208, 1307, and1509.

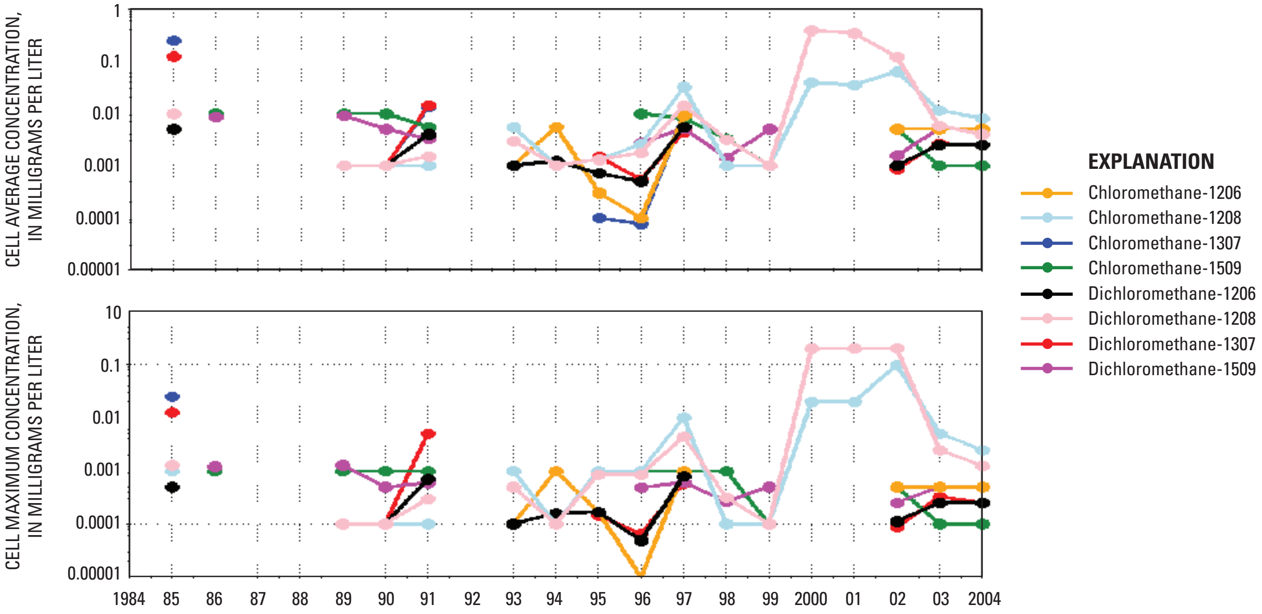


Figure 21. Average and maximum Class D analyte concentrations for cells 1206, 1208, 1307, and 1509.

Analysis of Inferential Analytes

An attempt was made to determine if the contaminants could be estimated inferentially using other analytes. As noted above, chlorides and carbon dioxide are degradation end products, and oxygen is an indicator of possible anaerobic degradation. Bivariate Pearson correlation coefficients (R) and coefficients of determination (R^2) for the contaminants in cell 1208 and candidate predictor analytes for inferential analytes are listed in table 4. Cell 1208 had the most data and exhibited the most variability in chlorinated hydrocarbon concentrations. As described previously, the data used to generate the statistics were noisy and sparse; however, consistently higher correlations having the same sign of R are seen in depth to water, nitrate concentration, and total dissolved solids (TDS).

Three-Dimensional Visualization

Two examples are given on how the GDV can be used to visualize data from the C-Area. The GDV was set up to show a 3-year sequence (2000, 2002, and 2004) of maximum cis-1,2-dichlorenthylene concentration (fig. 22). The data are spatial and temporal averages of 3 × 3 cells (9 total cells) and 2 years. The viewer shows a two-dimensional plan view and a three-dimensional view. The outline of the TCE plume (fig. 4) is shown in the plan views. Note the apparent decreasing trend in cis-1,2-dichloroethylene concentrations.

A 6-year sequence of Class B analytes is shown in figure 23. From 1999 to 2000, higher concentrations of 1,1-dichlorethylene and chloroethylene appear north and west of where samples had previously been collected. Subsequent wider-scale sampling from 2001 to 2004 further delineates the plumes, during which time concentrations are seen to decline. Decrease in concentrations may be due to advection, dispersion, or degradation. Spatial shifts in peak concentration might be indications of transport and could be confirmed with known ground-water-flow direction.

Summary and Conclusions

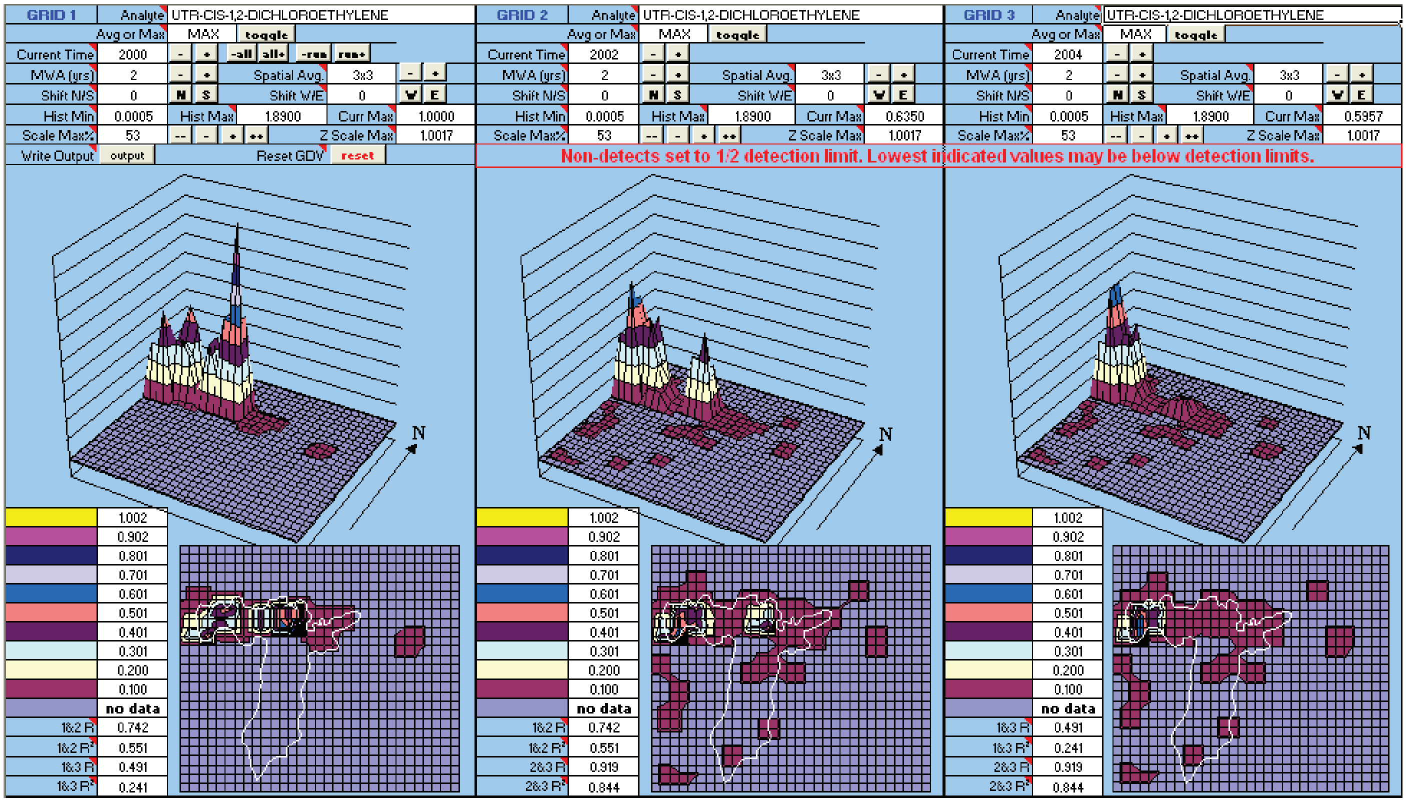
This project demonstrated how the C-Area database records could be organized into time series, representing 21 years of temporal and spatial variability. The collection of time series was analyzed to determine its overall data density and quality, suggesting limits about what is possible to learn from the data. Trend and correlation analyses can potentially describe degradation processes and options for inferential estimates of analytes of interest. Particular issues for the C-Area data include spatial and temporal sparseness, a lack

Table 4. Pearson correlation coefficients (R) and coefficients of determination (R^2) for cell 1208 chlorinated hydrocarbons and candidate predictor analytes.

[Colors represent the Class A–D of volatile organic compounds. Class A is pink, Class B is tan, Class C is green, and Class D is white. Average coefficients of determination greater than 0.25 are highlighted in yellow]

R	Air temperature	Alkalinity (as $CaCO_3$)	Calcium	Chloride	Depth to water	Iron	Magnesium	Nitrate	pH	Phosphorus	Silica	Specific conductance	Sulfate	Total dissolved solids	Total organic carbon	Total organic halogens	Phenolphthalein alkalinity
1,1,2,2-Tetrachloroethane	0.38	0.17	-0.41	0.07	0.61	-0.18	0.02	-0.45	-0.01	0.61	0.58	-0.18	0.07	-0.86	0.41	-0.11	-0.27
1,1,1-Trichloroethane	0.14	0.41	0.28	-0.21	0.12	-0.32	-0.23	0.50	0.23	-0.35	-0.21	0.13	-0.24	0.36	-0.20	0.30	-0.68
1,1,2-Trichloroethane	0.39	0.17	-0.41	0.32	0.61	-0.17	0.02	-0.88	-0.01	0.61	0.58	-0.19	0.32	-0.86	0.40	-0.11	-0.27
1,1-Dichloroethane	0.39	0.17	-0.41	0.32	0.61	-0.17	0.02	-0.88	-0.01	0.61	0.58	-0.19	0.32	-0.86	0.40	-0.11	-0.27
1,2-Dichloroethane (EDC)	0.41	0.21	-0.09	-0.09	0.63	-0.19	-0.13	-0.50	0.01	0.34	-0.24	-0.17	-0.10	0.82	0.38	-0.04	-0.27
Chloroethane	0.38	0.13	-0.42	0.32	0.56	-0.18	0.03	-0.88	-0.06	0.61	0.58	-0.21	0.32	-0.86	0.42	-0.17	-0.27
Tetrachloroethylene	0.18	0.18	0.27	-0.22	0.13	-0.21	-0.23	0.25	0.00	-0.35	-0.21	-0.04	-0.19	0.38	-0.18	0.15	-0.60
trans-1,2-Dichloroethylene	0.00	0.00	-0.79	-0.14	0.33	-0.22	0.73	-0.02	0.20	0.24	0.48	0.06	-0.27	-0.98	0.94	-0.23	-0.11
1,1-Dichloroethylene	0.40	0.17	-0.40	-0.07	0.61	-0.19	-0.04	0.88	0.00	-0.08	0.04	-0.19	-0.07	-0.27	0.39	-0.09	-0.28
Chloroethylene	0.39	0.14	-0.41	0.03	0.56	-0.21	-0.02	0.88	-0.06	0.10	0.20	-0.21	0.03	-0.54	0.40	-0.14	-0.29
Carbon tetrachloride	0.14	0.41	0.28	-0.21	0.12	-0.32	-0.23	0.50	0.23	-0.35	-0.21	0.13	-0.24	0.36	-0.20	0.30	-0.68
Chloromethane	0.29	0.00	-0.42	0.32	0.33	-0.18	0.03	-0.88	0.17	0.61	0.58	-0.04	0.32	-0.86	0.42	-0.17	0.36
Dichloromethane	0.39	0.20	-0.48	0.22	0.64	-0.15	0.10	-0.27	0.03	0.85	0.73	-0.16	0.22	-0.75	0.39	-0.05	-0.28

R^2	Air temperature	Alkalinity (as $CaCO_3$)	Calcium	Chloride	Depth to water	Iron	Magnesium	Nitrate	pH	Phosphorus	Silica	Specific conductance	Sulfate	Total dissolved solids	Total organic carbon	Total organic halogens	Phenolphthalein alkalinity
1,1,2,2-Tetrachloroethane	0.14	0.03	0.17	0.01	0.37	0.03	0.00	0.20	0.00	0.37	0.34	0.03	0.01	0.73	0.17	0.01	0.07
1,1,1-Trichloroethane	0.02	0.17	0.08	0.04	0.01	0.10	0.05	0.25	0.05	0.12	0.04	0.02	0.06	0.13	0.04	0.09	0.46
1,1,2-Trichloroethane	0.15	0.03	0.17	0.10	0.38	0.03	0.00	0.77	0.00	0.37	0.34	0.04	0.10	0.73	0.16	0.01	0.07
1,1-Dichloroethane	0.15	0.03	0.17	0.10	0.38	0.03	0.00	0.77	0.00	0.37	0.34	0.04	0.10	0.73	0.16	0.01	0.07
1,2-Dichloroethane (EDC)	0.17	0.04	0.01	0.01	0.39	0.04	0.02	0.25	0.00	0.11	0.06	0.03	0.01	0.68	0.14	0.00	0.07
Chloroethane	0.14	0.02	0.17	0.10	0.32	0.03	0.00	0.77	0.00	0.37	0.34	0.04	0.10	0.73	0.18	0.03	0.07
Tetrachloroethylene	0.03	0.03	0.07	0.05	0.02	0.04	0.05	0.06	0.00	0.12	0.05	0.00	0.03	0.14	0.03	0.02	0.36
trans-1,2-Dichloroethylene	0.00	0.00	0.62	0.02	0.11	0.05	0.53	0.00	0.04	0.06	0.23	0.00	0.08	0.97	0.88	0.05	0.01
1,1-Dichloroethylene	0.16	0.03	0.16	0.00	0.37	0.04	0.00	0.77	0.00	0.01	0.00	0.04	0.00	0.07	0.15	0.01	0.08
Chloroethylene	0.15	0.02	0.17	0.00	0.31	0.04	0.00	0.77	0.00	0.01	0.04	0.05	0.00	0.29	0.16	0.02	0.08
Carbon tetrachloride	0.02	0.17	0.08	0.04	0.01	0.10	0.05	0.25	0.05	0.12	0.04	0.02	0.06	0.13	0.04	0.09	0.46
Chloromethane	0.08	0.00	0.17	0.10	0.11	0.03	0.00	0.77	0.03	0.37	0.34	0.00	0.10	0.73	0.18	0.03	0.13
Dichloromethane	0.15	0.04	0.23	0.05	0.41	0.02	0.01	0.07	0.00	0.72	0.54	0.03	0.05	0.56	0.15	0.00	0.08
Average	0.11	0.05	0.17	0.05	0.25	0.05	0.06	0.44	0.01	0.24	0.21	0.02	0.05	0.51	0.19	0.03	0.16



GRID 1
Analyte: UTR-CIS-1,2-DICHLOROETHYLENE
Avg or Max: MAX
Current Time: 2000
MWA (yrs): 2
Spatial Avg.: 3x3
Shift N/S: 0
Shift W/E: 0
Hist Min: 0.0005
Hist Max: 1.8900
Curr Max: 1.0000
Scale Max%: 53
Z Scale Max: 1.0017
Write Output
Reset GDV

GRID 2
Analyte: UTR-CIS-1,2-DICHLOROETHYLENE
Avg or Max: MAX
Current Time: 2002
MWA (yrs): 2
Spatial Avg.: 3x3
Shift N/S: 0
Shift W/E: 0
Hist Min: 0.0005
Hist Max: 1.8900
Curr Max: 0.6350
Scale Max%: 53
Z Scale Max: 1.0017

GRID 3
Analyte: UTR-CIS-1,2-DICHLOROETHYLENE
Avg or Max: MAX
Current Time: 2004
MWA (yrs): 2
Spatial Avg.: 3x3
Shift N/S: 0
Shift W/E: 0
Hist Min: 0.0005
Hist Max: 1.8900
Curr Max: 0.5957
Scale Max%: 53
Z Scale Max: 1.0017

Non-detects set to 1/2 detection limit. Lowest indicated values may be below detection limits.

Grid 1		Grid 2		Grid 3	
🟨	1.002	🟨	1.002	🟨	1.002
🟪	0.902	🟪	0.902	🟪	0.902
■	0.801	■	0.801	■	0.801
▨	0.701	▨	0.701	▨	0.701
🟦	0.601	🟦	0.601	🟦	0.601
🟥	0.501	🟥	0.501	🟥	0.501
■	0.401	■	0.401	■	0.401
▨	0.301	▨	0.301	▨	0.301
▨	0.200	▨	0.200	▨	0.200
■	0.100	■	0.100	■	0.100
▨	no data	▨	no data	▨	no data
1&2 R	0.742	1&2 R	0.742	1&3 R	0.491
1&2 R²	0.551	1&2 R²	0.551	1&3 R²	0.241
1&3 R	0.491	2&3 R	0.919	2&3 R	0.919
1&3 R²	0.241	2&3 R²	0.844	2&3 R²	0.844

Figure 22. Maximum *cis*-1,2-dichloroethylene concentration for the Upper Three Runs aquifer for 2000, 2002, and 2004. Note the white trace outline of the trichloroethylene plume in the plan views at the bottom.

of concurrency in making measurements, and the accuracy of older measurements made by analytical chemistry methods.

The GDV provides a means for quickly evaluating all of the time series in an interactive environment with visualization and statistical tools. Data-quality issues identified in the time-series analysis are more comprehensively defined in GDV, such that future data-collection activities could be modified to provide better knowledge at lower cost. In particular, efforts should be considered to better identify plume boundaries to target limited sampling resources more closely; sampling should be concurrent and at fixed intervals so that dynamic behaviors can be ascertained more readily; data should be archived in an information system that avoids input errors and facilitates time-series analyses; and possible predictor analytes such as oxygen, chlorides, and carbon dioxide should be measured with the contaminants to determine their effectiveness in inferential estimation.

Findings from the time-series analysis include the following:

- Spatial and temporal aggregation of measurement records into grid cells and time steps made it possible to analyze record-oriented data as time series, which is necessary to ascertain water chemistry behaviors.

- Historical chlorinated hydrocarbon measurements obtained by analytical chemistry methods are possibly less reliable than those obtained using gas chromatography.

- Few different analytes were measured in most of the cells, making the time-series data spatially sparse. The time series of cells also were found to be temporally sparse. The measurement populations for the 146 Upper Three Runs aquifer and 54 Gordon aquifer cells having measurements were only 7.6 percent and 5.1 percent filled for 46 and 28 analytes, respectively.

- Of the four Upper Three Runs aquifer cells having the most measurements, only one cell (1208) exhibited significant chlorinated hydrocarbon concentrations and temporal variability. This suggests that many of the historical data provide little information about transport and degradation processes.

- Inferential indications of degradation behavior might be obtainable from analytes such as chloride, carbon dioxide, oxygen, and possibly others by means of a multivariate empirical model; however, measurements of candidate predictor analytes are sparse in the C-Area data.

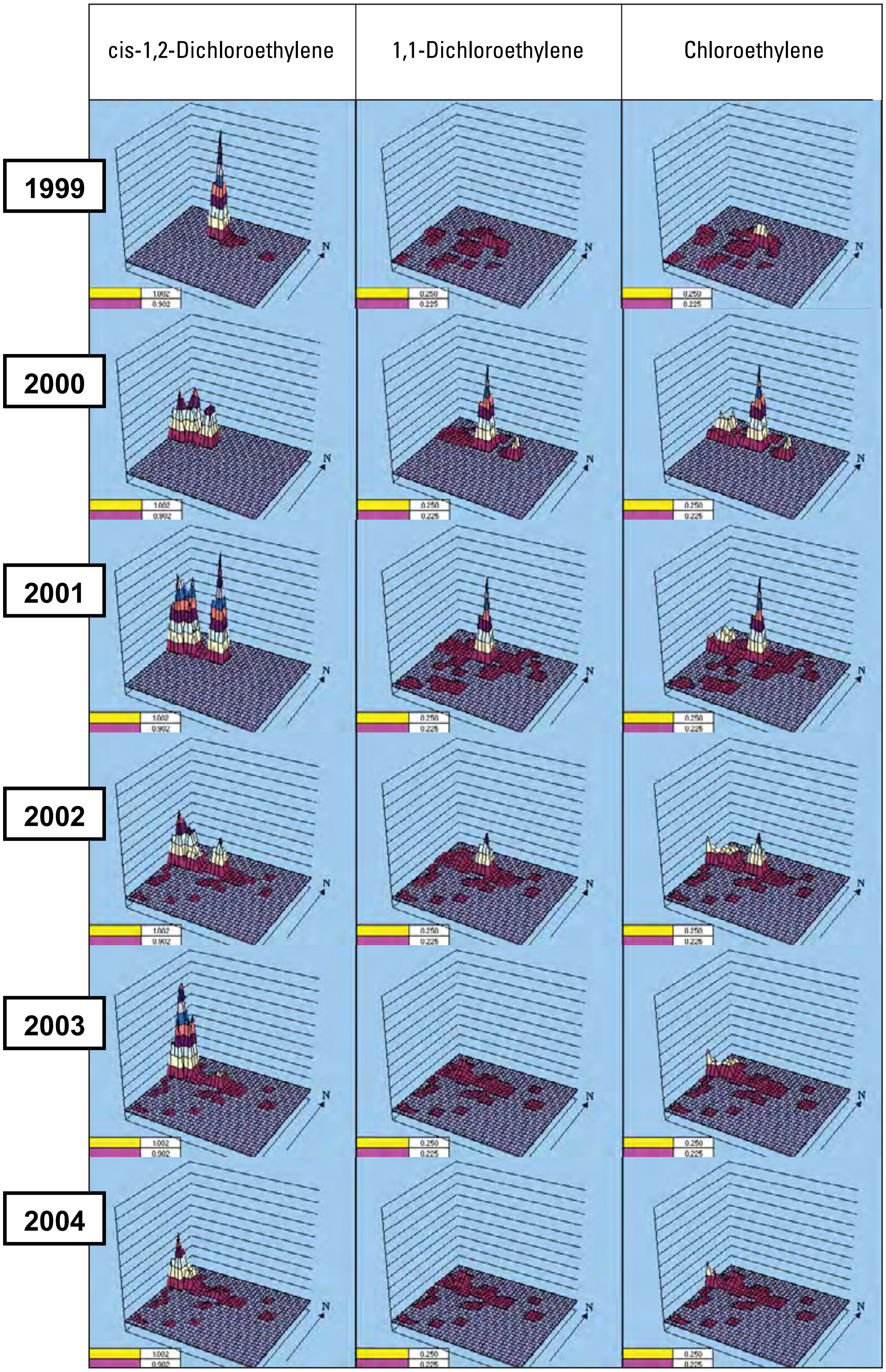


Figure 23. Maximum Class B analyte concentrations for the Upper Three Runs aquifer from 1999 to 2004. Note that the *cis*-1,2-dichloroethylene scale (left) is four times that of the 1,1-dichloroethylene (center) and chloroethylene (right) concentrations.

The conversion of record-oriented data into time series is essential to analyzing behaviors over time. The integration of time series with visualization and analytical tools can greatly improve the depth, breadth, and quality of the knowledge that can be obtained from costly data-collection efforts. The quality and timeliness of acquired knowledge directly affects the ability of site environmental managers to attain the goal of optimally managing a contaminated ground-water site. The following steps could increase the utility and improve the interpretation of data at both the SRS and other similar sites.

1. Review data archival processes to identify needs and remedies for ensuring the quality and completeness of future analyte measurement records.
2. Extend data archival and retrieval infrastructure to include the automatic conversion of database records into time series as described, in this report, and provide a means to export the time series for use by external applications, such as Microsoft Excel™.
3. In the case of SRS, extend the current GDV application to include parent analytes, such as tetrachloroethylene and trichloroethylene; other areas, such as L- and P-Areas; Kriging to perform spatial interpolation of analyte concentrations—an enhancement over the currently implemented spatial averaging; and conversion of the GDV and the existing record database into a client/server application. The GDV, which is a spreadsheet application and easily and inexpensively distributed, could be programmed to retrieve database records and convert them to time series for visualization and analyses.

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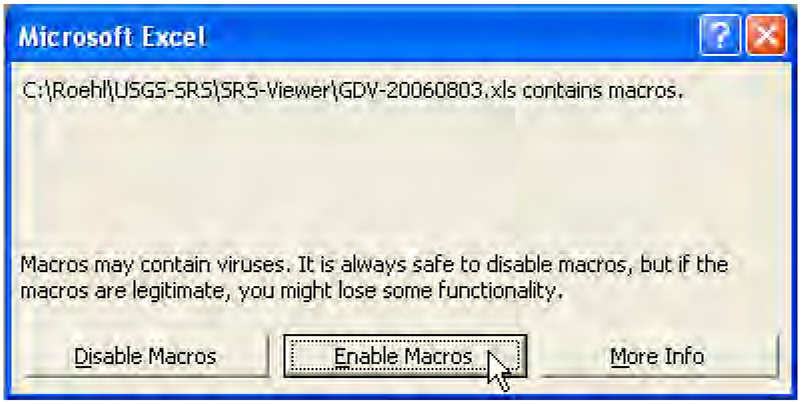
Appendix 1: User's Manual for the Ground-Water Data Viewer (GDV)

An important part of the U.S. Geological (USGS) mission is to provide scientific information for the effective management of the Nation's water resources. Often, ground-water and surface-water systems of concern, such as the C-Area system, have large historical databases that are underutilized and not well interpreted for addressing contemporary water-quality issues. The techniques used to develop the Ground-Water Data Viewer (GDV) demonstrate how valuable information can be extracted from existing databases to assist local, State, and Federal agencies in making water-management decisions. The application of data-mining techniques to the ground-water data for C-Area at the Savannah River Site (SRS) demonstrates how disparate historical monitoring networks can be integrated using a Decision Support System (DSS) to interrogate and visualize historical data and assist water-resource managers in evaluating future monitoring approaches. The techniques are readily applicable to other systems for evaluation of historical data and for alternative monitoring strategies.

This manual is distributed as an appendix to U.S. Geological Survey Scientific Investigations Report 2007–5140, "Visualization and Time-Series Analysis of Ground-Water Data for C-Area, Savannah River Site, South Carolina, 1984-2004." To differentiate figures in the appendix from those in the main body of the report, figures in the appendix use a numbering scheme that includes "A" as a prefix, for example, figure A1.

1. INSTALLATION, LAUNCH, SHUTDOWN, AND REMOVAL

The GDV is a Visual Basic for Applications™ (VBA) application distributed as a single Excel™ (.xls) file named GDV-yyyymmdd.xls. GDV may be launched by double clicking the program's icon, from any drive connected to your computer. As shown in figure A1, the user is asked via a pop-up window if macros are to be enabled. The Enable Macros button must be clicked to enable the VBA components of GDV and for the program to operate normally.



C:\Roehl\USGS-SRS\SRS-Viewer\GDV-20060803.xls contains macros.

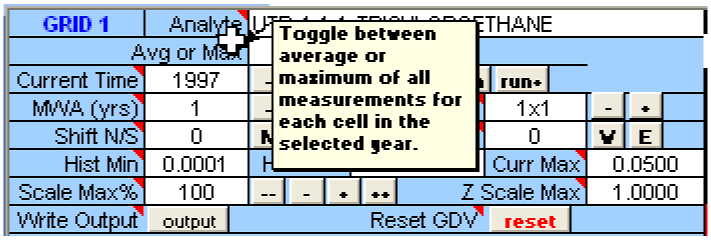
Macros may contain viruses. It is always safe to disable macros, but if the macros are legitimate, you might lose some functionality.

Figure A1. Pop-up window asking the user whether to enable macros.

The GDV can be exited at any time using Excel File>Exit menus. The user will be asked to save the file. Any control settings changes that the user wishes to keep for the next time GDV is launched can be retained using File>Save at any time. The GDV may be removed from your computer by simply deleting the GDV-yyyymmdd.xls file.

2. OPERATION

The GDV and its graphical user interface (GUI) are composed of a number of worksheets that are detailed below. The GDV is operated through a number of buttons and text and numerical fields. As shown in figure A2, text fields label buttons and other fields indicate current settings. Moving the mouse over a label marked with a red caret will provide a description of the header variable.


GRID 1

Analyte UTR 1,1,1-TRICHLOROETHANE

Avg or Max

Toggle between average or maximum of all measurements for each cell in the selected year.

Current Time 1997

MWA (yrs) 1

Shift N/S 0

Hist Min 0.0001

Curr Max 0.0500

Scale Max% 100

Z Scale Max 1.0000

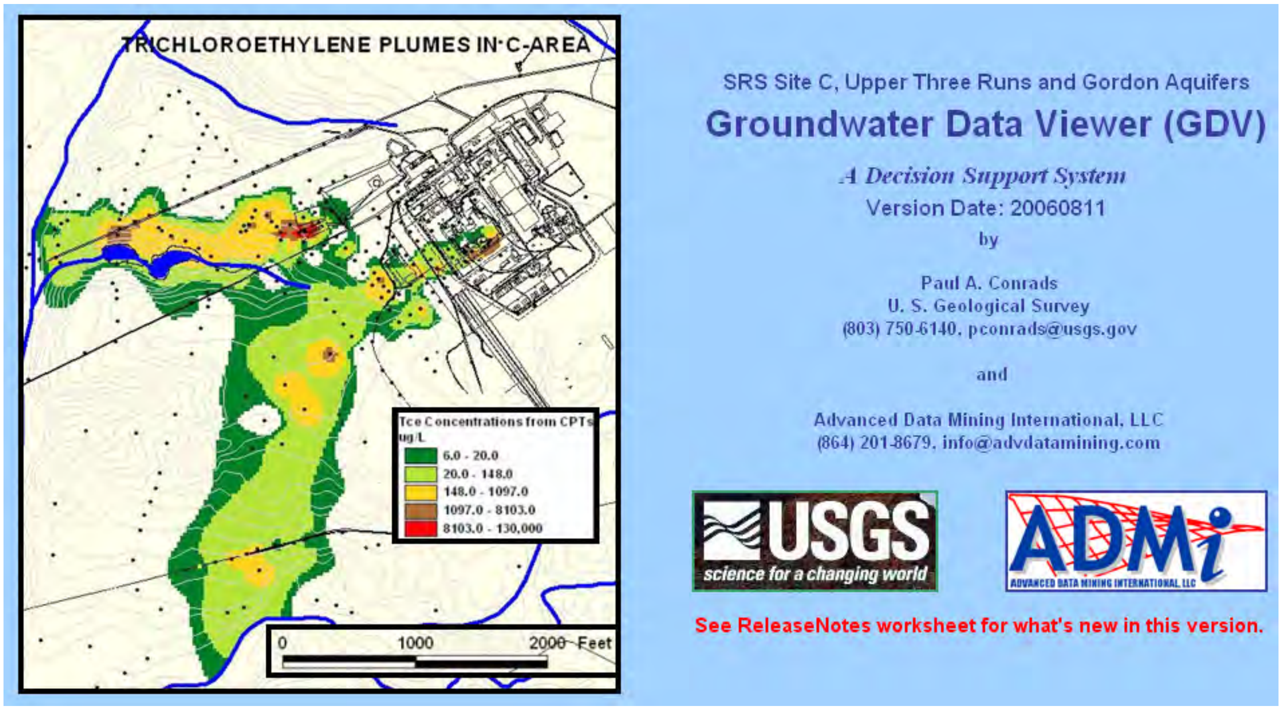
Write Output

Reset GDV

Figure A2. On-line description of “Avg” or “Max” button on the 3DVis worksheet.

2.1 Info Worksheet

The Info worksheet is displayed automatically when GDV is first loaded (fig. A3). The Info worksheet contains the program’s version date and the contact information of the developers. The C-Area TCE plume shown in figure A3 is included at the left for convenient reference while using GDV.



SRS Site C, Upper Three Runs and Gordon Aquifers

Groundwater Data Viewer (GDV)

A Decision Support System

Version Date: 20060811

by

Paul A. Conrads

U. S. Geological Survey

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and

Advanced Data Mining International, LLC

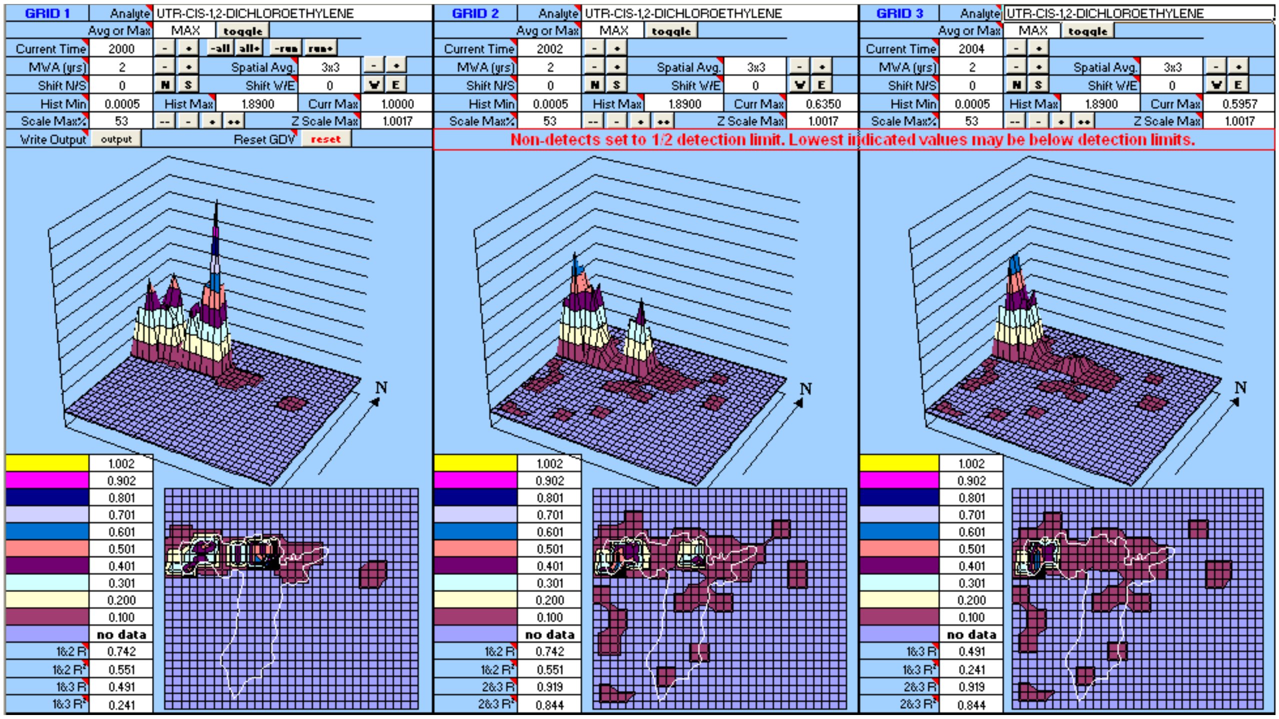
(864) 201-8679, info@advdatamining.com

See ReleaseNotes worksheet for what's new in this version.

Figure A3. “Info” worksheet.

2.2 3DVis Worksheet

The 3DVis (three-dimensional visualization) worksheet is the GUI component that enables the user to visualize and analyze analyte time-series data. As shown in figure A4, data are plotted in three-dimensional and plan views, with the horizontal plane corresponding to the grids shown in figures 6 and 7 of the report. The location and extent of the TCE plume shown in figure A4 are depicted in the plan views by a white outline. The vertical coordinate corresponds to a concentration or other value of an analyte selected by the user. The GDV provides three panels (referred to as Grid 1, Grid 2, and Grid 3) for side-by-side visualization and several features for manipulating the time series in the GDV database. Note that “non-detects” were set to one-half the detection limit in the time series, so the actual lowest measured values are possibly censored by the detection limits.



GRID 1
Analyte: UTR-CIS-1,2-DICHLOROETHYLENE
Avg or Max: MAX
Current Time: 2000
MWA (yrs): 2
Spatial Avg.: 3x3
Shift N/S: 0
Shift W/E: 0
Hist Min: 0.0005
Hist Max: 1.8900
Curr Max: 1.0000
Scale Max%: 53
Z Scale Max: 1.0017
Write Output
Reset GDV
1&2 R: 0.742
1&2 R²: 0.551
1&3 R: 0.491
1&3 R²: 0.241

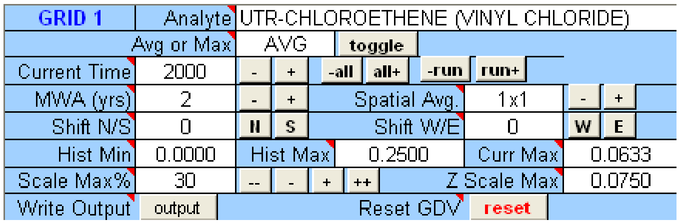
GRID 2
Analyte: UTR-CIS-1,2-DICHLOROETHYLENE
Avg or Max: MAX
Current Time: 2002
MWA (yrs): 2
Spatial Avg.: 3x3
Shift N/S: 0
Shift W/E: 0
Hist Min: 0.0005
Hist Max: 1.8900
Curr Max: 0.6350
Scale Max%: 53
Z Scale Max: 1.0017
1&2 R: 0.742
1&2 R²: 0.551
2&3 R: 0.919
2&3 R²: 0.844

GRID 3
Analyte: UTR-CIS-1,2-DICHLOROETHYLENE
Avg or Max: MAX
Current Time: 2004
MWA (yrs): 2
Spatial Avg.: 3x3
Shift N/S: 0
Shift W/E: 0
Hist Min: 0.0005
Hist Max: 1.8900
Curr Max: 0.5957
Scale Max%: 53
Z Scale Max: 1.0017
1&3 R: 0.491
1&3 R²: 0.241
2&3 R: 0.919
2&3 R²: 0.844

Non-detects set to 1/2 detection limit. Lowest indicated values may be below detection limits.

Figure A4. Screenshot from the Ground-Water Data Viewer (GDV). Shown from left to right are spatial and temporal averages of 3 x 3 cells and 2 years of maximum (MAX) Upper Three Runs aquifer *cis*-1,2-dichloroethylene concentrations for 2000, 2002, and 2004. Note the white trace outline of the TCE plume in the plan views at the bottom.

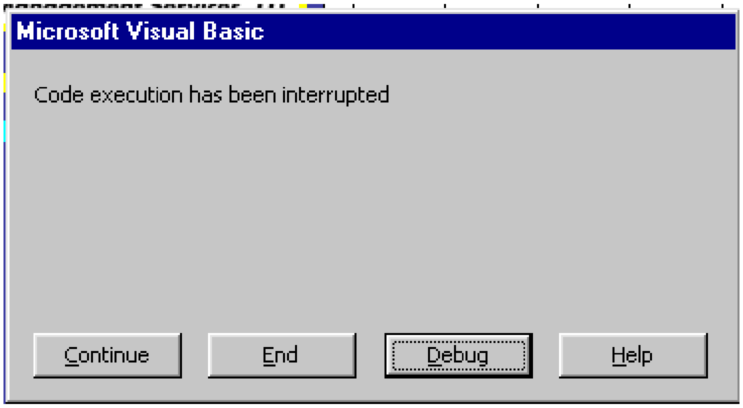
The controls of Grid 1, which are the same as those of Grids 2 and 3 except that Grid 1 has a few extra controls for time stepping all three grids together, writing output, and resetting GDV if the user interrupts a simulation, are shown in figure A5. The 3DVis controls are detailed below.



GRID 1
Analyte: UTR-CHLOROETHENE (VINYL CHLORIDE)
Avg or Max: AVG
Current Time: 2000
MWA (yrs): 2
Spatial Avg.: 1x1
Shift N/S: 0
Shift W/E: 0
Hist Min: 0.0000
Hist Max: 0.2500
Curr Max: 0.0633
Scale Max%: 30
Z Scale Max: 0.0750
Write Output
Reset GDV

Figure A5. 3DVis worksheet controls.

- **Analyte** – Select analytes in the “drop-down menu” to be displayed. Analytes are listed in order of their codes. Upper Three Runs aquifer (UTR) or Gordon aquifer (GOR) prefixes indicate from which aquifer the measurements are displayed. A complete list of analytes and codes is shown on the AnalyteInfo worksheet.
- **Avg or Max** – The “toggle” button allows the user to select the average or maximum of all measurements in each cell for the selected analyte and the selected Current Time.
- **Current Time** – The year to be displayed. The time step is 1 year, from 1984 to 2004. The “-” and “+” buttons decrease/increase time step by 1 year. The “-all” and “all+” buttons decrease/increase time stamps of Grids 1, 2, and 3 by 1 year. The “-run” and “run+” buttons automatically time step all Grids to run a simulation forward to 2004 or backward to 1984, respectively. A simulation may be stopped by holding down the “Esc” key, after which a pop-up window will appear like that shown in figure A6. Click on the “End” button to stop the simulation, then click the “reset” button shown at the lower right in figures A2 and A5. The “reset” button activates Excel’s automatic calculation feature (autocalc). Because the GDV programmatically manipulates autocalc for performance reasons, aborting a simulation can sometimes leave the model in a state where autocalc is not activated, which is remedied by clicking the “reset” button.



Code execution has been interrupted

Figure A6. Pop-up window that appears when a simulation is interrupted using the "Esc" key.

Other features on the 3DVis worksheet include

- **MWA (yrs)** – "Moving window average" size in years. The "-" and "+" buttons decrease/increase MWA by 1 year and will automatically increase the current time as needed. The maximum MWA allowed is 6 years. MWAs provide a means for temporally smoothing data to diminish the effects of measurement errors and temporal measurement gaps.
- **Spatial Avg.** – Spatially averages cell values. 1x1 is no averaging. 3x3 is three cells square. 5x5 and above are approximately radial. The maximum average allowed is 11x11 cells. Spatial averaging spatially smoothes data to diminish the effects of measurement errors and spatial gaps.
- **Shift N/S** – "N" and "S" buttons spatially shift a grid north or south by 1 cell per click, with a range of +/- 3 cells either direction.
- **Shift W/E** – "W" and "E" buttons spatially shift a grid west or east by 1 cell per click, with a range of +/- 3 cells in either direction.
- **Hist Min** – Shows the historical minimum value of the selected analyte's time series.
- **Hist Max** – Shows the historical maximum value of the selected analyte's time series.
- **Curr Max** – Shows the current maximum value being displayed for the selected analyte.
- **Scale Max%** – Buttons allow vertical scale to be set to a percent of the historical maximum. "-" and "+" decrease or increase scale by 1 percent per click. The "--" and "++" decrease or increase scale by 10 percent per click.
- **Z Scale Max** – Shows the current maximum value of the vertical scale.
- **Write Output** – Writes current values of all three grids to the Output worksheet. The contents of the Output worksheet can then be copied into another Excel workbook for further study. The contents of the Output worksheet are overwritten each time the button is clicked.
- **Reset GDV** – Turns Excel's autocalculation on in case calculations are interrupted and GDV stops working. See "Current Time" above for more information.

The color key at the lower left in each grid panel automatically changes with analyte selections and vertical scale settings. Below the keys are bivariate Pearson coefficients (R) and determination coefficients (R^2) calculated for grid pairings 1 & 2, 1 & 3, and 2 & 3. Depending on the data quality, using two or more grids at a time allows the following analyses to be performed. Results may be enhanced using spatial and temporal smoothing.

- Analyte degradation – The same analyte in multiple grids will show concentration changes over time.
- Degradation from parent into daughter analytes.
- Correlations – Shows correlations between candidate predictor variables and contaminants, for example, carbon dioxide and chloroethylene.

2.3 DegradationMap Worksheet

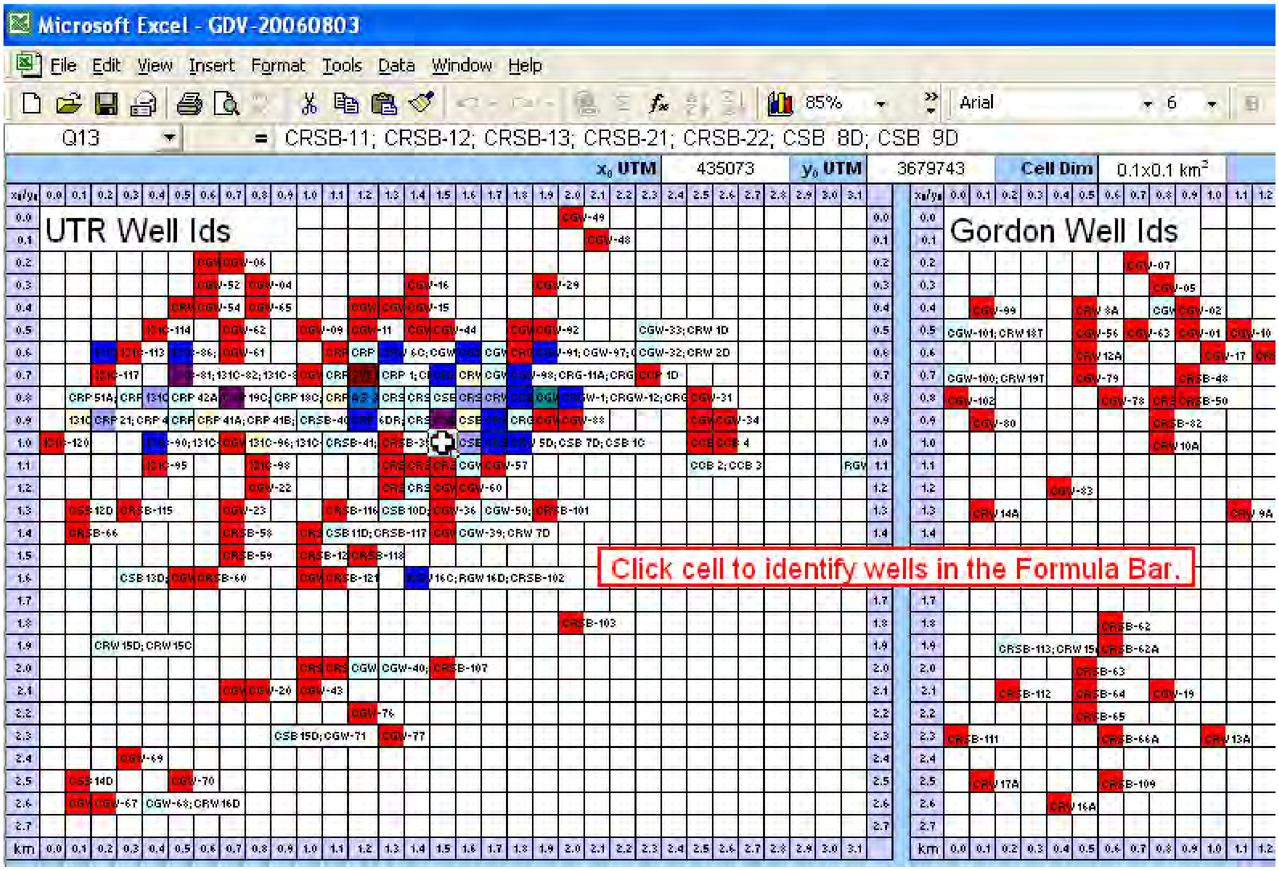
The DegradationMap worksheet provides convenient referencing of the degradation map (fig. 9 of the report) developed for this project by the U.S. Geological Survey.

2.4 AnalyteInfo Worksheet

The AnalyteInfo worksheet provides a handy reference of the list of analytes for which there were entries among the historical records supplied to this project (table 1 of the report). None of the analytes had actual measurements. The list indicates which analytes are included in GDV's database and also gives the SRS (Savannah River Site) code for each analyte.

2.5 WellInfo Worksheet

The WellInfo worksheet shows information about the Upper Three Runs aquifer and Gordon aquifer grids. It includes the number of wells per cell shown in figures 6 and 7 of the report and the well names associated with each cell (fig. A7).



Q13 = CRSB-11; CRSB-12; CRSB-13; CRSB-21; CRSB-22; CSB 8D; CSB 9D

x_0 UTM 435073 y_0 UTM 3679743 Cell Dim 0.1x0.1 km^2

UTR Well Ids

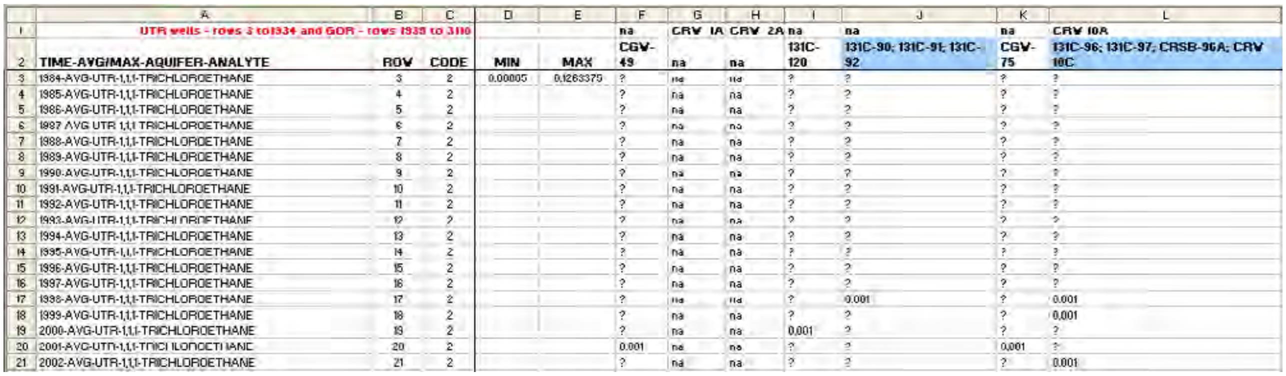
Gordon Well Ids

Click cell to identify wells in the Formula Bar.

Figure A7. Screenshot of grid showing the names of the wells associated with each cell in the study area. Clicking the mouse in each cell will list the associated wells in Excel's formula bar (red oval).

2.6 Database Worksheet

The Database worksheet contains all of the time series derived from the raw records of historical data supplied for this project (fig. A8). Columns F and greater represent the Upper Three Runs and Gordon aquifers' cells that contain wells. A listing of wells associated with each cell is given in rows 3 to 1934 for the Upper Three Runs aquifer and in rows 1935 to 3110 for the Gordon aquifer. As indicated by the first column header, TIME-AVG/MAX-AQUIFER-ANALYTE, each row corresponds to a vector of maximum or average values for an analyte, aquifer, and year. The ROW, CODE, MIN, and MAX columns contain data used to look up and scale data for display in the 3DVis worksheet. Missing values are indicated by "?". Cells marked "na" indicate that the column's associated cell had no well for the aquifer indicated in the TIME-AVG/MAX-AQUIFER-ANALYTE column.

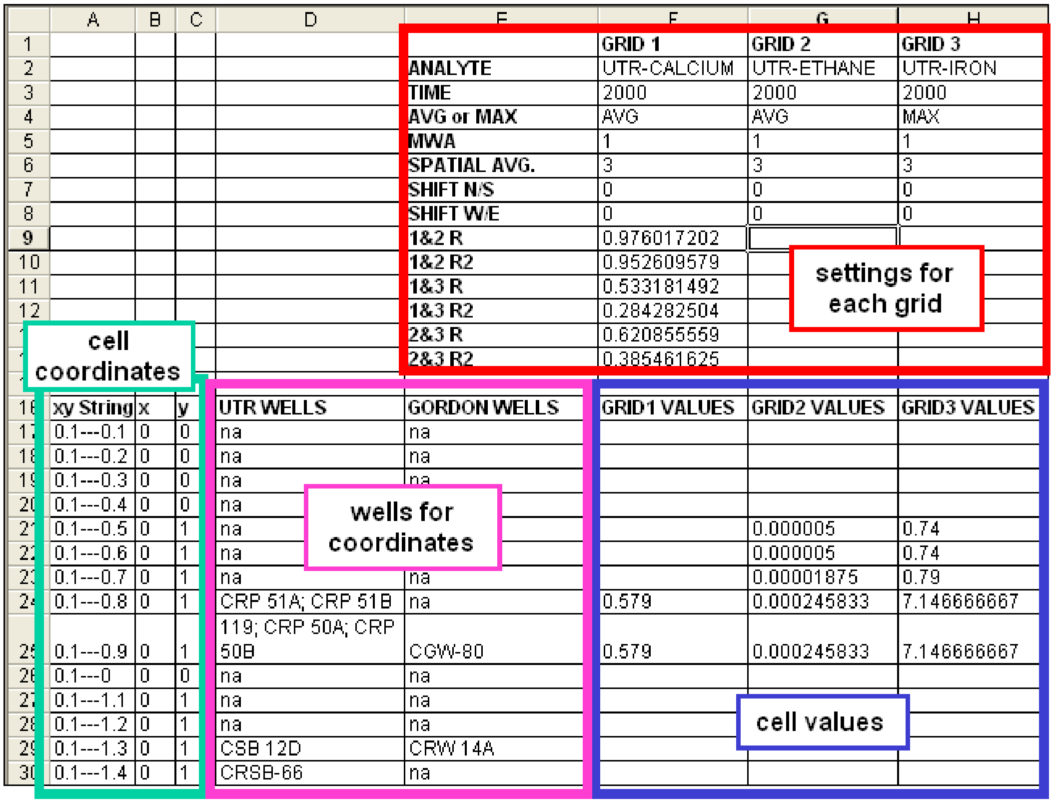


	A	B	C	D	E	F	G	H	I	J	K	L
1	UTR wells - rows 3 to1934 and GOR - rows 1935 to 3110					na	CRW 1A	CRW 2A	na	na	na	CRW 10A
2	TIME-AVG/MAX-AQUIFER-ANALYTE	ROW	CODE	MIN	MAX	CGW-49	na	na	131C-120	131C-90; 131C-91; 131C-92	CGW-75	131C-96; 131C-97; CRSB-96A; CRW 10C
3	1984-AVG-UTR-1,1,1-TRICHLOROETHANE	3	2	0.00005	0.1263375	?	na	na	?	?	?	?
4	1985-AVG-UTR-1,1,1-TRICHLOROETHANE	4	2			?	na	na	?	?	?	?
5	1986-AVG-UTR-1,1,1-TRICHLOROETHANE	5	2			?	na	na	?	?	?	?
6	1987 AVG UTR 1,1,1 TRICHLOROETHANE	6	2			?	na	na	?	?	?	?
7	1988-AVG-UTR-1,1,1-TRICHLOROETHANE	7	2			?	na	na	?	?	?	?
8	1989-AVG-UTR-1,1,1-TRICHLOROETHANE	8	2			?	na	na	?	?	?	?
9	1990-AVG-UTR-1,1,1-TRICHLOROETHANE	9	2			?	na	na	?	?	?	?
10	1991-AVG-UTR-1,1,1-TRICHLOROETHANE	10	2			?	na	na	?	?	?	?
11	1992-AVG-UTR-1,1,1-TRICHLOROETHANE	11	2			?	na	na	?	?	?	?
12	1993-AVG-UTR-1,1,1-TRICHLOROETHANE	12	2			?	na	na	?	?	?	?
13	1994-AVG-UTR-1,1,1-TRICHLOROETHANE	13	2			?	na	na	?	?	?	?
14	1995-AVG-UTR-1,1,1-TRICHLOROETHANE	14	2			?	na	na	?	?	?	?
15	1996-AVG-UTR-1,1,1-TRICHLOROETHANE	15	2			?	na	na	?	?	?	?
16	1997-AVG-UTR-1,1,1-TRICHLOROETHANE	16	2			?	na	na	?	?	?	?
17	1998-AVG-UTR-1,1,1-TRICHLOROETHANE	17	2			?	na	na	?	0.001	?	0.001
18	1999-AVG-UTR-1,1,1-TRICHLOROETHANE	18	2			?	na	na	?	?	?	0.001
19	2000-AVG-UTR-1,1,1-TRICHLOROETHANE	19	2			?	na	na	0.001	?	?	?
20	2001-AVG-UTR-1,1,1-TRICHLOROETHANE	20	2			0.001	na	na	?	?	0.001	?
21	2002-AVG-UTR-1,1,1-TRICHLOROETHANE	21	2			?	na	na	?	?	?	0.001

Figure A8. Screenshot of portion of the Database worksheet.

2.7 Output Worksheet

The Output worksheet contains data representing the three grids displayed on the 3DVis worksheet. Data are written to the Output worksheet when the Write Output button on the 3DVis worksheet is clicked. The contents of the Output worksheet can then be copied and pasted into another Excel workbook for further study. The contents of the Output worksheet are overwritten each time the Write Output button is clicked. As shown in figure A9, the settings of the three grids on the 3DVis worksheet are recorded at the upper right, with cell coordinates, associated well names, and grid values listed below.



A	B	C	D	E	F	G	H
					GRID 1	**GRID 2**	**GRID 3**
				ANALYTE	UTR-CALCIUM	UTR-ETHANE	UTR-IRON
				TIME	2000	2000	2000
				AVG or MAX	AVG	AVG	MAX
				MWA	1	1	1
				SPATIAL AVG.	3	3	3
				SHIFT N/S	0	0	0
				SHIFT W/E	0	0	0
				1&2 R	0.976017202		
				1&2 R2	0.952609579		
				1&3 R	0.533181492		
				1&3 R2	0.284282504		
				2&3 R	0.620855559		
				2&3 R2	0.385461625		
xy String	**x**	**y**	**UTR WELLS**	**GORDON WELLS**	**GRID1 VALUES**	**GRID2 VALUES**	**GRID3 VALUES**
0.1---0.1	0	0	na	na			
0.1---0.2	0	0	na	na			
0.1---0.3	0	0	na	na			
0.1---0.4	0	0	na				
0.1---0.5	0	1	na			0.000005	0.74
0.1---0.6	0	1	na			0.000005	0.74
0.1---0.7	0	1	na	na		0.00001875	0.79
0.1---0.8	0	1	CRP 51A; CRP 51B	na	0.579	0.000245833	7.146666667
0.1---0.9	0	1	119; CRP 50A; CRP 50B	CGW-80	0.579	0.000245833	7.146666667
0.1---0	0	0	na	na			
0.1---1.1	0	1	na	na			
0.1---1.2	0	1	na	na			
0.1---1.3	0	1	CSB 12D	CRW 14A			
0.1---1.4	0	1	CRSB-66	na			

Figure A.9. Screenshot of portion of the Output worksheet.

2.8 ReleaseNotes Worksheet

The ReleaseNotes worksheet provides information about updates and changes to GDV.

3. TECHNICAL ASSISTANCE

Please contact Paul Conrads of the U.S. Geological Survey in Columbia, SC, at (803) 750-6140, pconrads@usgs.gov, if you have problems with GDV.

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