GEOGRAPHIC INFORMATION SYSTEMS (GIS) MAPPING OF GROUNDWATER CONTAMINATION AT THE SAVANNAH RIVER SITE (SRS)

by

SILAS EUGENE MATHES

(Under the direction of Todd Rasmussen)

ABSTRACT

This thesis presents methodologies for mapping groundwater contamination at the Savannah River Site using a Geographic Information System and measurements of groundwater chemistry. The Savannah River Site (SRS) is a US Department of Energy facility located in South Carolina where special nuclear materials for national defense have been manufactured since the 1950s. Groundwater at SRS is contaminated in several locations as a result. We established appropriate extents, GIS coverages, and scales for displaying groundwater contamination concentrations of trichloroethylene and tritium at SRS. We also developed and tested a novel methodology for interpolating zones of potential contamination for tritium and tetrachloroethylene through the identification of aquifer water quality signatures. To identify signatures, we used principal components analysis and cluster analysis techniques to group geochemical and contaminant concentrations measured at monitoring wells. Maps of contamination potentials for 1993-1995 geochemical data compared favorably to contaminant concentrations measured at wells during 1999.

INDEX WORDS: Geographic Information Systems, GIS, Savannah River Site, SRS, Atlantic Coastal Plain, Groundwater, Monitoring wells, Hydrochemical facies, Geochemistry, Factor analysis, Principal components analysis, Cluster analysis, Tritium, Tetrachloroethylene, Trichloroethylene, Aquifer, Aquifer water quality signature

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I thank John Reed and Jim Bollinger of the Savannah River Site for providing me with well monitoring data and advice on this project.

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PREFACE

Chapter Four and Appendix I of this document were originally part of a report submitted to the Westinghouse Savannah River Company (WSRC) in August 2001 as part of a groundwater contamination mapping project at the Savannah River Site. Some sections refer to a support CD containing GIS coverages, printable maps in PDF format, and ArcView scripts. This CD can be obtained by contacting the authors.

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CHAPTER 1

INTRODUCTION

1.1 Background

The Savannah River Site (SRS) is a U.S. Department of Energy facility located near Aiken, South Carolina, on the Georgia-South Carolina border. Groundwater is contaminated at multiple locations on the site due to the release of industrial and radioactive contaminants as by-products of nuclear weapons materials production from the 1950s until the 1990s. Groundwater in the surrounding region is the major source of water for human consumption (Arnett et al., 1995).

Understanding the location of contaminated groundwater at SRS is imperative to maintaining both public safety and mitigating risk perception. To this end, investigators at SRS have drilled thousands of monitoring wells and maintain a quarterly sampling program for the detection of contaminants (Arnett et al., 1995). Despite extensive data collection efforts, monitoring data has been difficult to process for integration into historical or current maps of the contamination.

Further, the underlying aquifer systems of the Southeastern Coastal Plain are complex; numerical groundwater flow modeling efforts traditionally used at SRS have been limited to relatively small portions of the site where detailed hydrostratigraphic characterizations are available. This project introduces an alternative to numerical simulation modeling of groundwater flow patterns that relies instead on a statistical analysis of groundwater quality data to infer zones of potential contamination.

1.2 Objectives

The goal of this study is to establish a methodology for generating maps of groundwater contamination with field water quality data at the Savannah River Site. The study employs a

Geographic Information System (GIS) and methods of multivariate statistics to analyze data collected as part of the SRS well monitoring program. Maps of aquifer water quality provide insight into both the extent and history of groundwater contamination problems at SRS. In addition, these maps may help to answer the question of future contamination — In what direction is contamination moving, and will this movement pose a threat to public or environmental health?

The four main objectives of this study are to:

- Explore appropriate methods for representing the aerial extent of contamination at SRS.
- Use statistical tools including principal components analysis and factor analysis to group monitoring wells by water quality signature.
- Correlate aquifer water quality signatures with tetrachlroethylene and tritium concentrations to indicate areas of potential contamination.
- Use interpolation and other GIS tools to generate maps that depict areas of potential contamination.

1.3 Approach

This project introduces 1) methods for geographic representation of single well contaminant concentration results using a GIS and 2) statistical procedures for grouping wells and interpolating contamination based on the concept of aquifer water quality signatures. The primary assumption is that groundwater dissolves minerals and organic materials as it passes through geologic media, developing a unique signature based on geochemical concentrations. This aquifer water quality signature of groundwater extracted from a well can be identified through statistical analysis of groundwater chemical concentrations and field parameters. The signature can be compared with those from other wells and can be used to identify areas where groundwater and thus contamination may move. Using principal components analysis (PCA) as a data reduction technique, we identify these signatures based on the historical results from ground water monitoring at SRS.

Our approach has key advantages. First, the methods described in this thesis rely on data that has already been collected; no additional parameters need to be measured to gain insight into historical and present groundwater conditions at SRS. Second, this project utilizes field data, avoiding the uncertainty involved with contaminant transport modeling in the complex southeastern coastal plain environment. Third, the procedures outlined in this project are implemented with the widely available ArcView 3.2 Geographic Information Systems software program and any statistical package capable of principal components and factor analyses. This approach to mapping groundwater contamination potential produces results quickly and inexpensively relative to current techniques, which require hydrogeologists to map contamination by hand after performing detailed hydrostratigraphic characterizations.

The resulting contaminant maps can be used by SRS researchers to roughly identify the most important candidate areas for future monitoring and environmental remediation. Finally, state and federal regulators as well as the public can utilize the maps for a rapid estimation of public risks from groundwater contamination at SRS.

CHAPTER 2

SETTING

2.1 Savannah River Site Location and History

The Savannah River Site is a 790 km^2 area operated by the US Department of Energy and the Westinghouse Savannah River Company. During the Cold War era the primary purpose of SRS was the manufacture of nuclear materials including tritium and plutonium for the nation's defense. SRS is located on the Atlantic Coastal Plain province, in southwestern South Carolina on the Georgia-South Carolina border (Figure 2.1). Major nearby cities include Aiken, South Carolina, and Augusta, Georgia.

Manufacturing, waste disposal, and reactor facilities are located at several different areas scattered across SRS (Figure 2.2). Facilities cover only a small proportion of the entire area of SRS. The majority of the site is rural, forested by pine plantations in uplands and extensive bottom-land hardwood wetlands along streams and the Savannah River. The site also contains several small elliptically shaped depressional wetlands known as Carolina bays; these features are unique to the Southeastern Coastal Plain. The site is relatively flat with elevations ranging from approximately 20 to 100 meters above mean sea level. Streams, including Upper Three Runs Creek, Four Mile Creek, Pen Branch, Steel Creek, and Lower Three Runs Creek drain to the southwest and empty into the Savannah River (Figure 2.2). Two large impoundments, L-Lake and PAR Pond, were built to supply cooling water to reactors and are located in the southern and eastern portions of the site, respectively.

Construction of reactors and manufacturing facilities at SRS began in 1951 and within two years, SRS was producing weapons-grade nuclear materials (Arnett et al., 1995). Production wastes included a variety of radionuclides, such as tritiated water, as well as more common industrial organic by-products such as trichloroethylene and tetrachloroethylene(Arnett et al., 1995). For almost 40 years, many of these wastes were disposed of in unlined seepage basins or buried in open pits; occasional accidental releases to the soil also occurred (Bollinger, 1999; Miller, 2000; WSRC, 2002). As a result, groundwater contamination is now a problem at several areas on the site and is one of the major environmental concerns at SRS (Bollinger, 1999; Miller, 2000; Jorque et al., 1997; Harris et al., 1997). With the end of the Cold War and the rise of public and government environmental awareness, the current focus of activities at SRS has shifted from weapons materials production to tritium recycling, waste storage, and environmental remediation (Arnett et al., 1995).

As part of environmental remediation efforts, recent groundwater modeling studies and monitoring wells on site have indicated that most contamination is vertically located in surficial aquifers, and has not reached the deeper aquifers that supply nearby residents with drinking water (Delaimi, 1996; Harris et al., 1997; Miller et al., 2000). These studies also indicate that the contamination has not yet moved horizontally into offsite groundwater. However, the same research has not ruled out the eventual migration of groundwater pollutants offsite and the resulting potential threat to public safety (Delaimi, 1996; Rine, et al., 1998; Arnett et al., 1995). Researchers at SRS acknowledge that groundwater contamination from the site poses a risk to the public (Arnett, et al., 1995; USDOE, 2000). The probability of contaminant exposure to residents living near the site through groundwater pathways is thought to be very low, although quantifying this risk has been difficult due to local complexities in hydrogeology (Arnett et al., 1995; Miller et al., 2000, Hamilton, et al., 1994).

Our research is focused on groundwater under two areas of the site, the Administrative and Manufacturing Area (A/M Area) and the General Separations Area (GSA) (Figure 2.2). We study three representative contaminants in these areas: tetrachloroethylene and trichloroethylene, both primarily found at the A/M area, and tritium found in groundwater beneath the GSA. Historically, most radioactive and industrial wastes were generated and stored in these two areas; the highest concentrations of contaminants anywhere at SRS are present in underlying groundwater.

The A/M area houses offices for site administration, research laboratories, and metallurgical facilities that produced fuel rods and other reactor components. The area is located in the northwest corner of the Savannah River Site (Figure 2.2). Volatile organic compounds (VOCs) commonly used as cleaning solvents for metals fabrication are found in groundwater beneath the A/M Area (Bollinger, 1999; SRS WSRC, 2002). Two VOCs found at particularly high concentrations are tetrachloroethylene and trichloroethylene, cleaning solvents used in nuclear fuel manufacturing and metals machining processes (Arnett et al., 1995; Bollinger, 1999; WSRC, 2002). Both solvents, as well as other volatile organic compounds and heavy metals were disposed in shallow, unlined seepage basins from 1952 until the mid 1980s. The M-Area Settling Basin in particular received large volumes of these wastes in liquid form. The basin periodically overflowed into a wetland area surrounding the Lost Lake Carolina Bay. The highest levels of solvent contamination at SRS have been recovered from wells located in the water table aquifer beneath this portion of the A/M Area (Arnett et al., 1995; WSRC, 2002). Trichloroethylene and tetrachloroethylene are thus focus contaminants in this study, and serve as indicators of the industrial groundwater pollution present at SRS.

The General Separations Area (GSA), located in the central portion of SRS, is comprised of waste disposal sites including high level radioactive waste tank farms and mixed waste burial grounds, and facilities for the separation of specific radionuclides from targets produced at the reactor areas. Groundwater beneath the GSA is contaminated with a wide variety of chemicals and radionuclides, most notably tritium. For 40 years, tritium-contaminated wastewater was released into several seepage basins at the GSA where it eventually migrated into the uppermost aquifers underlying the GSA (Arnett, et al., 1995). As with TCE in the A/M area, tritium in liquid form was also accidentally spilled at several locations in the GSA, contributing to groundwater contamination. Tritium is the other contaminant of focus in this study, serving as an indicator of radionuclide groundwater contamination at SRS.

2.2 Contaminant Behavior

When spilled or released via seepage basins, the large variety of contaminants generated at SRS move through unsaturated soils at different rates, depending on their propensity for chemical adsorption, or retardation (Fetter, 1994). As contaminants reach the water table, or saturated zone, they dissolve into, float on top of, or sink through the groundwater. This behavior creates complex contaminant plumes that develop according to groundwater movement and the chemical and physical behavior of each contaminant in geologic media and water.

The physical and chemical processes of advection, dispersion, diffusion and retardation all influence the movement contaminant solutes in the vadose and saturated zones (Fetter, 1994). While these processes control where contaminants move, they also help to attenuate high concentrations through dilution. Advection occurs when contaminant solutes move at the same rate as the groundwater flow. Dilution of contamination due to dispersion occurs because fluid flows through geologic media at different rates on the pore level: contaminated fluid flows faster through large pores than small ones; faster through the center of pores than at the edges; and faster when it encounters low tortuosity (Fetter, 1994). Diffusion acts upon contaminant solutes causing them to move from areas of high concentration to low concentration. Finally, retardation can slow the movement of contaminants due to chemical adsorption between solutes and porous media. These processes are dependent upon many variables including contaminant chemical properties, aquifer geochemical makeup, hydraulic conductivity, pore size and sorting, and the degree of aquifer heterogeneity and anisotropy.

Trichloroethylene (TCE) and tetrachloroethylene (PCE) are mobile volatile organic compounds capable of contaminating large volumes of groundwater from only a relatively small source mass (Kehew, 2001; Fetter, 1994). As halogenated hydrocarbons TCE and PCE are dense non-aqueous phase liquids (DNAPLs) with water solubility factors equal to 1100 mg/L and 200 mg/L, respectively (Kehew, 2001). As they migrate through soils in the vadose zone, TCE and PCE partition into the air in soil pores and fractures because of their high volatilities (Fetter, 1994). At high concentrations, DNAPLs that reach the water table may sink through the groundwater because their molecules are denser than water. The specific gravity for TCE is equal to 1.46, and 1.62 for PCE at 25 degrees Celsius (Kehew, 2001). At low dissolved phase concentrations, TCE and PCE move with the groundwater. Thus, DNAPLs like TCE and PCE are mobilized by not only groundwater flow but also by gravitational forces. These contaminants may migrate downward even against upward pressure gradients created by an underlying confined aquifer. DNAPLs may move through or along aquitard confining layers and contaminate deeper aquifers. It is important to note that PCE and TCE concentrations measured in groundwater represent only dissolved phase concentrations. Locating non-dissolved masses of DNAPL requires an analysis of dissolved concentrations, contaminant history, and groundwater flow patterns.

DNAPLs are naturally attenuated through advection, dispersion, and retardation. Several air stripping and pump-and-treat facilities remove TCE, PCE, and other volatile organic compounds from groundwater at SRS (WSRC, 2002).

In humans, TCE and PCE exposure through drinking water pathways increases cancer risk and can cause liver problems (USEPA, 1999). The maximum allowable contaminant level (MCL) in drinking water for both contaminants is currently set by the U.S. Environmental Protection Agency (USEPA) at 0.005 mg/L, or 5 μg/L (USEPA, 2002).

The other contaminant of focus in this study, tritium, is an isotope of hydrogen that, when exposed to water, forms tritium oxide, or tritiated water. Tritiated water cannot be separated from groundwater, except as concentrations diminish through natural radioactive decay processes. Thus, tritium plumes mimic groundwater flow pathways. Tritium has a relatively short half-life in comparison to plutonium or uranium; it loses half of its radioactive energy every 12.43 years. As a result, the threat posed by a tritium plume to drinking water supplies diminishes over time (Keyhew, 2001). Currently there exist no methods for removing tritium from groundwater; tritium remediation at SRS relies on careful monitoring and natural attenuation (USDOE, 2000).

As tritium decays, it emits radiation in the form of beta particles. Because dead skin cells and barriers as thin as paper block the energy of beta particles, the main pathway for tritium doses to humans is internally when inhaled as a gas or ingested as a liquid. At very high levels, tritium's radioactive energy can disrupt cellular activity and cause mutations. Research on human exposure to lower levels of tritium such as those found in SRS groundwater is limited, but exposure to tritium through drinking water is assumed to increase the risk of cancer. USEPA (2002) has set the MCL for tritium in groundwater at 20,000 pCi/L (picoCuries per Liter).

Understanding the transport of dissolved groundwater contaminants like tritium and tetrachloroethylene is in part a matter of following groundwater flow rates and patterns (Fetter, 1994). Because groundwater flow cannot be directly observed, it must modeled mathematically from aquifer hydraulic properties. Accurate estimations of these properties require aquifer pump tests and a thorough understanding of subsurface hydrostratigraphy. In relatively simple hydrogeologic environments subsurface characterization is straightforward and uncertainty in aquifer flow models can be minimized (Miller et al., 2000; Keyhew, 2001). If hydrostratigraphy is homogenous and accurately predicted, even the more complex groundwater behavior of non-aqueous phase DNAPLs can be simulated (Kehew, 2001). Unfortunately, the complex layering of aquifers and confining units present at SRS hampers the accurate calculation of aquifer hydraulic properties, adding a high degree of uncertainty to groundwater flow and contaminant transport models (Reed, pers. comm., 2000; Harris et al., 1997; Miller et al., 2000; Kehew et al., 2001).

2.3 Hydrogeology

The complexity of SRS hydrogeology is due to its location on the Upper Atlantic Coastal Plain. The region dips southeastward toward the Atlantic Ocean which is about 160 km away;

both groundwater and surface water flow in this general direction. Sediments of this region formed as the result of complex depositional environments and lie atop a basement layer of crystalline Piedmont bedrock (Miller et al., 2000; Aadland et al., 1995). Upper Atlantic Coastal Plain sediments consist of unconsolidated sandy and clayey hydrostratigraphic layers that dip seaward from the northwest to the southeast. Layers with high sand content form water bearing aquifers. Clay sediments act as confining layers for the sandy aquifers. Regional groundwater recharge is generated by the infiltration of rainfall at the Fall Line where the crystalline rocks of the Piedmont province meet outcropping coastal plain sediments. Aquifers discharge regionally into the Savannah River and where they outcrop offshore in the Atlantic Ocean. Local recharge of deeper aquifers occurs at an extensive wetland system located northwest of the Savannah River Site and local discharge occurs where rivers, streams, and wetlands incise these aquifers. Recent measurements of water tables levels suggest that recharge to the shallow aquifers occurs only after very large rain events; seasonal patterns in recharge have not been observed.

The sediments at SRS form a complex, stacked lithology of unconsolidated sands, clayey sands, sandy clays, and calcareous muds deposited by periodic oceanic transmigration and by river and stream channel migration (Aadland, et al., 1995) (Figure 2.4). The sandy sediment layers are highly porous and thus hold large quantities of water. These sandy aquifers are interbedded with low permeability clay and marl layers that act as aquitards, or confining units. Understanding how and when contaminated groundwater moves is hampered because hydrostratigraphic layers change abruptly (Miller et al., 2000). Confining layers frequently disappear and aquifers grade into one another. One significant break in the confining layers occurs at the Pen Branch Fault Line which offsets all aquifers. Here and at other discontinuities where upper and lower aquifers join, contaminated water can potentially mix with clean water. Adding to the complexity are ancient buried stream channels that conduct flow along preferential pathways. These features formed when the ocean receded and river systems cut and meandered through remaining marine sediments, depositing their own alluvial materials (Aadland et al., 1995; Rasmussen, pers. comm., 2000). Groundwater from the surface aquifers, not lost to deeper formations, ultimately drains into present day streams and the Savannah River (Arnett et al., 1992).

According to characterizations performed by Aadland et al., sediments underneath SRS can be grouped into three aquifer systems separated by three confining systems. These aquifer and confining systems are made up of aquifer and confining units. From the surface to the crystalline bedrock these systems are as follows: the Floridan aquifer system, the Meyers Branch confining system, the Dublin aquifer system, the Allendale confining system, the Midville aquifer system, and the Appleton Confinining system.

In the central and southeastern portions of SRS, the Floridan Aquifer system is composed of the Upper Three Runs aquifer, the Gordon Confining unit, and the Gordon aquifer. The Upper Three Runs aquifer is the water table aquifer, recharged by direct precipitation. In the northwestern corner of the site near the A/M area, the Upper Three Runs Aquifer and Gordon Aquifer coalesce to form the Steed Pond aquifer.

Beneath the Floridan Aquifer system is the Meyer's Branch Confining system which consists of a single confining unit, the Crouch Branch. In the northwestern portion of SRS the Crouch Branch confining unit is discontinuous, allowing flow between the Floridan aquifer and the underlying Dublin aquifer system. The Dublin Aquifer system is composed of the Crouch Branch Aquifer. In the northwestern corner of the site the Dublin aquifer system is separated from the Midville aquifer system by the McQueen Branch confining unit, the Allendale Confining System. From the center to the north of SRS, the McQueen Branch confining unit is disrupted and the Dublin and Midville Aquifer Systems are connected. The Midville Aquifer system unit is the McQueen Branch Aquifer. The bottom-most confining layer is the Appleton confining unit which separates the fluvial and marine deposited sediments of the coastal plain from the undifferentiated Piedmont crystalline bedrock (Aadland et al., 1995). Table 2.1 depicts the generalized lithostratigraphy and hydrostratigraphy for SRS (Aadland, et al., 1995). Figure 2.4 represents a hydrostratigraphic cross-section of SRS along a northwest to southeast transect. Table 2.2 and Figure 2.5 list selected hydrogeologic properties for hydrostratigraphic layers in the GSA and A/M Areas, respectively.

2.4 Well Monitoring Program

To monitor aquifer contamination, investigators at SRS have drilled almost 2,000 groundwater monitoring wells over the last 30 years (Bollinger, 1999). These wells were screened at varying depths thought to correspond with the locations of specific aquifers and/or aquitards. Historically, groups of monitoring wells were placed and constructed as part of small-scale projects at SRS. For instance, three or four wells might be drilled in both the suspected up-gradient and down-gradient directions of flow to check for the presence of contamination from an accidental spill in an isolated area. Thus concentration data from monitoring wells at SRS is clustered primarily around known contaminated areas, leaving large spatial gaps where water quality data are unavailable (Figure 2.3: Map of monitoring wells).

Data from existing wells have not been fully integrated into plans for understanding site-wide or regional groundwater contamination, and new wells are simply added on an as-needed basis (Delaimi, 1996). Construction of older wells was not always properly documented; the aquifer-aquitard sequence under many of these wells can now only be inferred from stratigraphic models (Bollinger, 1999). Wells at SRS are generally sampled on a semi-annual basis. Water samples are taken to several different laboratories that perform quantitative analysis with extensive quality assurance/quality control for an entire suite of contaminants and water quality parameters. Commonly measured contaminants found at SRS include tritium, TCE and PCE (John Reed, WSRC, pers. comm., 1999). SRS stores the information from these analyses in its Geochemical Information Management System (GIMS). Field data from this rather extensive database could be used to improve studies of historical or future groundwater contaminant movement (Todd Rasmussen, WSFR, pers. comm., 1999).

In the late 1990s engineers at SRS developed a Geographic Information System (GIS) interface for the GIMS contaminant database. This interface adds a spatial component to the well collection data, and allows investigators to produce maps showing the locations of monitoring wells with high contaminant levels (Bollinger, 1999). Mapping this information is an important step in understanding contaminant transport at SRS; however, the maps of such data remain static and do not show how contaminant levels change with groundwater movement through time. In addition, it is difficult to accurately fill in the blanks, or interpolate the contamination in areas between wells. Standard methods of interpolating raw concentrations such as inverse distance weighting and kriging (Burrough, 1998) need improvement to incorporate the complexity of Coastal Plain hydrogeology (John Reed, WSRC, pers. comm. 2000). Delineation of contaminant plumes is still being performed by hand on site. These mapping efforts can benefit from the statistical simplification and GIS automation techniques presented in this paper.

<table>
<tr><th>Age</th><th colspan="3">Lithostratigraphy</th><th colspan="3">Hydrostratigraphy</th></tr>
<tr><td>Micocene</td><td>Hawthorne</td><td colspan="2">Altamaha (Upland Unit)</td><td rowspan="3">Surficial Aquifer</td><td rowspan="7">Upper Three Runs Aquifer</td><td rowspan="10">Floridan Aquifer System</td></tr>
<tr><td rowspan="9">Eocene</td><td rowspan="5">Barnwell</td><td colspan="2">Tobacco Road</td></tr>
<tr><td rowspan="3">Dry Branch</td><td>Irwinton Sand</td></tr>
<tr><td>Twiggs Clay</td><td>Tan Clay Aquitard</td></tr>
<tr><td>Griffins Landing</td><td rowspan="3">Barnwell-McBean Aquifer</td></tr>
<tr><td colspan="2">Clinchfield</td></tr>
<tr><td rowspan="3">Orangeburg</td><td colspan="2">Tinker/Santee</td></tr>
<tr><td colspan="2">Warley Hill</td><td colspan="2">Green Clay Aquitard</td></tr>
<tr><td colspan="2">Congaree</td><td colspan="2" rowspan="2">Gordon Aquifer</td></tr>
<tr><td rowspan="3">Black Mingo</td><td colspan="2">Fishburne/Fourmile</td></tr>
<tr><td rowspan="2">Paleocene</td><td colspan="2">Snapp/Williamsburg</td><td colspan="2" rowspan="2">Crouch Branch Aquitard</td><td rowspan="2">Meyers Branch Confining System</td></tr>
<tr><td colspan="2">Ellenton</td></tr>
<tr><td rowspan="2">Cretaceous</td><td rowspan="2">Lumbee</td><td colspan="2">Steel Creek/Peedee</td><td colspan="2" rowspan="2">Crouch Branch Aquifer</td><td rowspan="2">Dublin-Midville Aquifer System</td></tr>
<tr><td colspan="2">Black Creek</td></tr>
</table>

Table 2.1: SRS Lithostratigraphic (Group/Formation/Member) and Hydrostratigraphic Units (System/Aquifer/Zone)

Table 2.2: Hydrogeologic Properties at the Savannah River Site (GSA).

Hydrogeologic Zone	Thickness	Hydraulic Conductivity		Storativity	Transmissivity	Storage Coefficient	Hydraulic Diffusivity	Hydraulic Leakance
		Horizontal	Vertical					
	b (m)	K_h (m/s)	K_v (m/s)	S_s (1/m)	$T = K_h b$ (m^2/s)	$S = S_s b$	$D = T/S$ (m^2/s)	$L = K_v / b$ (s^{-1})
Surficial Aquifer	3 to 12	1.0 E-4	-	6.00 E-4	8.0 E-4	1.2 E-2	0.07	-
Tan Clay Aquitard	1.5 to 8	-	2.11 E-9	-	-	-	-	3.0 E-10
Barnwell-McBean Aquifer	12 to 40	3.0 E-5	-	8.1 E-6	6.0 E-4	1.6 E-4	4	-
Green Clay Aquitard	0.6 to 3	-	6.4 E-10	-	-	-	-	3.2 E-10
Gordon Aquifer	20 to 30	1.6 E-4	-	1.0 E-5	2.5 E-3	2.5 E-4	10	-
Crouch Branch Aquitard	18	-	1.1 E-9	-	-	-	-	5.8 E-11
Crouch Branch Aquifer	75	4.1 E-4	-	5.3 E-6	3.1 E-2	4.0 E-4	78	-

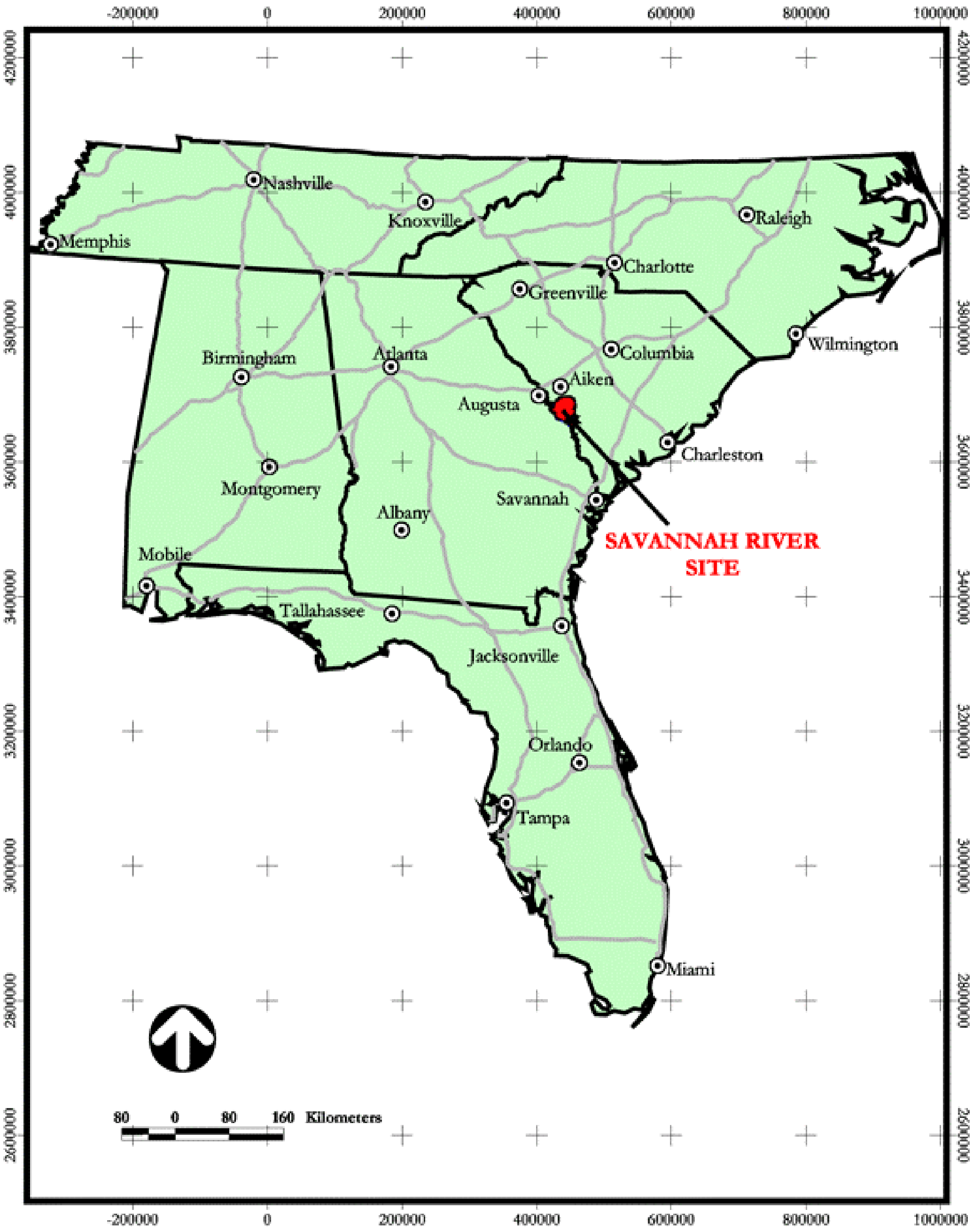


Figure 2.1: Savannah River Site Location

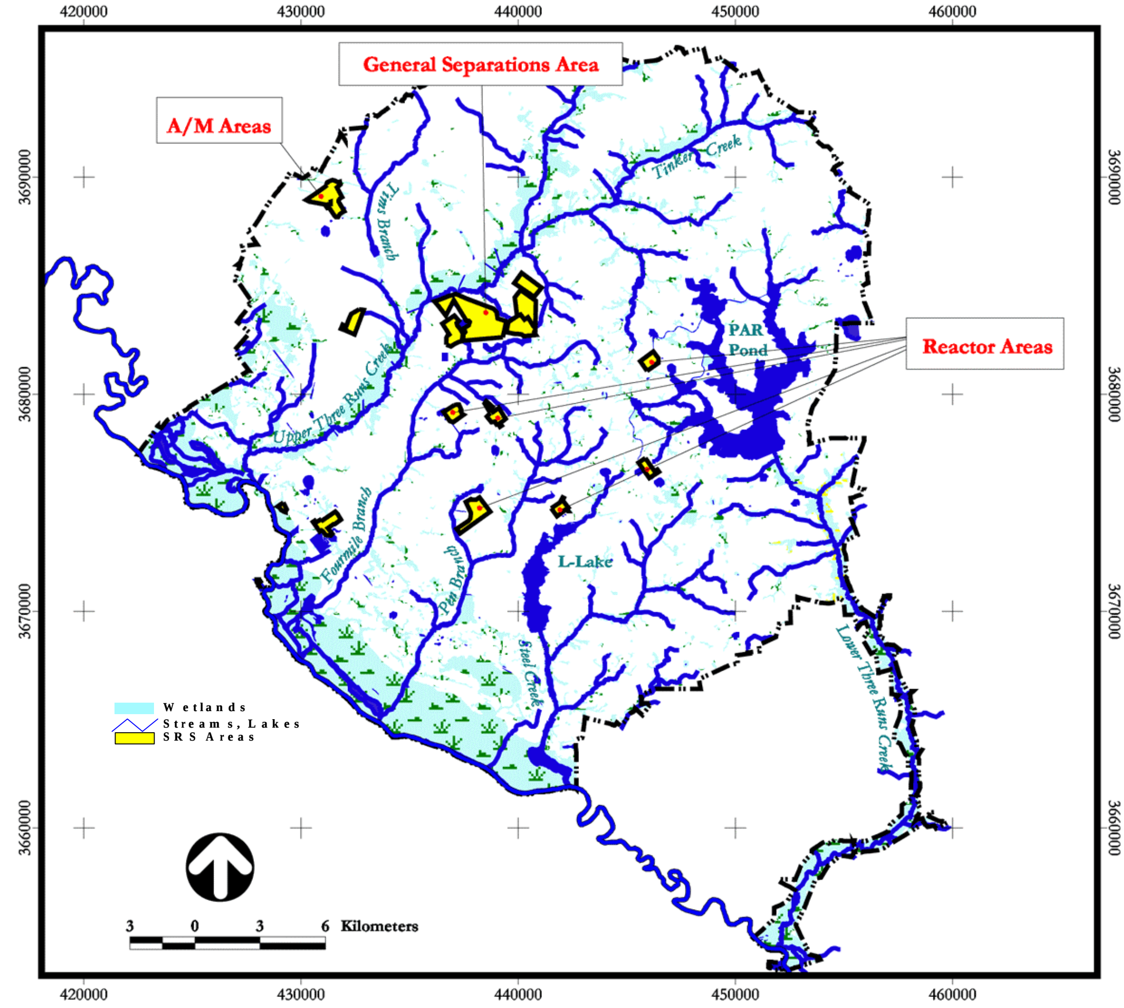


Figure 2.2: Savannah River Site Areas, Streams, Lakes, and Wetlands.

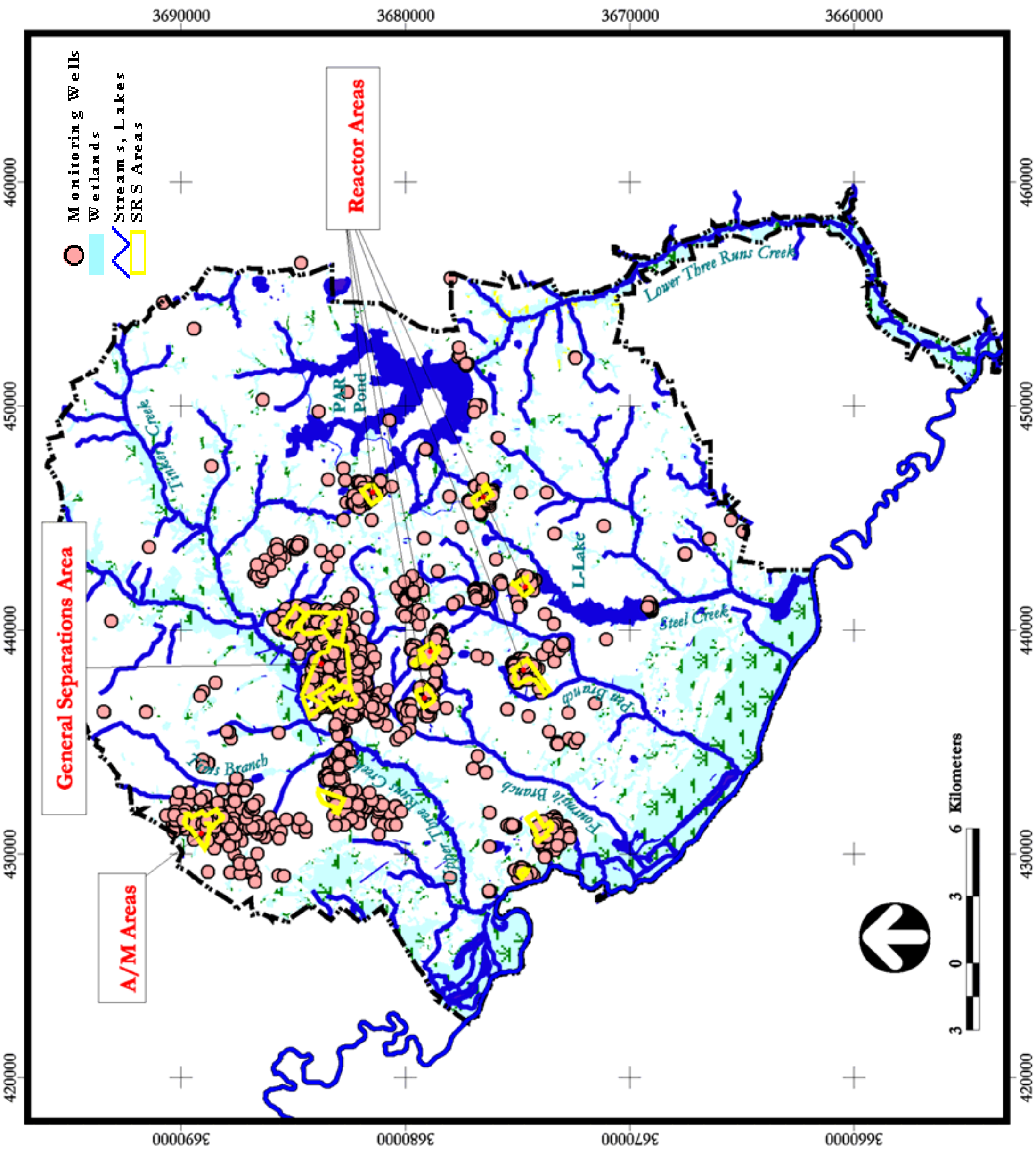
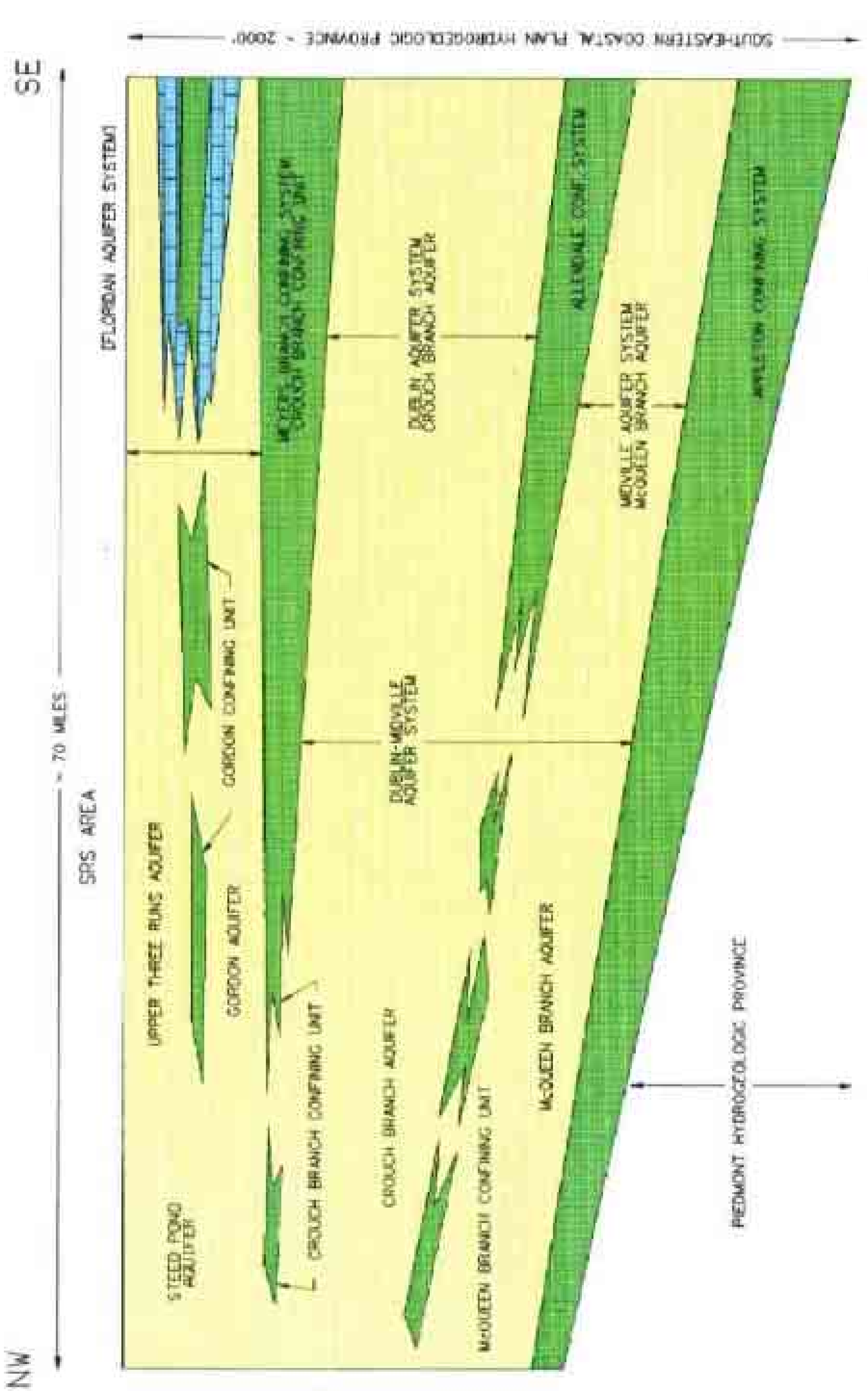


Figure 2.3: SRS Monitoring Wells (pink circles).



Aadland et al. (1995)

Figure 2.4: Savannah River Site hydrostratigraphy, NW to SE transect.

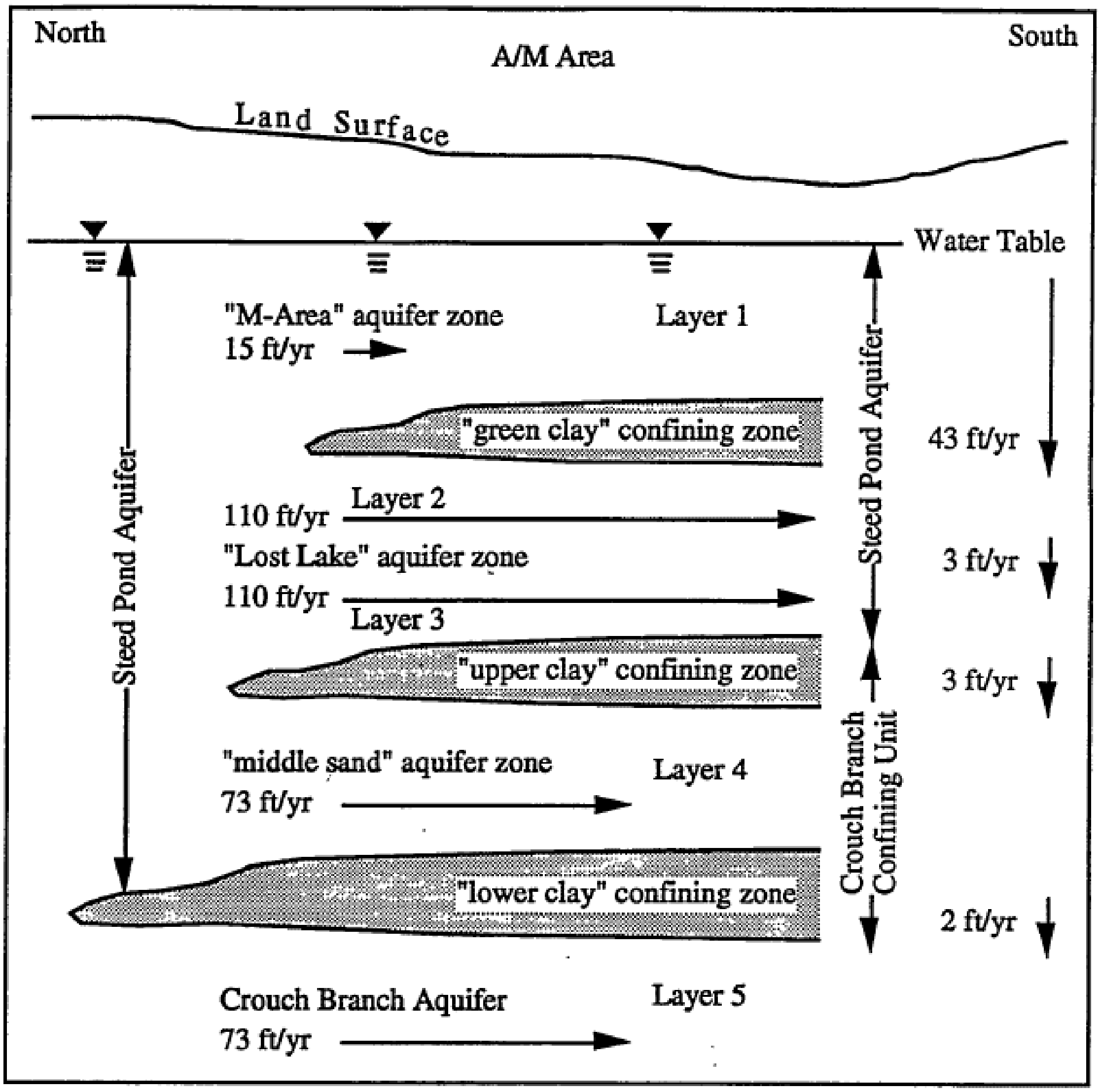


Figure 2.5: Vertical and horizontal hydraulic conductivity for aquifer units beneath the A/M area (Van Pelt, et al., 1994).

CHAPTER 3

LITERATURE REVIEW AND CONCEPTS

3.1 Previous Groundwater Studies at the Savannah River Site

Published scientific research from the Savannah River Site contains few discussions of the use of aquifer water quality signatures to predict groundwater and contaminant movement. At SRS, most previous attempts to predict the direction of groundwater flow and contaminant transport have not focused on the use of water quality data from well monitoring activities. Instead, groundwater studies have relied upon numerical simulation flow modeling (Coleman Research Group, 1995; Flach and Harris, 1997; Flach et. al., 1998, Flach et al., 1999; Rine, 1998; Van Pelt et al., 1994). Researchers acknowledge the high degree of uncertainty introduced into their conceptual models by the simulation of the complex hydrostratigraphy at SRS (Flach and Harris, 1997). Historically, field data has been difficult to incorporate into these numerical simulation flow models because of the "considerable effort required to process raw data into formats directly usable by groundwater codes through input" (Flach and Harris, 1997).

Independent regional studies, undertaken to determine whether radioactive contaminants would migrate beneath the Savannah River into Georgia, predicted that the Savannah River would act as a sink, drawing contaminants from deeper aquifers up into the river (Delaimi, 1996; Clarke and West, 1998). Observations at monitoring wells on the Georgia side of the Savannah River support the modeling by Delaimi (1996) and hydrogeologic characterization by Clarke and West (1998). Delaimi emphasized that his model did not account for vertical flow between discontinuous aquifer layers, and that for verification, more monitoring wells should be constructed to obtain a better understanding of field conditions. Clarke and West (1998) noted that the deepest aquifer layers may in fact transport groundwater beneath the Savannah River and that further field study was necessary to ascertain the likelihood of contaminants reaching these aquifers.

Numerical simulation techniques have been primarily used at SRS for modeling individual areas at high risk for contamination (Rine, 1998; Pelt et al., 1994; Flach and Harris, 1997; Flach et al., 1999). Many of these models are time-consuming and costly to produce because they require detailed characterization of localized hydrogeology. Incorporation of historical contaminant or other groundwater chemistry data for validation may improve the predictive ability of numerical flow models (Todd Rasmussen, pers. comm., 1999).

Flach and Harris (1997), for example, modeled groundwater flow beneath the GSA based on an extensive hydrostratigraphic characterization. Aquifer units were discretized into zones using fine-scale field characterizations and assigned hydraulic conductivity values based on field measurements. Citing errors in the field measurements, the researchers were forced to globally adjust, or smooth out field measured hydraulic conductivity coefficients for the Gordon aquifer unit and confining layer in order to calibrate their model with known aquifer recharge and discharge rates.

Jackson et al. (1996) developed a conceptual heuristic model of DNAPL (trichloroethylene and tetrachloroethylene) contamination for the Green Clay confining zone beneath the A/M area. This model relied on hydrostatic force balance, mass balance, and particle tracking as opposed to numerical flow simulation used in previous A/M area studies. An important model input was DNAPL concentration field data collected from well sampling; however, the model was not designed to include other ground water quality measurements and relied heavily upon previous detailed hydrostratigraphic studies.

SRS researchers have simulated groundwater and contaminant flow for other areas at SRS using less detailed hydrostratigraphic field measurements. To date, these models primarily have been used to identify further hydrogeologic characterization needs (Harris, 1997).

Rine et al., (1998) used a novel, GIS-based stack-unit mapping approach to identify surface groundwater contamination potential for a portion of the GSA. The researchers generated surface elevation maps for six aquifer units (all above the Crouch Branch Aquifer) and rated the contamination potential for each of these layers by their elevations and corresponding aquifer hydraulic properties. These six layers were then stacked within a GIS and spatial contamination potential from surface sources was summed using logarithmic techniques. Few analogous GIS-based groundwater contaminant mapping studies have been performed elsewhere in the Coastal Plain hydrogeologic environment (Rine, 1998).

3.2 Previous Studies Employing Statistical Analyses of Groundwater Quality Data

Research by Suk and Lee (1999) offers an alternative approach to the fine-scale hydrogeological characterization required by present groundwater flow models at SRS. Suk and Lee used multivariate analysis and GIS to correlate contaminant data with groundwater quality parameters for the purpose of identifying contaminated aquifer zones. They performed a principal components analysis (PCA) to reduce several measured aquifer water quality variables into a smaller series of underlying factors. Suk and Lee then ran factor scores generated by the PCA through a cluster analysis to group monitoring wells based on underlying water-rock interactions and recharge characteristics. These grouped wells were then mapped as aquifer zones using GIS software; zones identified by the researchers compared favorably with zones delineated with traditional hydrogeologic techniques (Suk and Lee, 1999).

Suk and Lee's (1999) multivariate analysis of geochemical data operated on the concept that each aquifer zone has its own unique groundwater quality signature, based upon the chemical makeup of the sediments that comprise it (Fetter, 1994; Kehew, 2001). Groups of water in aquifer zones delineated in this manner are known as hydrochemical facies (Fetter, 1994). Groundwater dissolves minerals and other geochemical constituents from the geologic media that it inhabits. The dissolved mineral and chemical composition is unique to the water in each aquifer, forming a groundwater quality signature of chemical constituent concentrations and field parameter readings that can serve to identify the parent aquifer. Signatures may vary when the physical and mineral makeup of aquifer geologic media changes, or at confining layer discontinuities that allow water from different aquifers to mix. Groundwater quality measurements from individual wells can thus be statistically grouped to identify such characteristics using a combination of factor and cluster analyses. One significant limitation to using aquifer water quality signatures to delineate physical aquifer structure is that different geologic units with differing geochemical makeup can behave as a single hydrogeologic unit based on shared hydraulic properties. Aquifer structure may remain the same, but may have different geochemical facies.

Using statistical methods to group monitoring wells by water quality, researchers have produced accurate maps of aquifer systems (Suk and Lee, 1999; Ceron, et al., 2000). In northwestern Spain, Vidal et al. (2000) performed a principal components analysis to reduce 14 water quality variables to two factors correlated with saline and organometallic contamination. Vidal et al. plotted the two sets of factor scores from the PCA against each other, graphically labeling each observation according to spatial location (either a well or spring sampling point). Sampling points fell into different clusters on the graph, illustrating those that shared common groundwater quality signatures. The location of the sampling points on the graph ranked their respective aquifers according to vulnerability to saline and/or organometallic contamination.

Abu-Jaber et al. (1997) used a similar multivariate statistical exploration of geochemical data to identify predominant chemical interactions in known aquifer zones and to determine zone sensitivity to pollution from domestic sewer leakage. Meng and Maynard (2001) processed geochemical data using cluster and factor analyses; these ground-water classifications were then used as a basis for developing a conceptual geochemical model of their study area. Ochsenkühn

(1997) performed a cluster analysis on groundwater geochemical data to identify major trend axes representing dominant groundwater flow pathways. Other studies have used similar principles to correlate groundwater pesticide contamination with different crop rotations and for the inference of groundwater flow direction (Grande, et al., 1996; Zanini, et al., 2000).

The success of these studies suggests the benefit of employing similar statistical analyses to map potential for groundwater contamination at SRS, especially in light of the fact that the GIMS database includes measurements of the water quality parameters used to describe signatures.

3.3 Groundwater Constituent Behavior

The following provides a brief introduction to some of the geochemical processes that may control concentrations of the naturally occurring groundwater constituents analyzed in this study. This information has been summarized from three textbooks that explain the geochemistry of groundwater in far greater detail (Fetter, 1996; Kehew, 2001; Drever, 1988).

Nine of the thirteen groundwater variables, or analytes, analyzed in this study are commonly found as natural constituents of groundwater. Table 3.1 lists these variables and their natural concentration ranges. In general there are eight major ions which usually make up more than 90% of all dissolved solids in groundwater. These are Na^+, Ca^{2+}, K^+, Mg^{2+}, SO_4^{2-}, Cl^-, HCO_3^-, and CO_3^{2-} (Fetter, 1994; Drever, 1988; Kehew, 2001). Concentrations of these major ions are usually greater than 1 mg/L (1000 µg/L) (Fetter, 1994). The six major ions examined by this study include Na^+, Ca^{2+}, K^+, Mg^{2+}, SO_4^{2-}, Cl^-. Iron and aluminum concentrations were also analyzed; these ions are considered common minor (0.01 to 10.0 mg/l) or trace (<0.1 mg/L) constituents of groundwater (Kehew, 2001)(Table 6.1). Silica, another common groundwater constituent studied here, is usually not found in ionic form and instead remains in aqueous phase.

The concentrations of these ions in groundwater are directly related to rock, soil, and gas interactions with water and thus help define aquifer water quality signatures. Several different chemical processes control the interactions of groundwater as it moves toward chemical equilibrium with surrounding minerals and gases. Kinetics describe the speed with which these equilibrium reactions occur in groundwater. The residence time of groundwater in an aquifer then is important in determining the degree of chemical equilibrium groundwater has reached.

Dissociation is the term given to the process that occurs when a compound in aqueous solution breaks down into its constituent ions. Dissociation is a reversible reaction controlled by the solubility properties of a compound in water. For example, NaCl dissociates in an aqueous solution into its constituent ions, Na^+ and Cl^-. Dissociation of inorganic salts such as NaCl is governed by diffusion, as water molecules do not play a chemical role in the breakup of the salt (Fetter, 1996). More complex compounds dissociate when their ions are chemically attracted to the H^+ and OH^- ions that make up water. Among these types of reactions are carbonate equilibrium reactions. Dissociation can also occur in groundwater during reduction-oxidation reactions most commonly involving electron transfer among H^+ and OH^- ions and iron, sulfur, or nitrogen compounds. When dissociation occurs, free ions may also exchange places with ions bound to minerals or other compounds groundwater contacts. These types of ion exchange reactions are driven by solute concentrations and by the chemical bonding properties of the ions involved (Drever, 1988).

The weak-acid strong base carbonate equilibrium system is one of the most dominant drivers of groundwater geochemical interactions (Kehew, 2001; Fetter, 1996, Drever, 1988). Carbon dioxide in the air dissolves in groundwater to form a weak acid known as carbonic acid. Carbonic acid dissociates in water to form bicarbonate and excess hydrogen ions. These hydrogen ions decrease the pH of groundwater, affecting the rates of other reactions including ion exchange and reduction-oxidation. Bicarbonate also dissociates in groundwater to form carbonate. Finally, calcium carbonate found in soil and aquifer rock dissociates to calcium and carbonate ions (Fetter, 1996). When excess carbonate is present the reactions move from in the opposite direction, and pH can be increased. A major control of the carbonate equilibrium system is pH change due to the presence of external acids and bases, either from natural sources or from anthropogenic pollution.

Groundwater chemically weathers different silicate minerals by dissolution at variable rates. These reactions release dissolved silica as silicic acid and metal cations including calcium, sodium, magnesium and potassium (Kehew, 2001). When aluminum and iron are present, clay minerals are formed as secondary products of silica mineral weathering. Because clay particles have highly charged surfaces they react strongly with ions dissolved in groundwater and play a role in the formation of aquifer water-quality signatures. Groundwater interactions with clay particles generally fall into the class of ion exchange reactions, although very slow dissolution also takes place.

Ion exchange occurs when the surfaces of porous geologic media and soil particles gain ions from groundwater and release other more weakly-held ions to groundwater. The relative strength of ion exchange for major cations is Na+ > K+ > Mg2+ > Ca2+. As an illustration, a common ion exchange that takes place in aquifers on the Atlantic Coastal Plain is that of “adsorbed sodium for calcium and magnesium in solution” (Kehew, 2001). Clay layers often provide the sodium ions for the exchange.

Reduction-oxidation (redox) reactions generate chemical conditions in groundwater that “directly or indirectly control the species and mobility of many elements” (Kehew, 2001). Redox reactions in groundwater usually involve electron transfer among H^+ and OH^- ions and iron, sulfur, carbon or nitrogen compounds. The valences and thus the chemical properties of species change as a result of the electron transfer. Oxidization occurs when species lose electrons while reduction takes place when species gain them. For example, oxygen dissolved from the atmosphere accepts electrons from iron cations in iron hydroxide and forms water. The iron in this example loses valence electrons and is thus oxidized. Eh is used as a measure of the oxidation potential (tendency to donate electrons) for an aqueous solution (Fetter, 1996).

In areas of recharge where unconfined aquifers are exposed to the atmosphere, redox conditions are usually oxidizing. The rate of oxidation in groundwater is often biologically controlled by microorganisms as they use redox reactions to gain energy (Kehew, 2001). As water in aquifers moves downgradient and becomes potentially confined, the oxygen used by aerobic microorganisms as an electron acceptor is no longer available and depletes, leading to a reducing environment. Under reducing conditions, anaerobes in groundwater preferentially deplete nitrate, then ferric iron, and then sulfate as electron acceptors.

All of the chemical processes described in this section are spatially influenced by variation in aquifer porous media and soils and by the location of recharge and discharge zones. The processes act together to define the concentrations of different groundwater constituents which in turn discriminate geochemical facies with unique aquifer water quality signatures.

3.4 Factor Analysis Using Principal Components

To identify aquifer water quality signatures, this study employs one of the most widely used forms of factor analysis, principal components analysis (PCA). PCA is a multivariate statistical procedure designed to classify variables based on their correlations with one another. The goals of a PCA and other factor analyses are first, to reduce the number of variables into a smaller set of latent factors and then second, to describe the structure of variables in relation to the system on which they were measured (Statsoft, 2002). PCA identifies which variables in a system are independent of one another, and patterns in correlated variables that may reflect the underlying processes governing the system (Tabachnik and Fidell, 2001). PCA works because variables often overlap in the amount and type of systematic variation they explain. In the case of groundwater, concentrations of different constituents may be correlated based on underlying physical and chemical processes such as dissociation, ionic substitution or carbonate equilibrium reactions. PCA helps to classify correlated variables into groups more easily interpreted as these underlying processes.

Principal components are identified through a matrix algebra-based analysis of correlations (or covariances, if so desired). Tabachnik and Fidell (2001) provide an example of the calculations necessary to produce a PCA. The graphical conceptualization of the mathematics behind PCA involves the plotting of all variables in a multidimensional space. A line known as an eigenvector can be drawn in this space so that it describes a maximal amount of the variation for all the plotted variables. A second line can be drawn to represent a majority of the remaining variation not explained by the first line, then a third line to describe the "left-over" variation from the second, and so forth. All lines drawn are independent of, or orthogonal to one another, because they explain entirely different groups of variation. The equation for each of these lines, or eigenvectors, is known as a factor, or component; the amount of variance described by each factor is represented by a number called an eigenvalue. In a typical PCA, eigenvalues representing variation are reported for each factor and also for factors cumulatively in a table format.

Researchers set the number of factors to extract from a particular dataset based on the amount of non-random variation they believe will adequately explain the underlying processes behind the measured variables. The more factors extracted, the greater is the cumulative amount of variation in the original data accounted for. When researchers do not have a priori knowledge of how much variation is necessary to describe a system, two other techniques are available to help them decide how many factors to extract (Statsoft, 2002). One decision rule is the Kaiser criterion where only factors with eigenvalues greater than one are extracted (Tabachnik and Fidell, 2001). The second technique is a scree test where the factor number is plotted on the x-axis against its corresponding eigenvalue on the y-axis. The number of factors to extract occurs where the slope of the line connecting the plotted points changes most dramatically from a steep (high) to shallow (low) negative value (Tabachnik and Fidell, 2001).

The coefficients of the equation for each eigenvector, or factor, are known as factor loadings. Factor loadings describe correlations between variables and factors; variables with high factor loadings can thus be grouped together by a common factor. Often, variables are strongly correlated with more than one factor, making the interpretation of results difficult. Interpretability can be simplified by rotating the original eigenvectors; this changes the positions of the original variable observations in the multidimensional space, but does not change variables' relationships to each other. Although an infinite number of rotations exist, the most commonly used method is the varimax procedure which maximizes the variance of the factor loadings within factors and across variables (Tabachnik and Fidell, 2001). PCA results generally include a table of factor loadings arranged by variable and corresponding factor.

Factor scores from a PCA often serve as a useful way to transform observations on individual variables to observations on the factors. "Factor scores are estimates of the scores [studied systems] would have received on each of the factors had they been measured directly," (Tabachnik and Fidell, 2001). Factor score coefficients can be calculated from the correlation matrix of the original variables and the factor loading matrix using regression techniques. These coefficients can then be used to calculate factor scores for each of the observations in the dataset.

PCA is a particularly useful data exploration tool because it does not require input data to be normally distributed. While this assumption is not necessary, normally distributed data can enhance PCA results because the analysis is sensitive to outliers, skewness, and kurtosis (Tabachnik and Fidell, 2001). Removal of suspected outliers and data transformation help to increase the stability of a PCA. Another important PCA consideration is the size of the dataset. Comrey and Lee (1992) suggest that a stable PCA requires at least 300 observations; however, if high correlations (>.80) exist among variables the sample size for a stable PCA can be as low as 150 (Guadagnoli and Velicer, 1988; Tabachnik and Fidell, 2001).

3.5 Cluster Analysis

In this study, we used a second multivariate statistical data reduction technique known as cluster analysis to group monitoring wells by aquifer water quality behavior. After research by

Suk and Lee (1999) and others, we performed our cluster analysis as tree clustering on factor scores generated by a PCA. Cluster analysis provided us with a tool to place monitoring wells (points where geochemical observations were taken) into geochemical zones of similar behavior (Suk and Lee, 1999). Conceptually, cluster analysis links variables hierarchically in the configuration of a tree with different branches. Branches that have linkages closer to each other indicate a stronger relationship among variables or clusters of variables.

The cluster analysis we used in this study calculates the Euclidean distance between observations. Our procedure then uses Ward's Method to analyze the distances among linkages for the entire group of observations. Ward's method is a regression approach designed to minimize the Error Sum of Squares between any two clusters at each hierarchical level (Statsoft, 2002).

The dendrogram generated from tree clustering provides a useful graphical tool for determining the number of clusters that adequately describe underlying processes that lead to spatial variation. Cluster membership can be saved for each observation and then mapped to show variation in the case of spatial data.

3.6 Inverse Distance Weighting For Map Interpolation

To map potential aquifer contamination we performed an inverse distance weighting (IDW) interpolation on factor scores from the two factors most correlated with the contaminant variables, tritium and tetrachloroethylene. IDW is an algorithm for spatially interpolating, or estimating values between measurements. We selected inverse distance weighting (IDW) because it is implemented in ArcView 3.2 GIS software and because it generated results preferable to ArcView's kriging and spline interpolation algorithms.

Each value estimated in an IDW interpolation is a weighted average of the surrounding sample points. Weights are computed by taking the inverse of the distance from an observation's location to the location of the point being estimated (Burrough and McDonnell, 1998). This distance term is often raised to a power "to control the significance of locational separation in the estimation" (Guan, et al., 1999). In a comparison of several different deterministic interpolation procedures, Burrough and McDonnell (1998) found that using IDW with a squared distance term yielded results most consistent with original input data.

CHAPTER 4

MAP REPRESENTATION OF POINT CONTAMINANT DATA AT SRS

4.1 Description of Work

We established methods for mapping analyte concentrations derived from the extensive quarterly ground water well monitoring program undertaken by workers at the Savannah River Site. Scripts and shapefiles were developed within an ArcView based Geographic Information System to produce ANSI D and E sized maps depicting tritium and trichloroethylene contamination at SRS Areas during 1999. These maps suggest that most contamination at SRS is located near production facilities and that outlying areas have groundwater with relatively low concentrations of tritium and trichloroethylene.

Our work with these basemaps established the sizes, scales, and aerial extents of that best communicate levels of contamination for different areas at SRS. Groundwater concentration levels of two of the most reliably measured analytes, tritium and trichloroethylene, were mapped for year 1999 sampling quarters and show the approximate areal extent of contamination at SRS. These maps are intended for use as basemaps for the display of analyte concentrations from other time periods. We created these basemaps for later use in displaying the results of our aquifer water quality analyses. A detailed description of our efforts can be found in Appendix I.

CHAPTER 5

ANALYSIS OF SRS GROUNDWATER DATA: METHODS

5.1 Procurement and Preprocessing of Data

Researchers at the Savannah River Site sampled ground water from several thousand monitoring wells and then analyzed the samples for a large suite of contaminants. To ensure cost effectiveness and quality control, analyses were performed at multiple laboratories on site and across the country. Sample spikes, blanks, and replicate analyses were all a routine part of the quality control/quality assurance (QA/QC) portion of the SRS Ground Water Monitoring Program. Results including QA/QC from the chemical analyses were stored in the Geochemical Information Management System (GIMS) an Oracle database maintained by a private contractor, Exploration Resources. The database is secure and can only be accessed by authorized personnel at the Savannah River Site.

To procure the data for this research we contacted Jim Bollinger, a chemical engineer/GIS analyst who works for the Environmental Remediation Section at SRS. Mr. Bollinger wrote ArcView Avenue scripts designed to access the GIMS database, return selected ranges of analyte data by time and/or geographic area, and attach the appropriate geospatial location to each well in the dataset. Using his scripts, Mr. Bollinger provided us with dBase files in single analyte format retrieved from the GIMS database by his interface script. The maximum temporal range of the analyte data retrieved from the GIMS database was from January 1979 to June 2001.

It is important to note that many analytes were not measured until the mid 1980s, resulting in smaller datasets for many groundwater constituents. In addition, wells were sampled at different time intervals. Wells located in areas of particularly high concern or at the location of ground water remediation projects were often sampled once or more each quarter. Monitoring wells in lower priority locations often were sampled only once yearly. Some old wells become abandoned as projects on site reach completion while other wells are installed when new remediation or characterization efforts begin.

Each analyte file consisted of a table of records with the fields listed and described in Table 5.1. The structure of the field parameter files was slightly different, and is illustrated in Table 5.2. Figure 5.1 provides a schematic overview of the methodology we used to analyze and map groundwater quality data at SRS.

Because our goal was to examine the relationships among analytes, the first step in our data screening process was to match records from analyte files based on the Sample ID field. The Sample ID numbers correspond to unique water sampling events at single well locations, and are used to track water samples through the chain-of-custody process from field to laboratory to database. After a thorough examination of the data we realized that matching analyte concentrations by Sample ID was not feasible because several observations in the analyte files were defined by the same Sample ID number. Such instances occurred when replicate analyses for a constituent were performed on the same ground water sample.

We considered averaging observations with the same Sample ID number but decided against this route because some water samples completely lacked a Sample ID number, and also because many samples were analyzed for only a few constituents. In addition, understanding the spatial variability of ground water quality required that we track analyte observations by well location. However, some wells were sampled more often than others; multiple observations at the same well would spatially bias factors generated by the principal components analysis. To avoid this spatial bias we chose to average sampling results over each quarter. In this way, a well tested six times during a quarter would not be weighted any more than a well tested only once.

We acknowledge that averaged results with low standard deviations generally provide more accuracy than single observations, making data from these two types of wells harder to compare, but given the irregularity of sampling events at SRS we decided that quarterly averaging would be the best way to capture enough data for factor and cluster analyses.

After examination of the data we found that during most years the majority of wells were sampled on one or two dates. Because principal components analysis requires a minimum of 300 observations for the most robust exploration of variable relationships, we focused on quarters 1993 through 1995 (Tabachnik and Fidell, 2001). Over these quarters, wells were sampled frequently and ground water was analyzed for the widest variety of constituents during any period of the SRS ground water monitoring program. The program performed its most extensive site-wide analyses during the early 1990s. The peak of the groundwater monitoring occurred during the first quarter of 1993 and during this time over 1000 wells were sampled for the analytes and field parameters chosen to represent ground water quality in this study.

The structure of the groundwater monitoring data supplied by Jim Bollinger led us to select 13 analytes/field parameters for statistical analysis. We chose 11 of these variables based on three criteria: 1)high spatial and temporal frequency of measurement, 2) their likeliness to represent naturally occurring chemical conditions, or aquifer water quality signature, and 3) availability.

Variables meeting these criteria included aluminum, calcium, chloride, iron, potassium, magnesium, sodium, pH, silica, sulfate, and total dissolved solids (TDS). Two additional variables, tritium and tetrachloroethylene, we selected because they represent radioactive and industrial ground water contamination, respectively.

5.2 Record Matching/Data Compilation

To perform multivariate analyses, statistical software packages usually require a flat, table-style database containing all variables of interest. What follows is the series of steps we used to convert the original GIMS data (Table 5.1) into a table containing quarterly observations for multiple analytes/field parameters (Table 5.4).

We averaged the original GIMS data by quarter using an ArcView 3.2 Avenue script, “Summarize” to process the dBase analyte files and convert them into ArcView shapefiles (Appendix I). The script matched well names from the original data to an existing UTM projection shapefile containing point locations of the wells. The script also created a field of unique names for wells called “wellqtr”, a field that combined the well name and quarter as a single string. Because analytes were often measured in different units, the script included a routine to standardize all units for each analyte. We converted chemical concentrations to micrograms per liter and tritium concentrations to picoCuries per liter.

The summarize script examined dates from the GIMS data and placed each observation in the appropriate quarter category using a dictionary-key scheme. All observations from the same well within each quarter category were counted and averaged, and standard deviations were calculated. The script also tracked the qualifier codes for each original observation by appending the code letters to a single string stored in the output “qualifier” field.

Lastly the script recorded the maximum detection limit for all observations of a single analyte. Table 5.3 describes the fields in the shapefile created by the summarize script. The processed shapefiles summarized the original GIMS data with unique, averaged observations at each well within each quarter.

We ran the summarize script for each of the thirteen analyte/field parameter files. We modified the averaging and standard deviation functions in the script to properly calculate values for pH using the following formulas:

$$\bar{x}_{pH} = -\log\left[\frac{\sum_{n}^{1} 10^{-pH_n}}{n}\right] \qquad s_{pH} = -\log\sqrt{\frac{\sum^{1}(10^{-pH_n} - 10^{-\overline{pH}})^2}{n-1}}$$

Measurements were not taken for every single well or for every type of analyte/field parameter during each quarter. We used Microsoft Access to join data for different analytes based on a field containing the well name and sampling quarter concatenated as a single string for each observation.

To accomplish the joins, we imported each of the resulting thirteen dBase files (part of the shapefiles generated by the summarize script) as tables in a Microsoft Access database. We then joined the files based on the wellqtr field. In Access this sort of field is known as a key; for records to properly match with one another the key field cannot contain duplicate entries. We set the wellqtr field as the key in the design view for each of the thirteen imported tables. We then ran a make table query: in the show tables dialog we connected all thirteen tables to each other based on the wellqtr key field; and then set up the query to extract the Well Name and Quarter fields for the first variable, and the Name, Result, and Standard Deviation fields for all 13 variables (Table 5.4).

5.3 Filtering and Outlier Analysis

To enhance subsequent principal components analyses we attempted to normalize the data. This was performed by removing quarterly observations based on 3 criteria: 1) those with Coefficient of Variation (CV) scores greater than 50%; 2) those identified as univariate outliers; 3) and those identified as multivariate outliers by Mahalanobis Distance tests.

We exported the 13 variable table resulting from the Microsoft Access query into a Microsoft Excel spreadsheet. In Excel, we calculated the coefficients of variation for all averaged observations and removed those observations with CV scores greater than 50%. We sorted the entire table in ascending order by the quarter field. Using the Subtotals option from the Data menu, we counted the number of observations for each quarter, and chose the 6 quarters with more than 300 observations: first quarter 1993, second quarter 1993, third quarter 1993, fourth quarter 1993, first quarter 1994, first quarter 1995. We also performed the statistical methodology described here on data from all quarters grouped into a single dataset.

To identify univariate outliers, we generated separate worksheets for the seven datasets and then sorted the worksheets by each analyte or field parameter. For most of the variables, two or three observations were several orders of magnitude higher or lower than the rest of the data; these we excluded from later analysis steps. We then scaled all remaining observations except those for pH with a logarithmic transformation.:

$$\textit{scaled observation} = \log[\textit{observation} + 1]$$

One was added to each observation before transformation to avoid negative numbers when raw measurements were between zero and one.

The resulting seven quarterly datasets were imported into the SPSS version 9.0 statistical analysis software package for multivariate outlier analysis. We fit each dataset to a linear regression model, using total dissolved solids (tds) as the dependent variable. TDS was chosen because it maximized the amount of variation explained by a regression model containing all the variables; for each quarterly dataset, R^2 values from the model were greater than 0.8. We saved Mahalanobis distance scores calculated by the regression model for each observation and used the chi-square distribution to determine the threshold for scores that identified outliers.

Mahalanobis distance defines observations in terms of their distance from the intersection of the means of all the variables, or the centroid of the data (Tabachnik and Fidell, 2001). For 13 degrees of freedom and $p<0.001$, the chi-square statistic is 32.909; any observations with Mahalanobis distance scores greater than this value were classified as multivariate outliers and removed from further analysis.

5.4 Principal Components Analysis

We ran the SPSS Factor Analysis module on the data for each quarter, specifying the principal components method with varimax rotation. After several trial runs, we found that extracting four factors during the analysis was sufficient to account for at least two-thirds of the variation in six of the seven datasets. For all quarterly datasets we extracted four factors and generated four corresponding groups of factor scores by multiplying the original observations by the appropriate factor-score coefficients. The factor scores were saved as four variables into the quarterly datasets for subsequent cluster analysis and for interpolation in ArcView. We also produced factor loading tables to show the strength of the relationship between each variable and factor.

After examination of the PCA results for several quarters, we found that high factor loadings repeatedly grouped the same variables together by component. However, due to rotation and differences in the amount of variation explained, the component position of these variable groups changed from quarter to quarter. To characterize patterns among quarters more clearly, we assigned each numbered component (1-4) a letter (A-D) based on the three quarters with almost identical PCA results. For these three quarters, variables with factor loadings greater than 0.4 for the first principal component were assigned to group A, group B for the loadings in the second component, C for the third, and D for the fourth (Table 5.1). Using this nomenclature, we identified subsets of analytes/field parameters related by similarly varying concentrations. We reserved those subsets containing the contaminant analytes, tritium and tetrachloroethylene, for subsequent GIS mapping.

5.5 Cluster Analysis

To group monitoring wells by geochemical zone (i.e., similar analyte/field parameter behavior during a quarter), we performed a cluster analysis on the previously saved principal components. In SPSS, we chose the hierarchical cluster analysis option to process observations from the four saved factor score variables in each dataset. (Factor score variables correspond to components identified by the PCA.) We labeled factor scores using the well name field, and specified the Ward method with squared Euclidean distance calculations for clustering. We chose to save the results as a cluster membership group number for each well. I was not possible to cluster the dataset with pooled observations from all quarters because it contained multiple observations for wells.

We saved cluster memberships from 3 classes to 10 with each class being a variable output to the dataset. To identify the number of classes necessary to distinguish between aquifer zones, we also generated cluster tree diagrams, or dendrograms by importing each dataset into the SAS statistical package. This step was necessary because SAS routines for generating dendrograms proved more robust for classifying hundreds of observations than those implemented by SPSS. Saving cluster membership at multiple levels provided for flexibility in later identifying the practical limits for resolving differences in aquifer water quality behavior among wells on GIS maps.

5.6 GIS Interpolation and Mapping of Statistical Results

We exported the quarterly datasets containing factor scores and cluster memberships from SPSS into dBase format for use in ArcView. In ArcView, we added the dBase files as tables and linked them by well name to well locations already spatially referenced in an ArcView shapefile. We saved each quarter as a new shapefile and then ran these files through a custom batch script that performed ArcView Spatial Analyst's inverse distance weighting interpolation for each set of factor scores. Thus, ESRI raster-based grid files were interpolated for each of the four factor score sets in each quarter. Because the extent of the aquifer beneath each well has been historically difficult to determine, we limited interpolations to a 500 meter distance from each well, and chose to use only factor scores from the nearest 12 wells for weighting purposes.

For each quarter, we then selected the two interpolated grids corresponding to the factors A and D. These two factors explained concentration variances for the contaminants, tritium and tetrachloroethylene, respectively. To map potential zones of contamination we overlayed the tritium and tetrachloroethylene grids onto the basemaps described in Chapter Three. Tritium grids were symbolized using a nine-class graduated color scale of light pink to dark red. Low factor scores in each grid indicated low potential for contamination and were colored pink, while the highest factor scores suggested high potential for contamination and were colored dark red. We symbolized tetrachloroethylene similarly, using shades of orange instead of red. We generated two maps for each contaminant in order to overlay both cluster analysis results and raw contaminant concentrations from 1999.

We color coded well points according to their cluster membership for the shapefiles discussed at the beginning of this section. Based on results from cluster diagrams, we chose five-levels to represent geochemical zones and labeled wells accordingly. We placed this layer on top of one set of the tritium and tetrachloroethylene potential maps for each quarter. To roughly estimate accuracy, we overlayed 1999 contaminant concentrations onto the other set of contamination potential maps. We accomplished this step using the symbology and procedures outlined in Chapter Three. We sized all the maps in 11 by 17 inch format for inclusion in this thesis.

Field Name	Function
Well_Name	Srs Name of Well
Samp_Date	Date of Sampling
Anal_Res	Result of Sample Analysis
Anal_Name	Name of Analyte
Res_Qcode	Qualifier Code for Analytical Result
Samp_ID	Sample ID Number
Record_ID	Record ID Number
Analyte_ID	Analyte ID Number
Ameth_Code	Type of Analysis
Lab_Code	Analytical Laboratory ID Number
Anal_Qcode	Analyte Laboratory Qualifier Code
Unit_Name	Units of Reported Analytical Result
Det_Limit	Method Detection Limit
Res_Prec	
Unit_ID	Unit ID Number
Validation	
UTM_E	Universal Transverse Mercator Easting
UTM_N	Universal Transverse Mercator Northing
SRS_E	SRS Easting
SRS_N	SRS Northing
Lat	Latitude
Long	Longitude
Samp_Type	Type of Sample
Field_Code	Field Conditions Code
Aquifer	Aquifer in Which Well Screen is Located

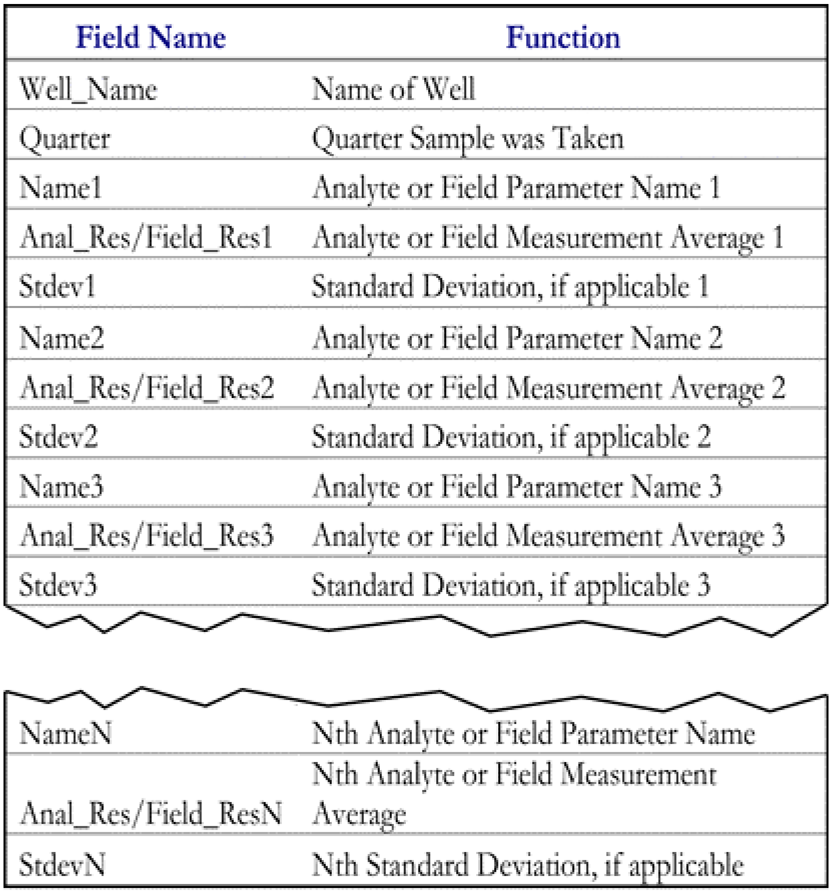
Table 5.1: Field names and functions for chemical analyte dBase files extracted from GIMS.

Field Name	**Function**
Well_Name	Srs Name of Well
Samp_Date	Date of Sampling
Field_Res	Results of Field Measurement
Units	Name of Analyte
Field_Parm	Field Parameter Name
Qual_Name	Qualifier Name
Samp_Prog	Sampling Program
UTM_E	Universal Transverse Mercator Easting
UTM_N	Universal Transverse Mercator Northing
SRS_E	SRS Easting
SRS_N	SRS Northing
Lat	Latitude
Long	Longitude
TOC	Top of Casing
TOS	Top of Screen
Record_ID	Record ID Number
Sample_ID	Sample ID Number
Aquifer	Aquifer in Which Well Screen is Located

Table 5.2: Field names and functions for field parameter dBase files extracted from GIMS.

Field Name	Function
Well_Name	Name of Well
Quarter	Quarter Sample was Taken
Anal_Res/Field_Res	Average of Concentrations or Field Measurements
Name	Analyte or Field Parameter Name
Qualifiers	Qualifier String
Stdev	Standard Deviation, if applicable

Table 5.3: Field names and functions for dBase files generated by the ArcView Avenue "Summarize" Script.



Field Name	Function
Well_Name	Name of Well
Quarter	Quarter Sample was Taken
Name1	Analyte or Field Parameter Name 1
Anal_Res/Field_Res1	Analyte or Field Measurement Average 1
Stdev1	Standard Deviation, if applicable 1
Name2	Analyte or Field Parameter Name 2
Anal_Res/Field_Res2	Analyte or Field Measurement Average 2
Stdev2	Standard Deviation, if applicable 2
Name3	Analyte or Field Parameter Name 3
Anal_Res/Field_Res3	Analyte or Field Measurement Average 3
Stdev3	Standard Deviation, if applicable 3
NameN	Nth Analyte or Field Parameter Name
Anal_Res/Field_ResN	Nth Analyte or Field Measurement Average
StdevN	Nth Standard Deviation, if applicable

Table 5.4: Field names and functions for quarterly dBase files created after linking average analyte/field parameters by well name and quarter.

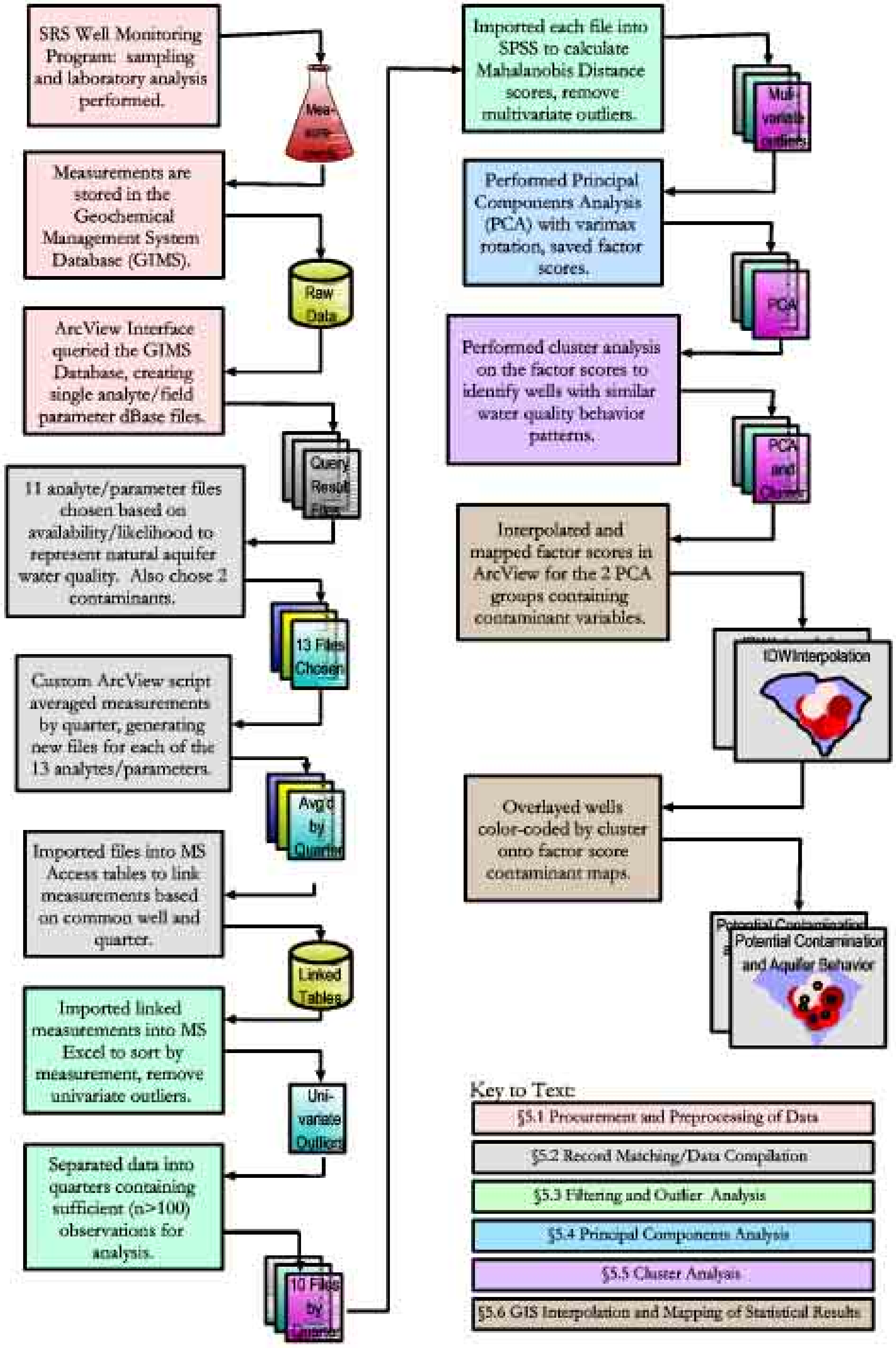


Figure 5.1: Schematic overview of aquifer water quality signature mapping methods.

CHAPTER 6

ANALYSIS OF SRS GROUNDWATER DATA: RESULTS AND DISCUSSION

6.1 Data Availability and Principal Components Analysis

After data preprocessing and outlier analysis steps, we found that six quarters yielded sufficient monitoring data (at least 300 observations) for stable principal components analysis. These quarters ranged from the beginning of 1993 to the beginning of 1995 and contained from 343 to 744 observations (Table 6.6). As a summary of time-averaged aquifer water quality conditions, we also performed a PCA on an aggregate group of all monitoring well observations where the 13 analytes of interest were measured. We identified 3914 acceptable observations for the aggregate PCA ranging from the fourth quarter of 1992 to the fourth quarter of 1999.

Table 6.1 is a summary of concentration data for the 13 analytes we studied. The table lists minimum detection levels, minimum and maximum concentrations, concentrations ranked by percentile, averaged concentrations, and coefficients of variation for the averages.

The spatial extent of the data for each quarter varied with where researchers at SRS sampled wells. For the first quarter of 1993, 744 wells were sampled for all 13 variables in this study. These wells were located in both the General Separations Area (400 observations) and the A/M Area (275 observations). For subsequent quarters, tritium monitoring efforts focused heavily on the General Separations Area and not on the A/M; around 90% of all observations we selected for this study by matching analytes were located in the GSA vicinity during these quarters. As a result, our analysis and mapping for the A/M Area relies heavily on data from the first quarter of 1993 and on the aggregate dataset.

After trial-and-error PCA runs, we found that extracting four components explained at least 2/3 of the variance for each quarterly dataset. Table 6.3, for example, reveals the eigenvalues and the percent of variance explained by each component for the fourth quarter 1994 PCA. Table 6.5 shows the percent of variance explained by each component for all datasets we analyzed. Components in this table are labeled by letters that correspond to common variable groupings explained in the following paragraph.

We examined the factor loadings generated for each quarterly PCA and the aggregate dataset. Because factor loadings show the correlation between analyte variables and components, we were able to group variables by their most highly correlated principal component. As an example, Table 6.2 illustrates factor loadings for the fourth quarter of 1993. Factor loadings greater than 0.4 are shown in red and designate a relatively high correlation between variables and components. For the fourth quarter of 1994, aluminum, magnesium, sodium, TDS, and tritium were strongly correlated with the first principal component. Calcium, potassium, pH, silica, sulfate, and TDS were strongly correlated with the second component. The third component was strongly correlated with aluminum, iron, and sulfate while the fourth component was most correlated with chloride and tetrachloroethylene. This pattern of variable grouping by component repeatedly occurred in PCAs for other quarters and for the aggregate dataset. To clarify these patterns, we renamed factors based on their variable groups with the lettering scheme shown in Table 6.4. Table 6.6 lists components with the absolute value of factor scores greater than 0.4 for all PCAs we performed in this study. This clearly illustrates a strong quarterly pattern of repeating component-variable groups. Table 6.7 summarizes these patterns across PCAs for all quarters and the aggregate PCA: Group (or component) A included aluminum, magnesium, sodium, tritium and TDS; group B included calcium, potassium, pH, silica, and also TDS variables; group C included aluminum, iron, and sulfate; and group D consisted of tetrachloroethylene and chloride.

The PCAs suggest that for the different hydrostratigraphic zones sampled by monitoring wells in this study, tritium concentrations behaved similarly to concentrations of aluminum, magnesium, and sodium cations and TDS. Tetrachloroethylene concentrations behaved similarly to those of chloride anions.

We calculated factor scores using the 13 original concentration/field parameter measurements made at each well. For each PCA, this procedure yielded four sets of factor scores corresponding to the four components of the PCA. We saved these scores for subsequent cluster analyses. Factor scores for groups A and D, the two component-variable groups containing the contaminants tritium and tetrachloroethylene, were stored in a GIS for later interpolation and mapping. The factor scores indicate the strength of correlation between components and the 13 measurements made at each well. Wells attributed with high factor scores for component group A may be more likely to receive tritium contamination. High factor scores for component group D suggest a stronger potential for tetrachloroethylene contamination.

6.2 Cluster Analysis

Dendrograms (tree clusters) generated by preliminary cluster analyses implied that monitoring wells could be best discretized into five zones. Dendrograms for the first quarters of 1994 and 1995 are provided as examples of the five zone dichotomy in Figure 6.1. This diagram shows that cluster analysis divided wells into five different groups based on aquifer water quality measurements. The Euclidean distance separating each of the five major clusters is greater than 100. In addition, we performed an exploratory correlation analysis of SRS-identified aquifer zones with different levels (3-10) of cluster organization. We found the highest correlation between well-screen aquifer zones and a 5-cluster system (Spearman's R = 0.225).

Using cluster analysis, we grouped each monitoring well into one of the five hierarchical cluster categories. On our maps, clusters showed a distinct spatial pattern for the first quarter of 1993 (Figure 6.7). GSA monitoring wells were grouped into four of the five cluster categories.

Wells of the category not represented at the GSA were prevalent at the A/M area and one of the GSA category wells was not present at the A/M. These differences indicate that potentially diverse aquifer geochemistry separates the A/M area from the GSA. In subsequent quarters, data was limited to the GSA. While all five cluster categories were represented at the GSA, the same three categories identified during the first quarter of 1993 were dominant. On a more local scale, neighboring wells screened at different depths within both areas often varied by cluster category.

6.3 GIS Maps

Table 6.8 lists the 18 maps we generated from the PCA and cluster analysis results. Maps included in this thesis are noted in the table. As detailed in Chapter Five, we performed inverse distance weighting interpolation on factor scores for components correlated with the two contaminant variables, tritium and tetrachloroethylene. The radial interpolation method we chose created continuous surfaces for 500 meters around each well based on the factor score values at the 12 nearest wells. We made no interpolations for portions of the site outside the 500 meter radius of any well. Interpolated surfaces reflected the coverage of wells; areas with high contamination potential often end abruptly on our maps.

We mapped interpolated factor scores using raster-based grid layers shaded to 9 levels (Figures 6.2-6.19). We used shades of orange to represent tetrachloroethylene contamination and shades of red to represent tritium contamination. The lightest shades corresponded to the lowest contamination potential, the middle shade (fifth in sequence) corresponded to the median contamination potential, and the darkest shades indicated the highest level of contamination potential. Factor scores moved into the positive range from the median to the highest contamination potential shade. Positive factor scores indicated a positive correlation with their respective contaminant bearing component.

In general, our map interpolations suggest that portions of the GSA possessed the highest potential for tritium contamination, while the portions of the A/M Area were most likely to receive tetrachloroethylene contamination. On a finer scale, interpolations for both tritium and tetrachloroethylene indicate a stronger likelihood of contamination near seepage basins and other waste disposal sites. For tritium, the trend of increasing contamination potential was directed from waste sites toward streams and seepage basins. Tetrachloroethylene contamination potentials did not reveal as clear a pattern as those for tritium.

The structure and extents of potentially contaminated zones changed slightly from quarter to quarter. In addition to the natural variation of analyte concentrations, the number of wells monitored changed over time. Well monitoring activity was reduced subsequent to the first quarter of 1993; wells on the periphery of the two SRS areas were not monitored during every quarter we studied, thus changing the extent of our interpolations. After the first quarter of 1993, fewer wells were monitored overall. While quarterly changes did not have a strong effect on the component structure of the PCAs in this study (Table 6.6), the reduction in data points is reflected in shifted extents and locations of potential contamination zones on the maps.

To roughly gage the accuracy of contamination potentials generated from 1993-1995 data, we overlayed unprocessed concentration data from all four quarters of 1999. We symbolized 1999 tritium and trichloroethylene concentration data using the graduated color legends described in Section 4.4. At SRS, trichloroethylene was often disposed of in the same locations and at the same time as tetrachloroethylene. The two contaminants share many similar chemical characteristics and behave similarly as DNAPLs in groundwater. Despite a 5-6 year time lag, areas with high contamination potential for both tritium and tetrachloroethylene strongly coincided with later point observations of relatively high tritium and trichloroethylene concentrations (Figures 6.2, 6.4, 6.6, 6.13). Factor scores interpolated for components uncorrelated with either of the contaminants did not correspond to 1999 locations of elevated tritium and trichloroethylene concentrations.

We also mapped groundwater quality zones at well locations (Figures 6.3,6.5, 6.7-6.12, 6.14-6.19). These zones were derived from cluster analyses of the factor scores generated by each PCA. Earlier work has established that clustering factor scores can help delineate geochemical facies with unique aquifer water quality signatures (Suk and Lee, 1999). Mapping the cluster analysis results to five levels indicated possible groundwater quality zones in the GSA and the A/M area. In several portions of the GSA, groups of wells repeatedly shared a common cluster membership over subsequent quarters. The largest repeating clusters of wells were located around the Burial Grounds and the F-Area and H-Area seepage basins. It is important to note that the statistical software assigned cluster number labels to the cluster groups based on analysis for a single quarter. Cluster number labels and their colors on the maps do not necessarily match each other from one quarter to the next. Green clustered wells in one quarter for example, may correspond with yellow coded wells on the map for a later quarter.

6.4 Discussion

In this study we present a novel contaminant mapping methodology for the Savannah River Site. The study demonstrates the ability of principal components and factor analyses to detect physical and chemical aquifer processes underlying groundwater quality variables. Our maps depict aquifer water quality signatures as contamination potential for both the GSA and the A/M Area at SRS. We believe that the procedures outlined here may help SRS workers with hydrogeologic characterization, contaminant plume delineation, and future well construction and monitoring decisions.

Maps of PCA factor scores as contamination potential imply the link between aquifer geochemistry and underlying physical aquifer hydraulic properties. This link is most strongly suggested for tritium at the GSA where potential contamination zones stretched from seepage basins and other source areas to streams, wetlands, and seeplines. One interpretation is that during the study period, tritium movement was regulated by a shallow flow regime where local topographical features dissect and receive discharge from the water table aquifer (the Upper Three Runs aquifer). However, this interpretation is confounded by recent evidence that groundwater levels show very little seasonality in the shallow aquifers at SRS (Todd Rasmussen, WSFR, personal communication, 2002).

Processes underlying tetrachloroethylene behavior were harder to characterize; comprehension may require comparison of the contamination potential maps with detailed hydrostratigraphy. Mapping DNAPL contamination potential using aquifer water quality signatures may not be appropriate, because concentrations in groundwater reflect only the dissolved portion of DNAPL. Significant amounts of non-dissolved DNAPL may actually exist in areas at SRS where our maps showed no contamination potential. Zones where low dissolved potential are surrounded by high PCE contamination potential may indicate the existence of plumes of non-dissolved PCE.

The most difficult step in this methodology was finding wells where all 13 analyte and field parameter variables were consistently measured. A single parameter not measured over a quarter would exclude a well from later statistical analysis. This is especially evident for the entire A/M area where many wells were not re-measured for tritium after the first quarter of 1993; the A/M area was, for practical purposes, excluded from PCA analyses of subsequent quarters. Unfortunately, such changes in the number of observations make inter-quarter comparisons unclear because they introduce variation that is difficult to separate from the natural fluctuations of analyte concentrations. The results of the PCAs in this study do suggest that a smaller, optimized number of groundwater quality variables may be measured to gain the same insight into aquifer water quality behavior. Matching a reduced number of geochemical variables would unquestionably incorporate more wells and provide a larger, higher resolution spatial picture of aquifer signatures and contamination potential.

Despite quarterly spatial differences in well monitoring, the variable-component structure of PCAs for different quarters was remarkably similar. The comparable temporal behavior of variables validates our assumption that aquifer water quality signatures were governed by underlying processes such as water-rock interactions and recharge-discharge relationships. Our aquifer water quality signature assumption is further validated because contamination concentrations measured in 1999 strongly corresponded to mapped locations of high contamination potential. These locations possessed positive factor scores for principal components highly correlated with contaminant variables.

Interpolation of factor scores incorporates underlying aquifer processes better than simple interpretation of raw contaminant concentrations. Using factor scores smooths out spikes in concentrations and identifies areas that may receive future contamination because of correlation with variables other than contaminants. The interpolations are meant to visualize the potential for contamination; we decided not to interpolate at a larger distance because the coverage of monitoring wells became increasingly sparse with distance away from SRS areas. As distance from large groups of monitoring wells increased, predicting the potential for contamination was less reliable because interpolations at these wells included fewer factor score observations.

An in-depth comparison of hydrogeology with the aquifer water quality zones delineated by cluster analysis is necessary to understand the aquifer processes represented by the zones. Seasonal differences in aquifer water quality may explain why some wells changed their cluster zone association over different quarters. These wells may draw water from shallow aquifers affected by local recharge and discharge. Many wells belonged to the same cluster zone for all quarters we analyzed; these wells may draw water from deeper aquifers with more stable geochemistry. Nested monitoring wells screened at different depths fell into separate clusters, further indicating the sensitivity of the statistical techniques to vertical differences in groundwater geochemistry.

Overall, the field-based analysis methods described in this research show promise for supplementing previous studies of groundwater flow and contaminant transport at SRS. Mapping contamination potentials with existing GIMS data proved inexpensive and relatively efficient; we relied on widely available statistical and GIS software packages, and after refinement of the methodology, the final data preparation and analysis steps took less than a week. Mapping results was time consuming and tedious, but we generated scripts to automate interpolations and other repetitive tasks. While our methods were partially validated by favorable comparison with later data, a full validation may require focused analysis on a selected portion of SRS where fine-scaled hydrostratigraphic information is available.

Further efforts in the direction of this research will benefit from the descriptions of our methodology, and the successes and pitfalls we encountered. Some recommendations to make our methods more efficient and to improve the interpretation of results include:

- a critical examination of our results by experts well-versed in SRS geochemistry.
- a test application of this methodology to a portion of the GSA where wells have been heavily monitored and hydrostratigraphy is well known. Known aquifer processes may be matched with aquifer water quality signatures; these relationships can then be extrapolated to other areas of the site.
- a background analysis of naturally occurring versus contaminant concentrations of all analytes used for this methodology.
- possible separation of contaminant data from the PCA to identify zones at high risk for contamination. Factor scores would be less heavily biased by contaminant concentrations. Contaminants could be matched to appropriate principal components after the PCA by calculating correlations between factor scores and raw contaminant concentrations.
- possible incorporation of other major, minor, and trace groundwater constituents for analysis.
- optimizing the number of water quality variables to increase spatial coverage and resolution of PCA and Cluster Analysis. Higher correlations among optimized variables

would reduce the number of observations necessary for a stable PCA (Tabachnik and Fidell, 2001).

- gaining better access to recent observations in the GIMS database and generating a historical summary of monitoring activities by well.
- using Visual Basic scripts in MS Access to automate the process of matching wells with analytes.
- using better methods of interpolation--possibly kriging as implemented in Surfer or software packages other than ArcView 3.2.

We believe that these suggestions combined with our methodology will add to the understanding of groundwater flow, hydrostratigraphy, and contaminant transport at SRS.

Table 6.1: Background levels and concentration ranges for analytes at SRS.

Analyte	*MCL*[1]	*Natural Range*[2]	*SRS Background*[3]	*Detection Limit*	*Min.*	*Max.*	*Percentiles*					*Mean*	*CV Score (%)*
							10th	*25th*	*50th*	*75th*	*90th*		
Aluminum	50	<100 (Trace)	27.40	1.93	3.54	155000	20	33.3	90.6	381	2101	2578.0	433.3
Calcium	--	>5000 (Major)	--	10.00	10.00	482000	616.2	1320	3830	13600	34010	13002.7	233.6
Chloride	250000	>5000 (Major)	--	28.00	250.00	44600	1620	2030	2550	3470	5510	3338.4	87.7
Iron	300	10-10000 (Minor)	31.80	1.90	4.00	48100	5.2	12.0	38.3	170.5	678.4	522.1	477.3
Potassium	--	>5000 (Major)	--	15.00	49.35	145000	500	500	833	1550	3271	2065.5	334.1
Magnesium	50	>5000 (Major)	7.72	2.00	2.16	40000	259	398	655.5	1220	2740	1357.1	194.5
Sodium	20000[*]	>5000 (Major)	--	4.70	495.00	360000	1820	2570	4660	12800	34150	14354.9	206.7
pH	6.5- 8.5	--	6.16	--	3.0	12.8	4.4	4.9	5.5	6.5	8	4.6	88.6
Silica	--	>5000 (Major)	--	42.80	152.00	158000	6063	7370	9380	13600	26200	13341.7	98.1
Sulfate	250000	>5000 (Major)	--	90.00	93.50	440000	1000	1000	1670	5467.5	10600	5565.7	309.4
PCE	5	--	--	0.026	0.03	19700	1	1	1	2.5	5	26.9	1842.5
TDS	500000	--	--	1000.00	23.00	1785000	23000	33000	60000	128000	265100	126583.3	164.0
Tritium	20000	--	1480.00	7.00	2.00	286000000	700	1630	11400	263000	3565000	1804393.8	571.8

Units are µg/L except for pH (unitless) and tritium (pCi/L).

[*] Sodium is under consideration by the USEPA for listing as a drinking water contaminant.

[1] Maximum Contaminant Level for drinking water set by USEPA, 2002.

[2] General ranges for naturally occurring major, minor, and trace ion concentrations in groundwater (Fetter, 1996).

[3] Background ion/contaminant concentrations for the General Separations Area at the Savannah River Site (Cresp et al., 2000).

Principal Components Analysis
Factor Loadings - Fourth Quarter 1993

	Component			
	1	*2*	*3*	*4*
Aluminum	0.759	-0.005	0.451	-0.181
Calcium	0.161	0.856	-0.236	0.100
Chloride	0.106	0.039	-0.031	0.833
Iron	0.023	-0.076	0.854	0.063
Potassium	0.203	0.749	0.176	0.093
Magnesium	0.780	0.218	-0.168	0.240
Sodium	0.865	0.182	0.138	0.134
pH	-0.494	0.698	-0.092	0.022
Silica	0.197	0.675	0.115	-0.302
Sulfate	-0.089	0.529	0.561	0.119
Tetrachloroethylene	-0.014	-0.019	0.114	0.690
Total Dissolved Solids	0.756	0.538	-0.004	0.017
Tritium	0.832	-0.176	-0.192	-0.091

Table 6.2: Factor Loadings for Fourth Quarter 1993 PCA

Principal Components Analysis
Variance - Fourth Quarter 1993

Component	*Eigenvalue*	*% of Variance*	*Cumulative %*
1	3.57	27.44	27.44
2	2.92	22.50	49.94
3	1.45	11.18	61.12
4	1.41	10.88	72.00

Table 6.3: Explained Variance for Fourth Quarter 1993 PCA

Component Group	*Aggregate Dataset*	**Order of Components for Each Group** *1993Q1*	*1993Q2*	*1993Q3*	*1993Q4*	*1994Q1*	*1995Q1*
A	1	2	1	1	1	1	1
B	2	1	2	2	2	2	2
C	4	3	3	4	3	3	3
D	3	4	4	3	4	4	4

Table 6.4: Order of original principal components and their component group letter assignment for six quarters.

	Percentage of Variance by Principal Component						
Component Group	*Aggregate Dataset*	*1993Q1*	*1993Q2*	*1993Q3*	*1993Q4*	*1994Q1*	*1995Q1*
A	23.2	21.7	25.4	27.3	27.4	25.7	25.8
B	22	24.4	21.2	21.9	22.5	20	21.6
C	11.3	10.7	12.1	10.1	11.2	12.3	11.5
D	11.3	9.7	10.4	10.8	10.9	11	10.6
Sum	67.8	66.5	69.1	70.1	72	69	69.5

Table 6.5: Percentage of variance explained by each principal component for six quarters.

	Principal Component Membership - Factor Loadings > 0.4						
	Aggregate Dataset	*1993Q1*	*1993Q2*	*1993Q3*	*1993Q4*	*1994Q1*	*1995Q1*
Aluminum	A,D	A,C	A	A,C	A,C	A,C	A
Calcium	B	B	B	B	B	B	B
Chloride	D	D	D	D	D	D	D
Iron	D	C	-C	C	C	C	C
Potassium	B	B	B	B	B	B	B
Magnesium	A	A	A	A	A	A	A
Sodium	A	A	A	A	A	A	A
pH	B(-A)	B	B(-A)	B(-A)	B(-A)	B(-A)	B(-A)
Silica	B	B	C	B(-D)	B	B	B
Sulfate	D,C	B,C	B	B,C	C,D	C	C
Tetrachloroethylene	D	D	D	D	D	D	D
Total Dissolved Solids	A,B	B,A	A,B	A,B	A,B	A,B	A,B
Tritium	A	A	A	A	A	A	A
Total Number of Wells	3914	744	362	368	343	383	347

*All Available Data category includes repeat measurements of the same wells for different quarters. Parenthesis () indicate that the variable posessed a second factor loading above 0.4. The greater factor loading of each pair is in the first position.

Negative signs indicate a negative factor score for the corresponding component.

Table 6.6: Principal Component Membership by Variable for Six Quarters

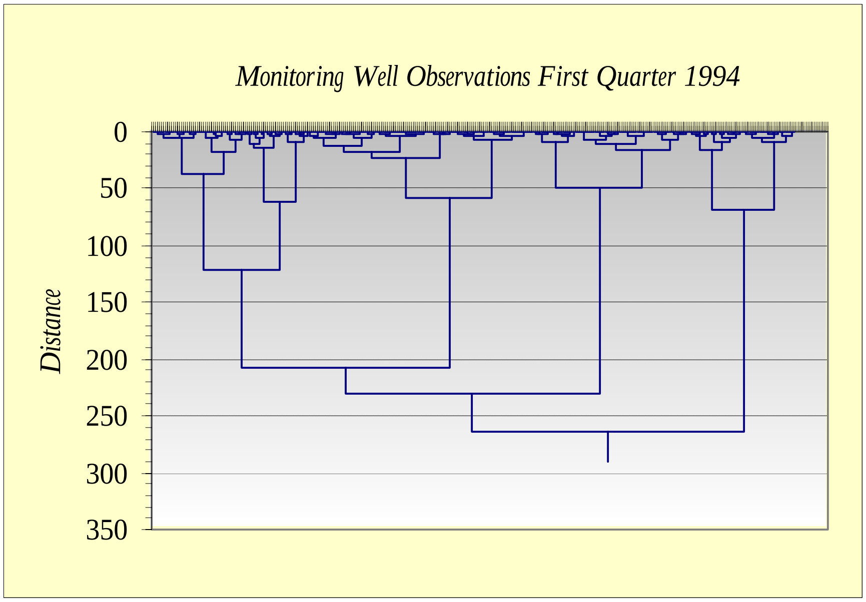
Generalized Component Membership

Group	*Variables*
A	Aluminum, Magnesium, Sodium, Tritium, TDS
B	Calcium, Potassium, pH, Silica, TDS
C	Aluminum, Iron, Sulfate
D	Chloride, Tetrachloroethylene

Table 6.7: Generalized Component Membership for Variables

Area	*Contaminant*	*Date*	*Overlay*	*Principal Component of Factor Scores*	*Figure Number in this Document*
A/M	PCE	Aggregate (1993 – 1995)	1999 TCE concentrations	3	6.2
A/M	PCE	1993 Quarter 1	aquifer zone	4	6.3
A/M	Tritium	Aggregate (1993 – 1995)	1999 Tritium concentrations	1	6.4
A/M	Tritium	1993 Quarter 1	aquifer zone	2	6.5
GSA	PCE	Aggregate (1993 – 1995)	1999 TCE concentrations	3	6.6
GSA	PCE	1993 Quarter 1	aquifer zone	4	6.7
GSA	PCE	1993 Quarter 2	aquifer zone	4	6.8
GSA	PCE	1993 Quarter 3	aquifer zone	3	6.9
GSA	PCE	1993 Quarter 4	aquifer zone	4	6.10
GSA	PCE	1994 Quarter 1	aquifer zone	4	6.11
GSA	PCE	1995 Quarter 1	aquifer zone	4	6.12
GSA	Tritium	Aggregate (1993 – 1995)	1999 Tritium concentrations	1	6.13
GSA	Tritium	1993 Quarter 1	aquifer zone	2	6.14
GSA	Tritium	1993 Quarter 2	aquifer zone	1	6.15
GSA	Tritium	1993 Quarter 3	aquifer zone	1	6.16
GSA	Tritium	1993 Quarter 4	aquifer zone	1	6.17
GSA	Tritium	1994 Quarter 1	aquifer zone	1	6.18
GSA	Tritium	1995 Quarter 1	aquifer zone	1	6.19

Table 6.8: Listing of GIS maps and their contaminant type, time frame, overlay, and component used for factor score interpolation.



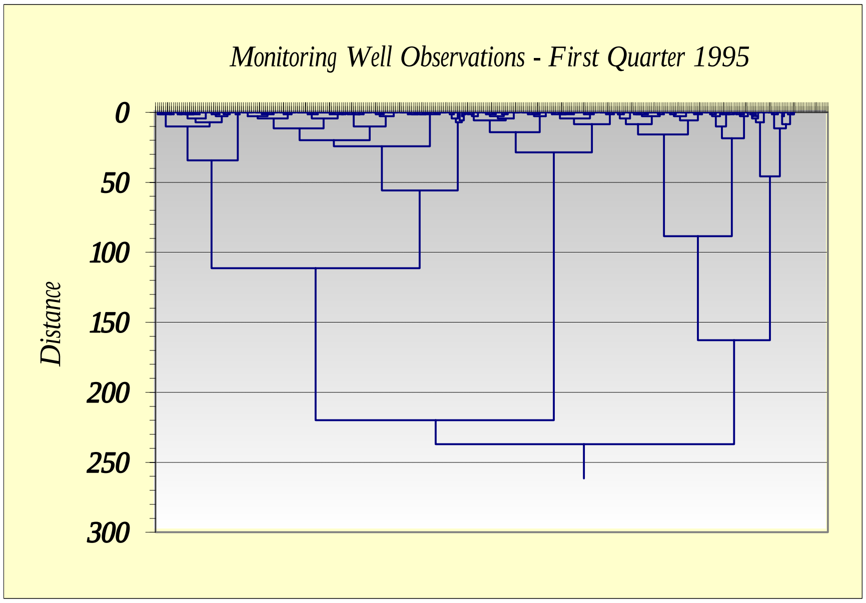


Figure 6.1: Cluster analysis dendrograms for First Quarters 1994 and 1995. These diagrams depict how five major cluster groups (squared Euclidean distance > 100) categorized monitoring wells at SRS.

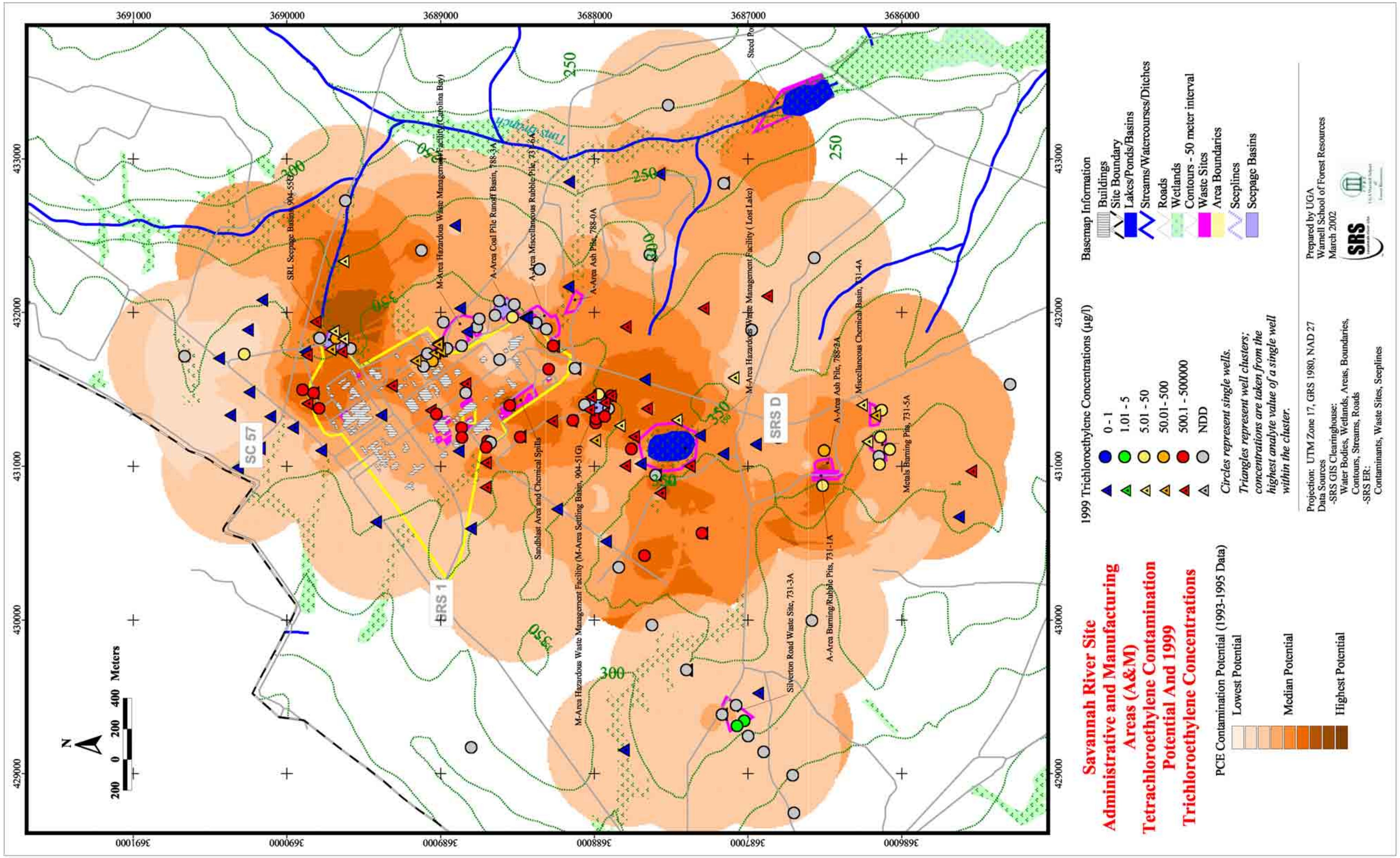


Figure 6.2: PCE Contamination Potential for 1993-1995 with 1999 TCE Concentrations Overlay, A/M Area.

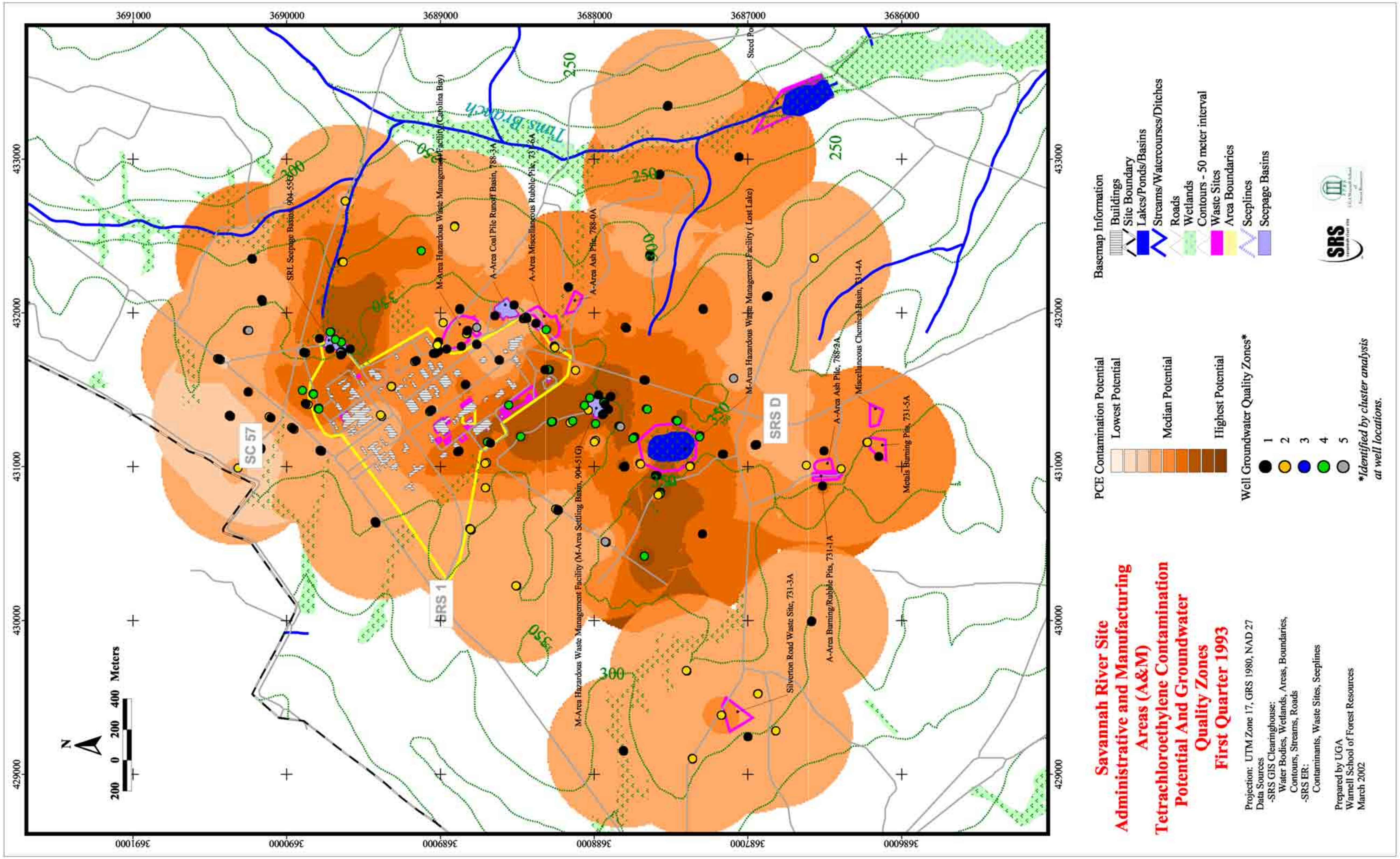


Figure 6.3: PCE Contamination Potential for First Quarter 1993 with Aquifer Zone Overlay, A/M Area.

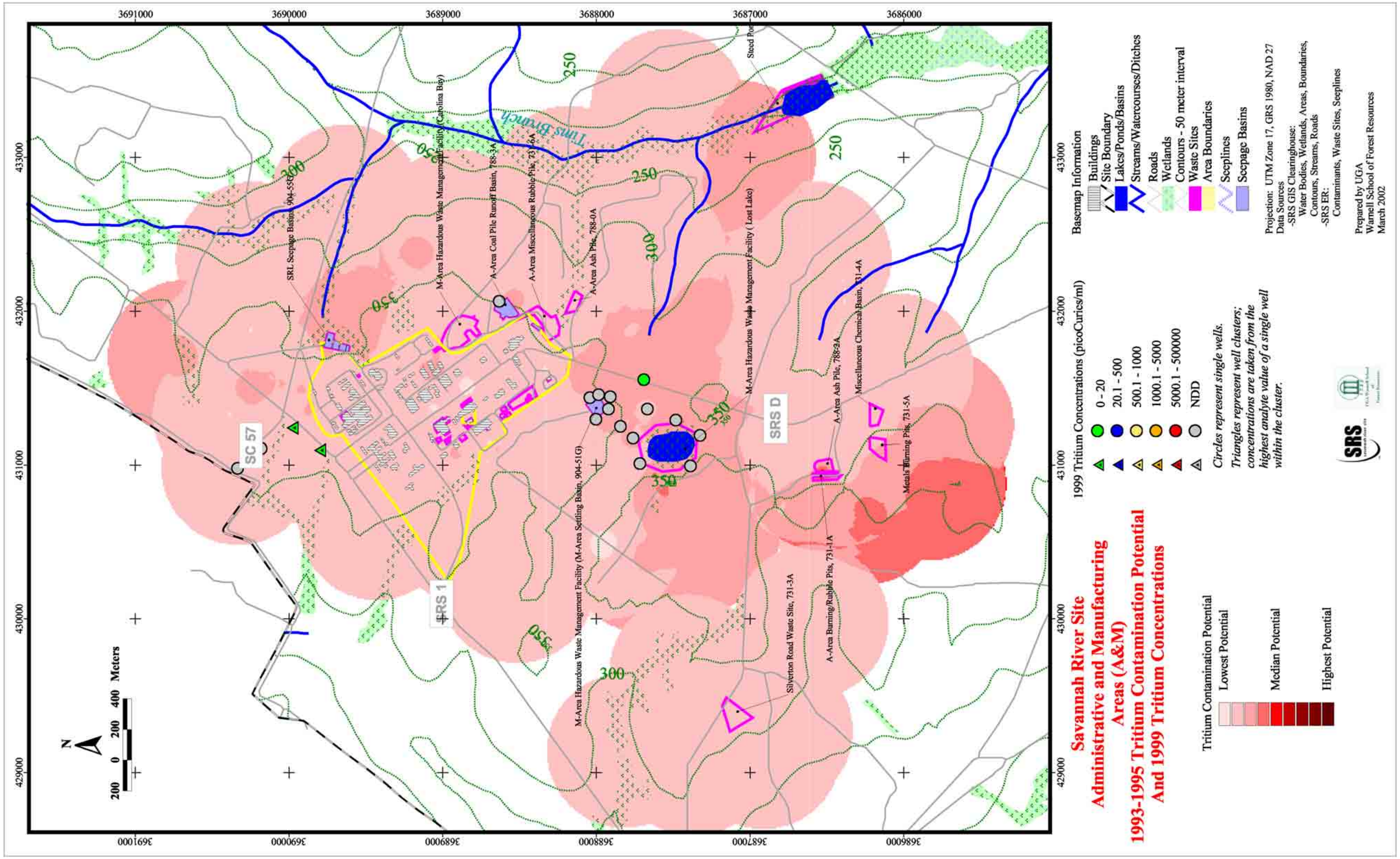


Figure 6.4: Tritium Contamination Potential for 1993-1995 with 1999 Tritium Concentrations Overlay, A/M Area.

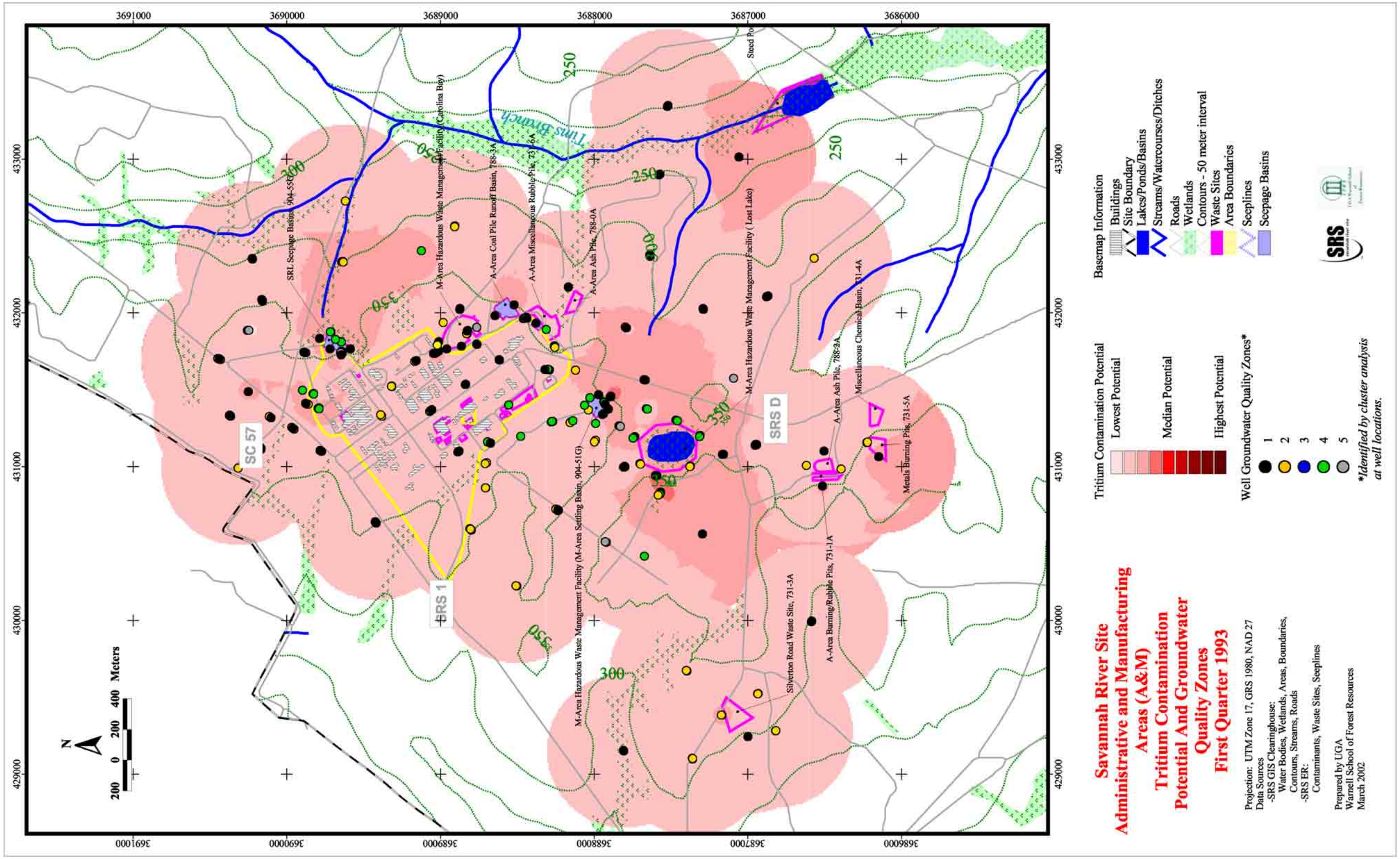


Figure 6.5: Tritium Contamination Potential for First Quarter 1993 with Aquifer Zone Overlay, A/M Area.

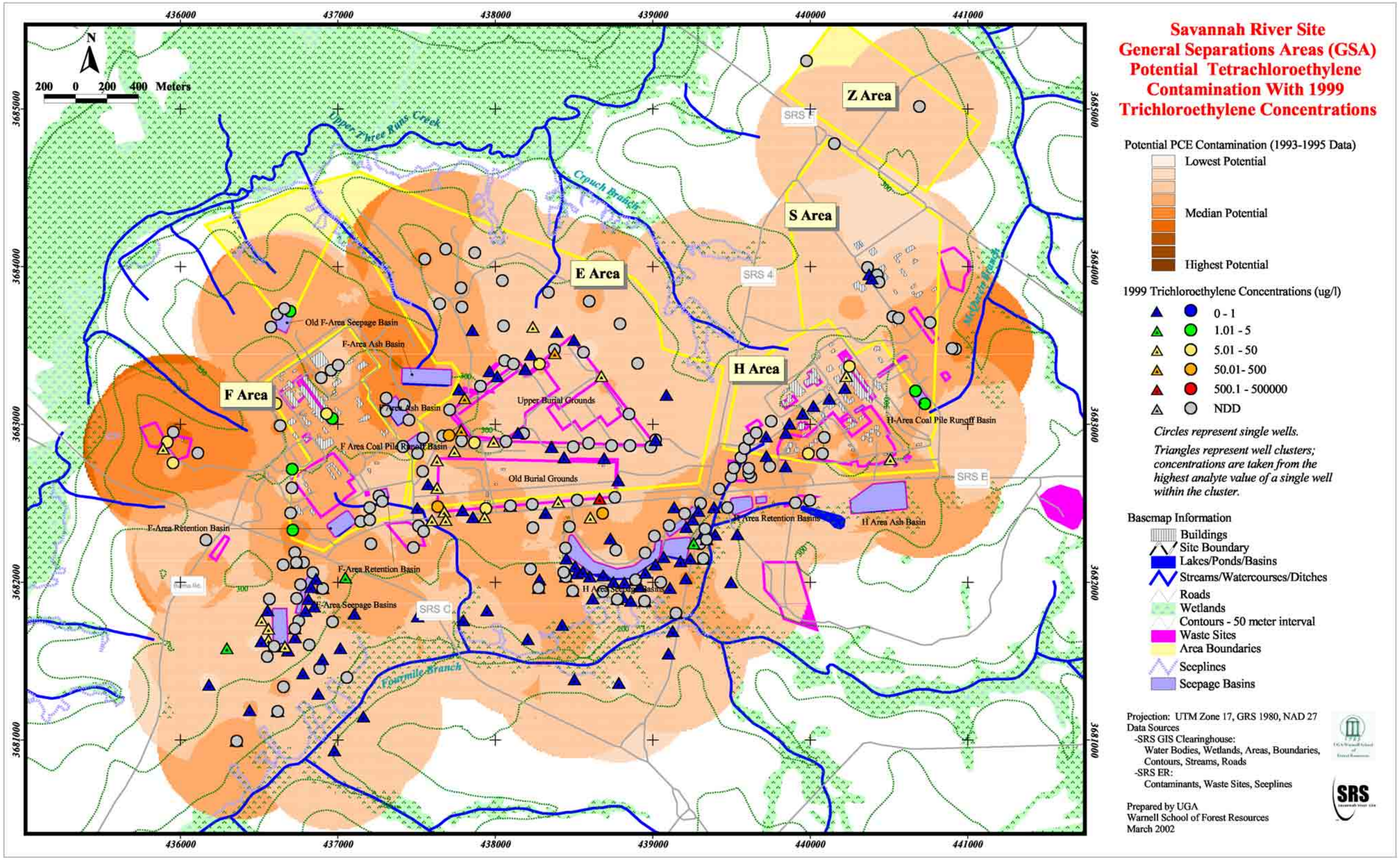


Figure 6.6: PCE Contamination Potential for 1993-1995 with 1999 TCE Concentrations Overlay, GSA.

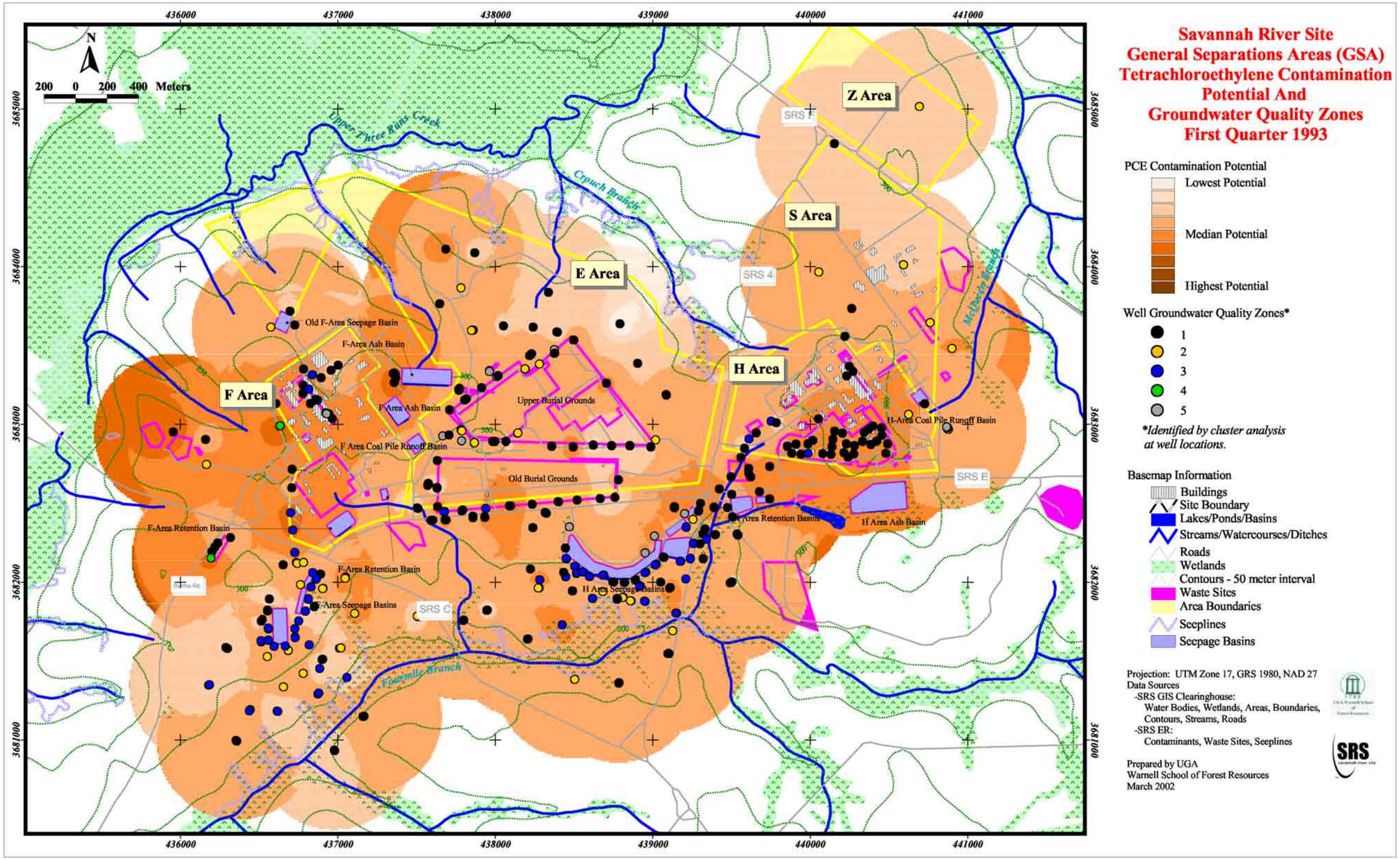


Figure 6.7: PCE Contamination Potential for First Quarter 1993 with Aquifer Zone Overlay, GSA.

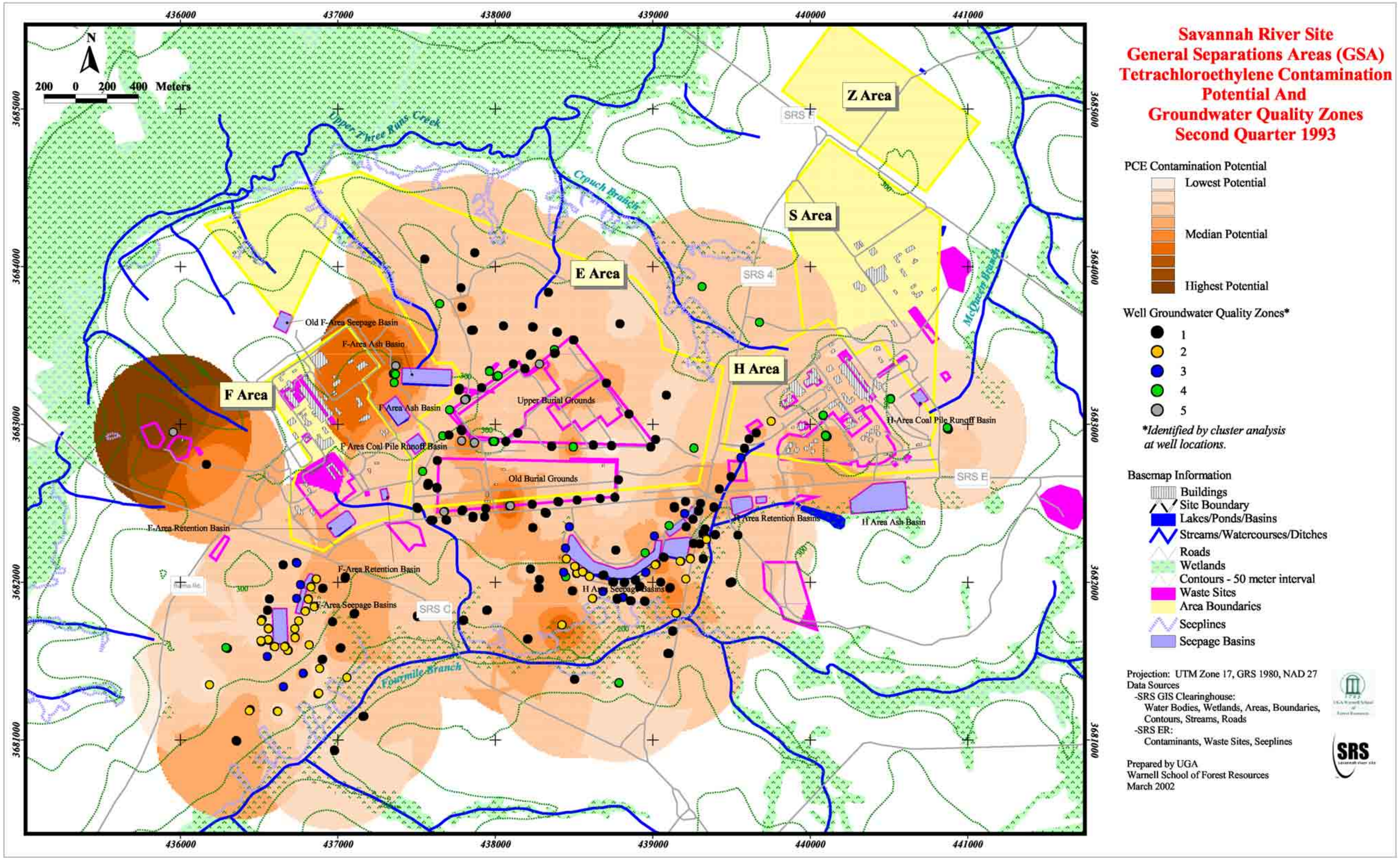


Figure 6.8: PCE Contamination Potential for Second Quarter 1993 with Aquifer Zone Overlay, GSA.

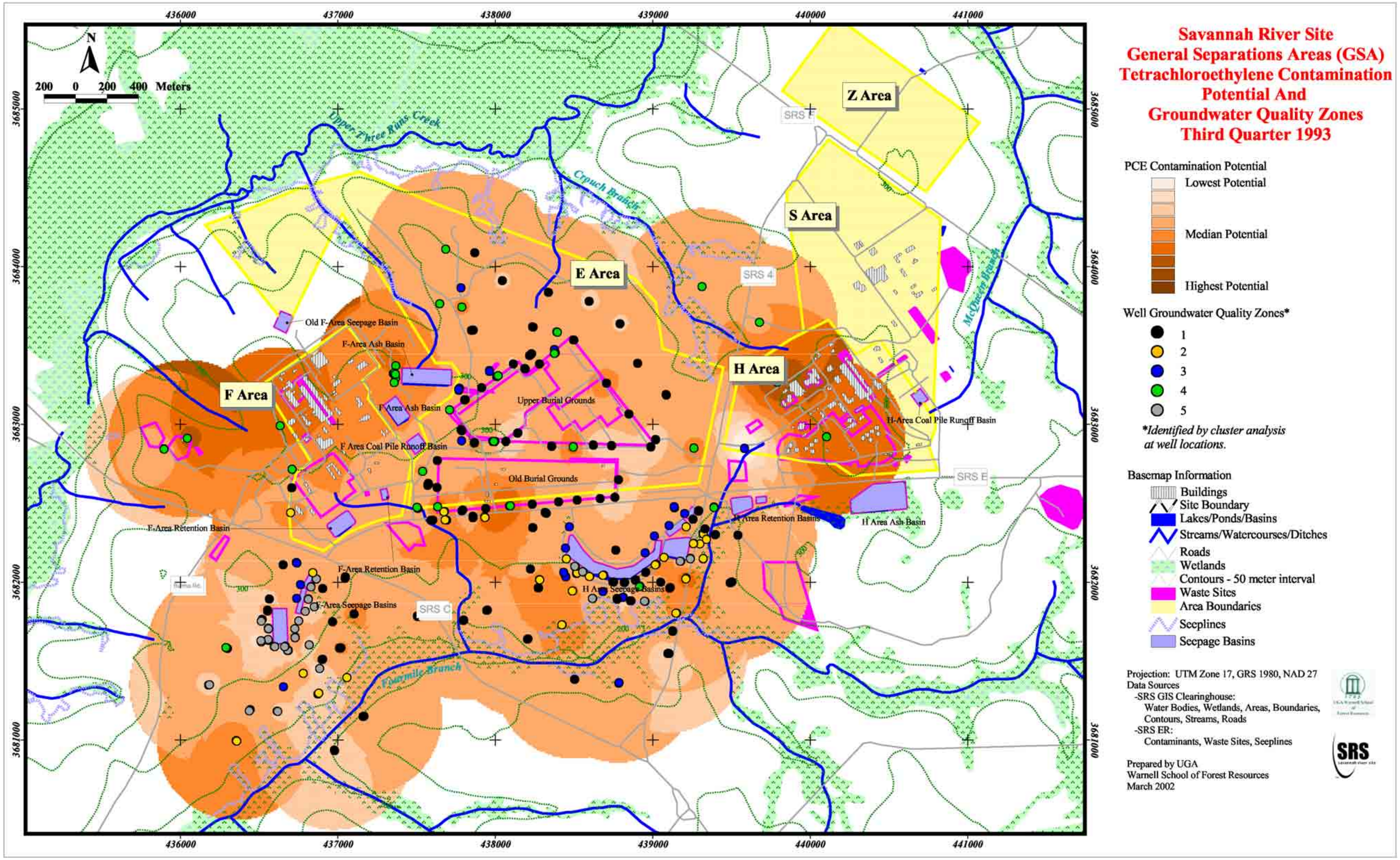


Figure 6.9: PCE Contamination Potential for Third Quarter 1993 with Aquifer Zone Overlay, GSA.

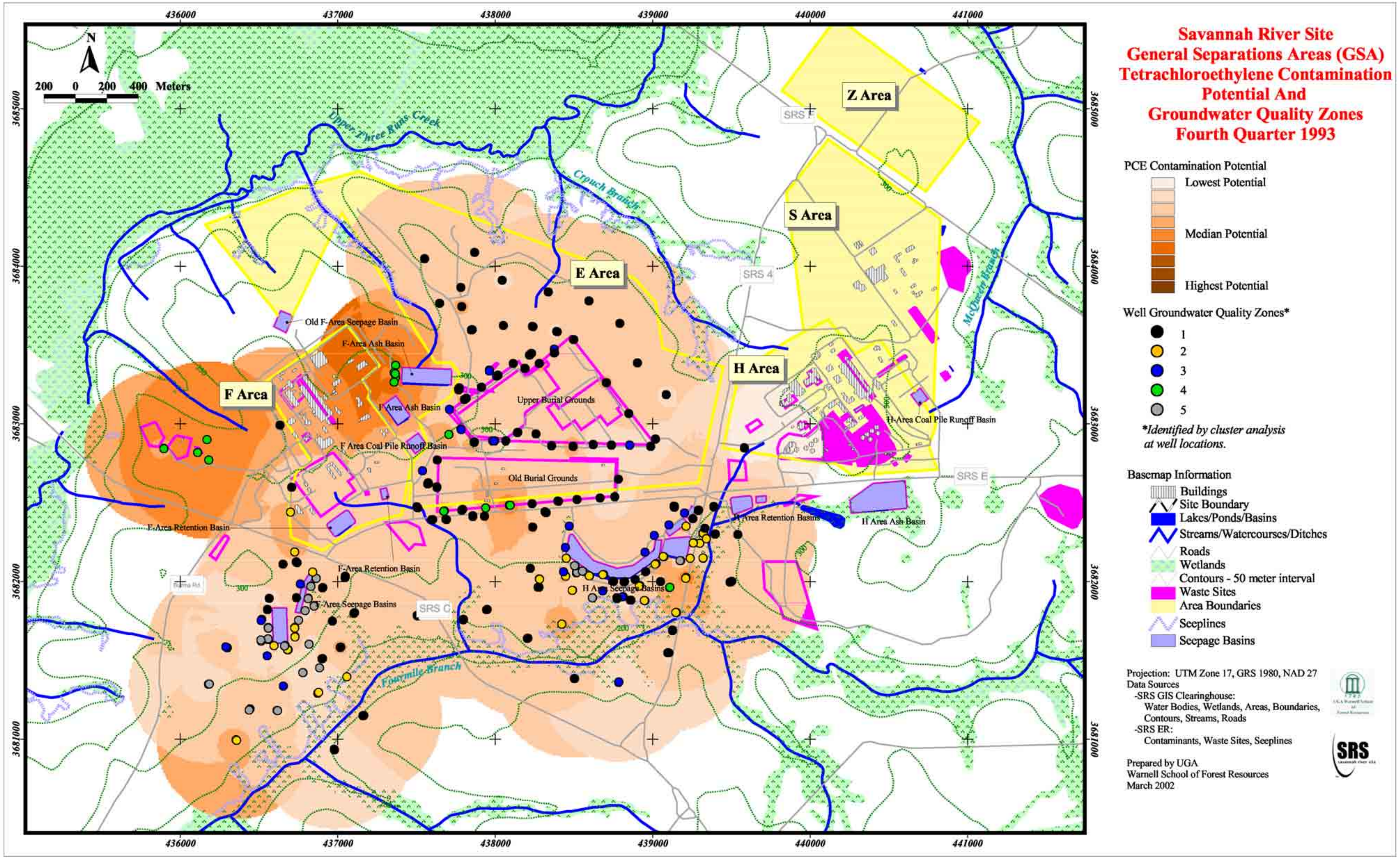


Figure 6.10: PCE Contamination Potential for Fourth Quarter 1993 with Aquifer Zone Overlay, GSA.

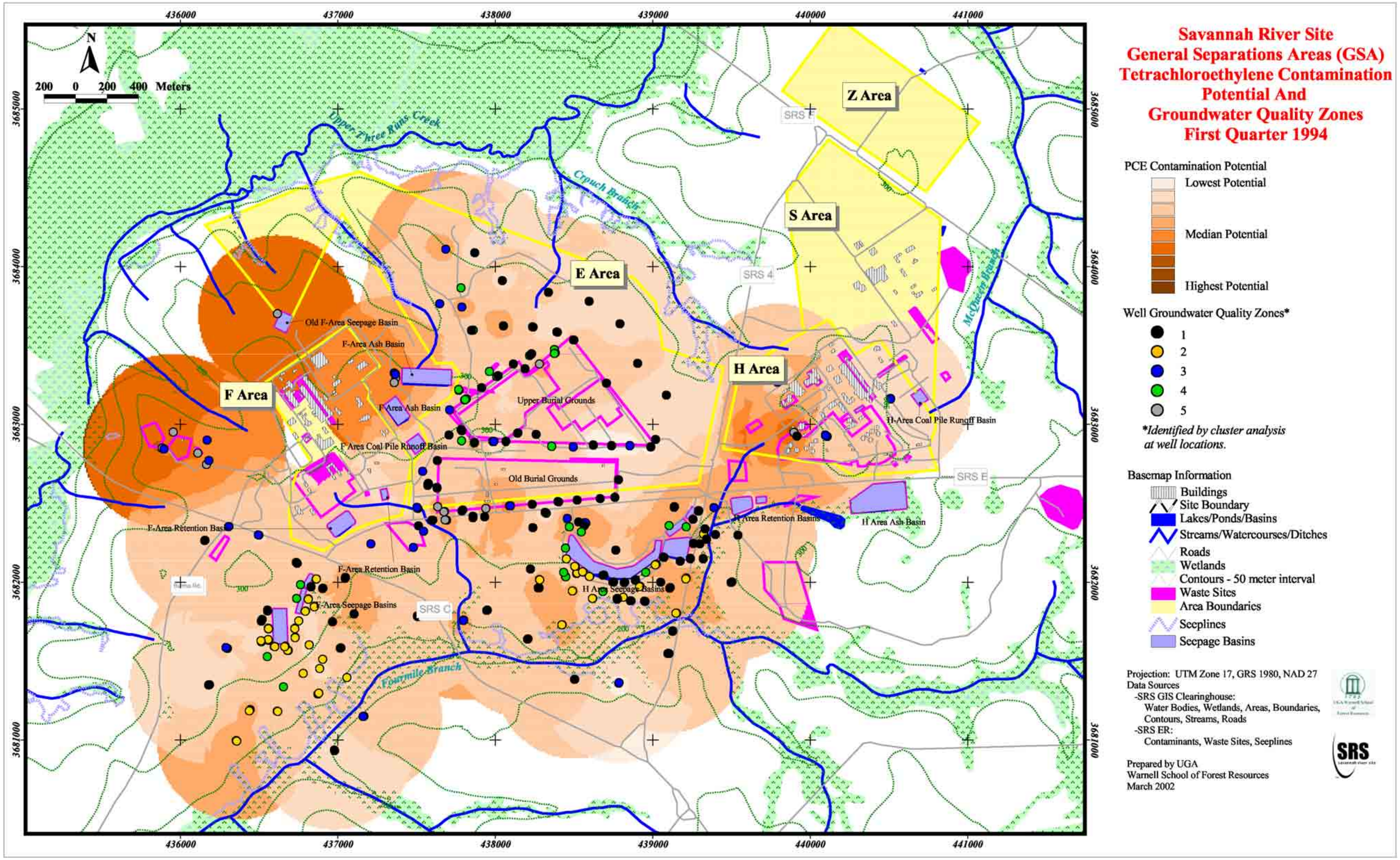


Figure 6.11: PCE Contamination Potential for First Quarter 1994 with Aquifer Zone Overlay, GSA.

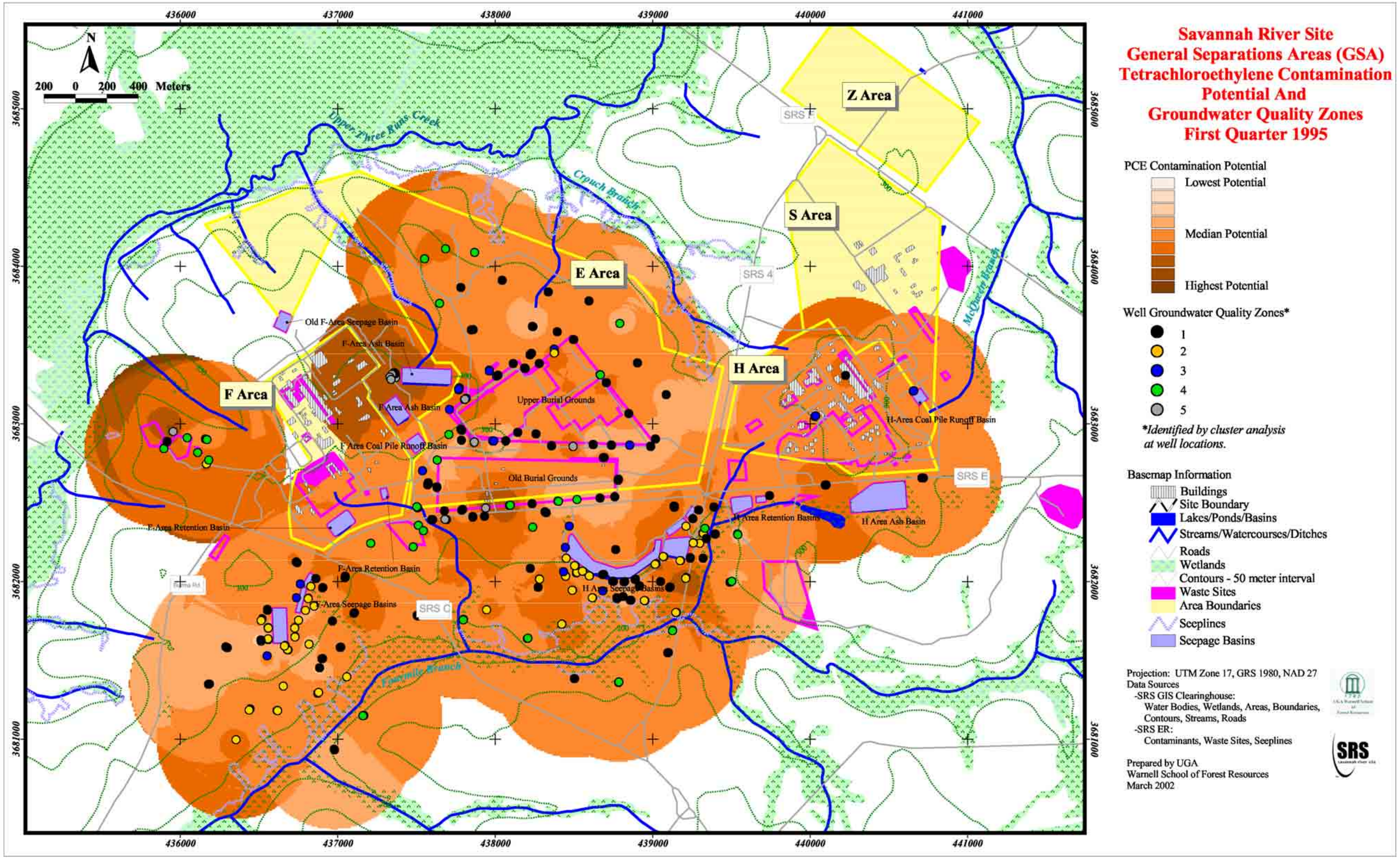


Figure 6.12: PCE Contamination Potential for First Quarter 1995 with Aquifer Zone Overlay, GSA.

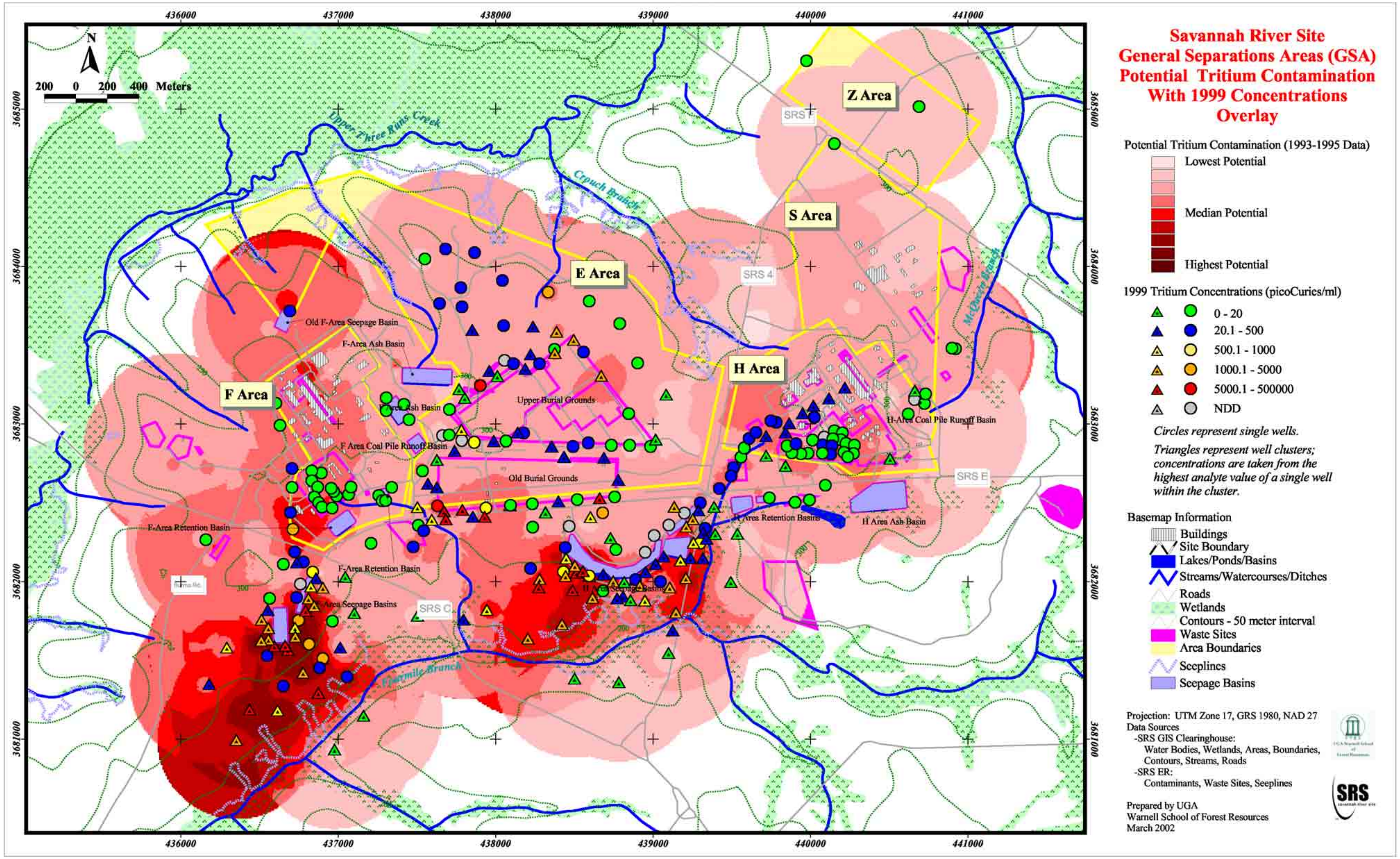


Figure 6.13: Tritium Contamination Potential for 1993-1995 with 1999 Tritium Concentrations Overlay, GSA.

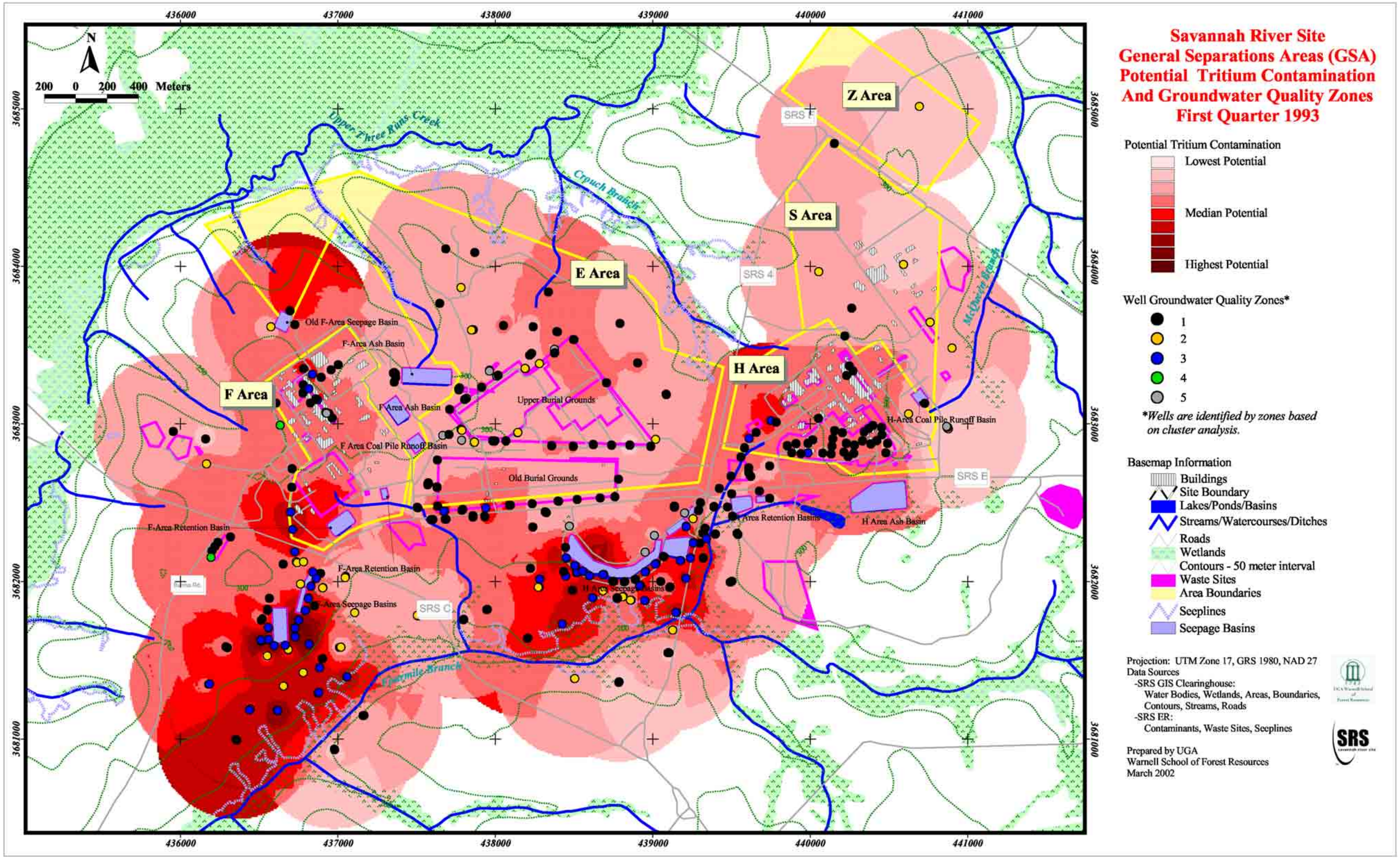


Figure 6.14: Tritium Contamination Potential for First Quarter 1993 with Aquifer Zone Overlay, GSA.

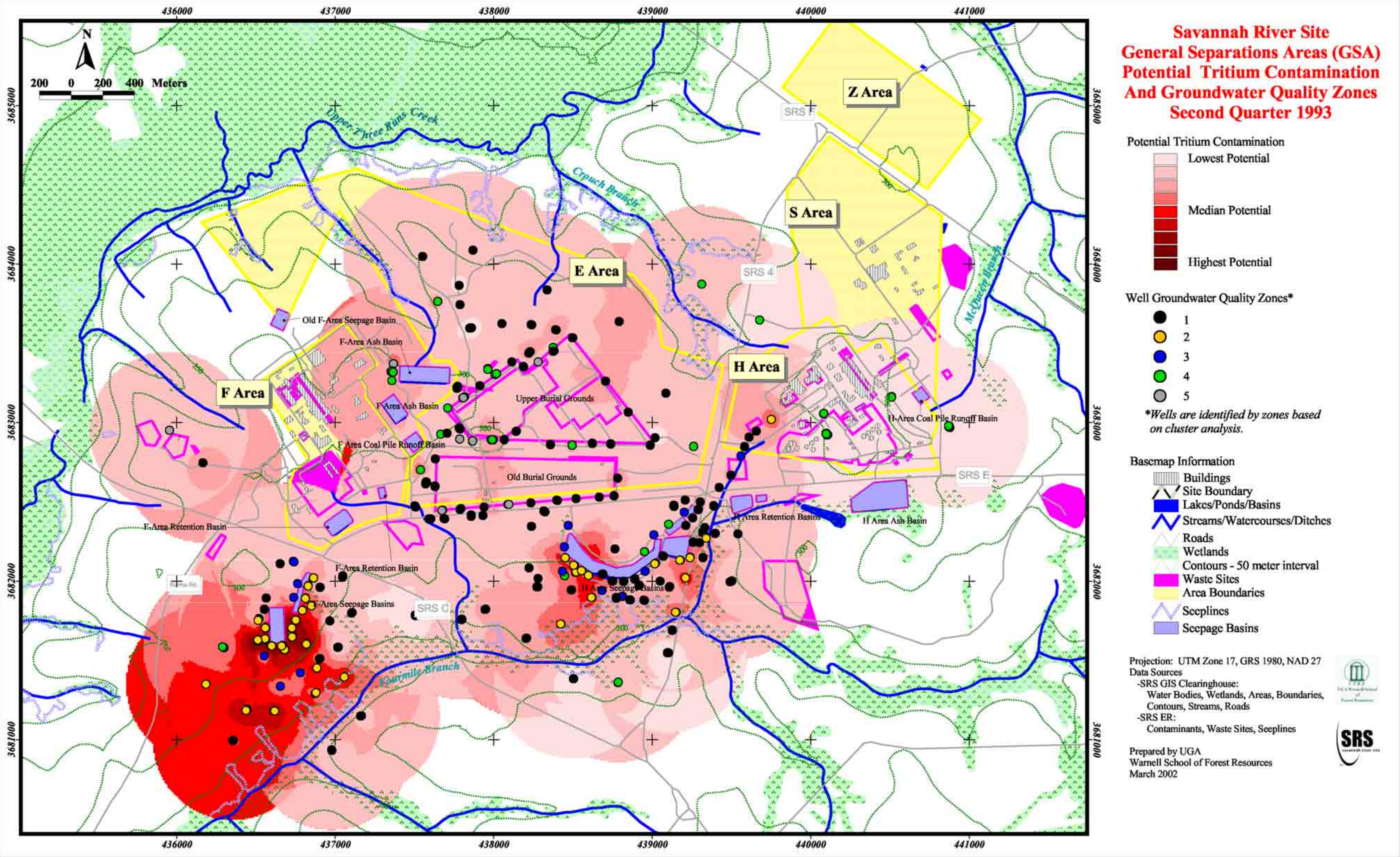


Figure 6.15: Tritium Contamination Potential for Second Quarter 1993 with Aquifer Zone Overlay, GSA.

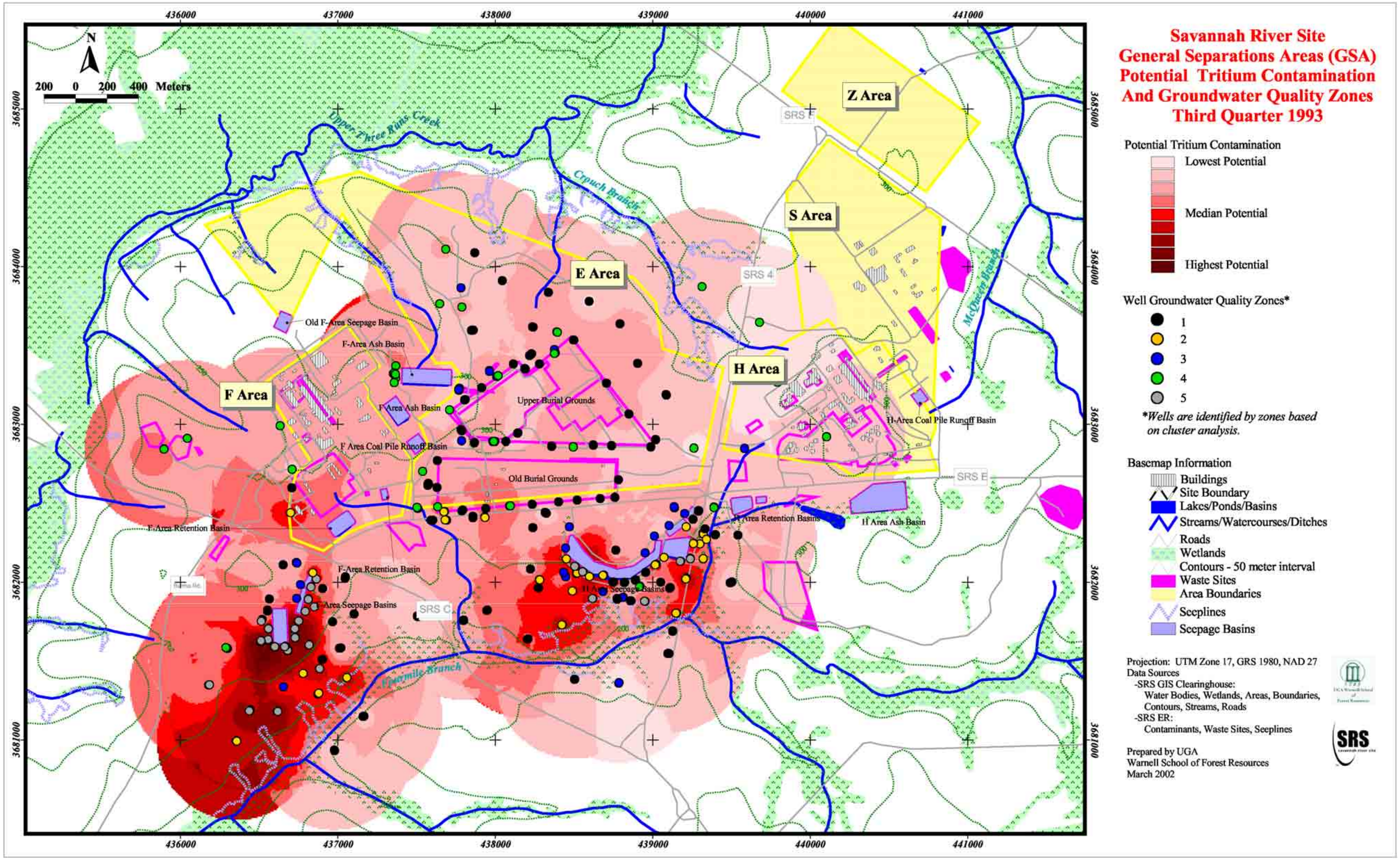


Figure 6.16: Tritium Contamination Potential for Third Quarter 1993 with Aquifer Zone Overlay, GSA.

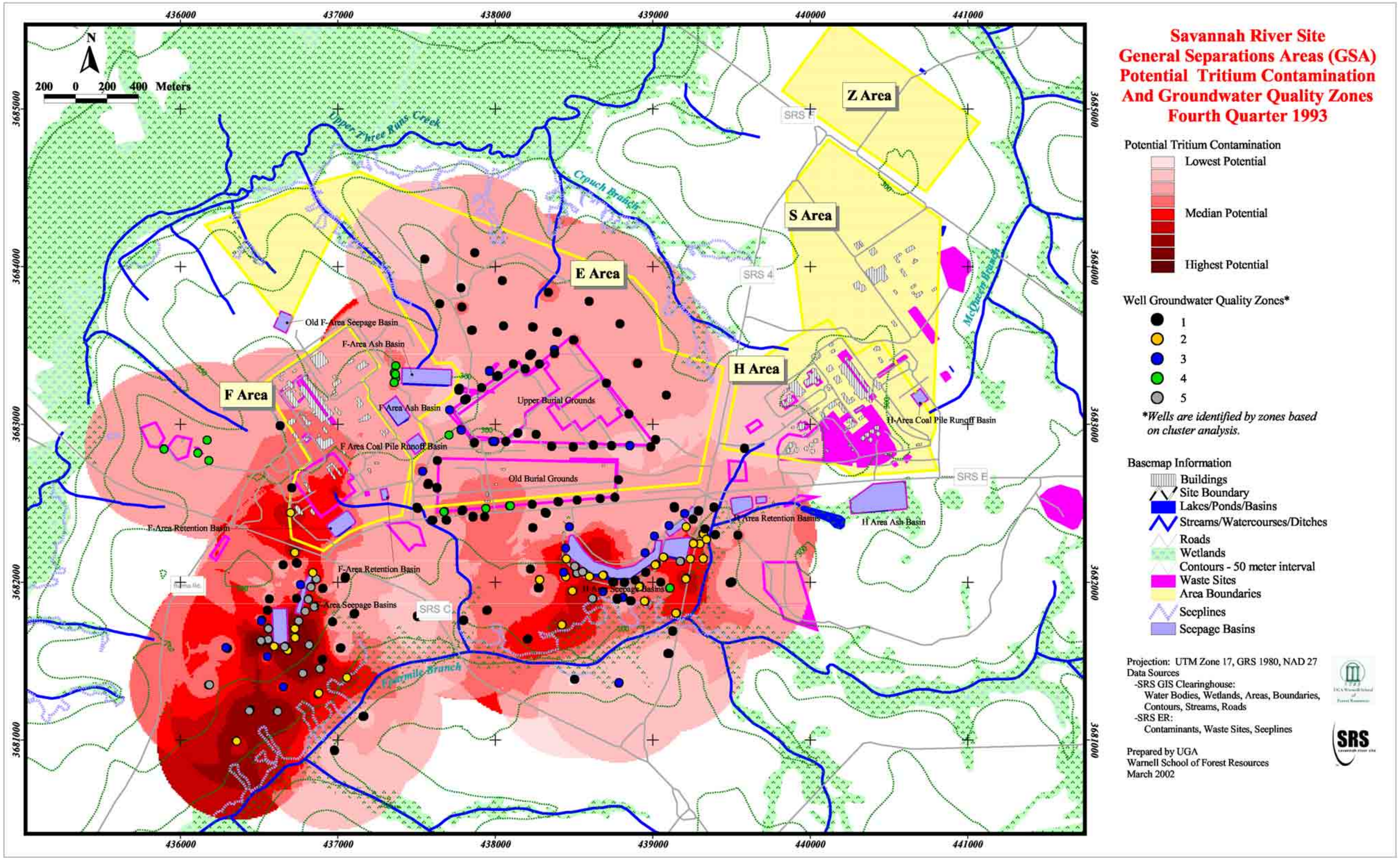


Figure 6.17: Tritium Contamination Potential for Fourth Quarter 1993 with Aquifer Zone Overlay, GSA.

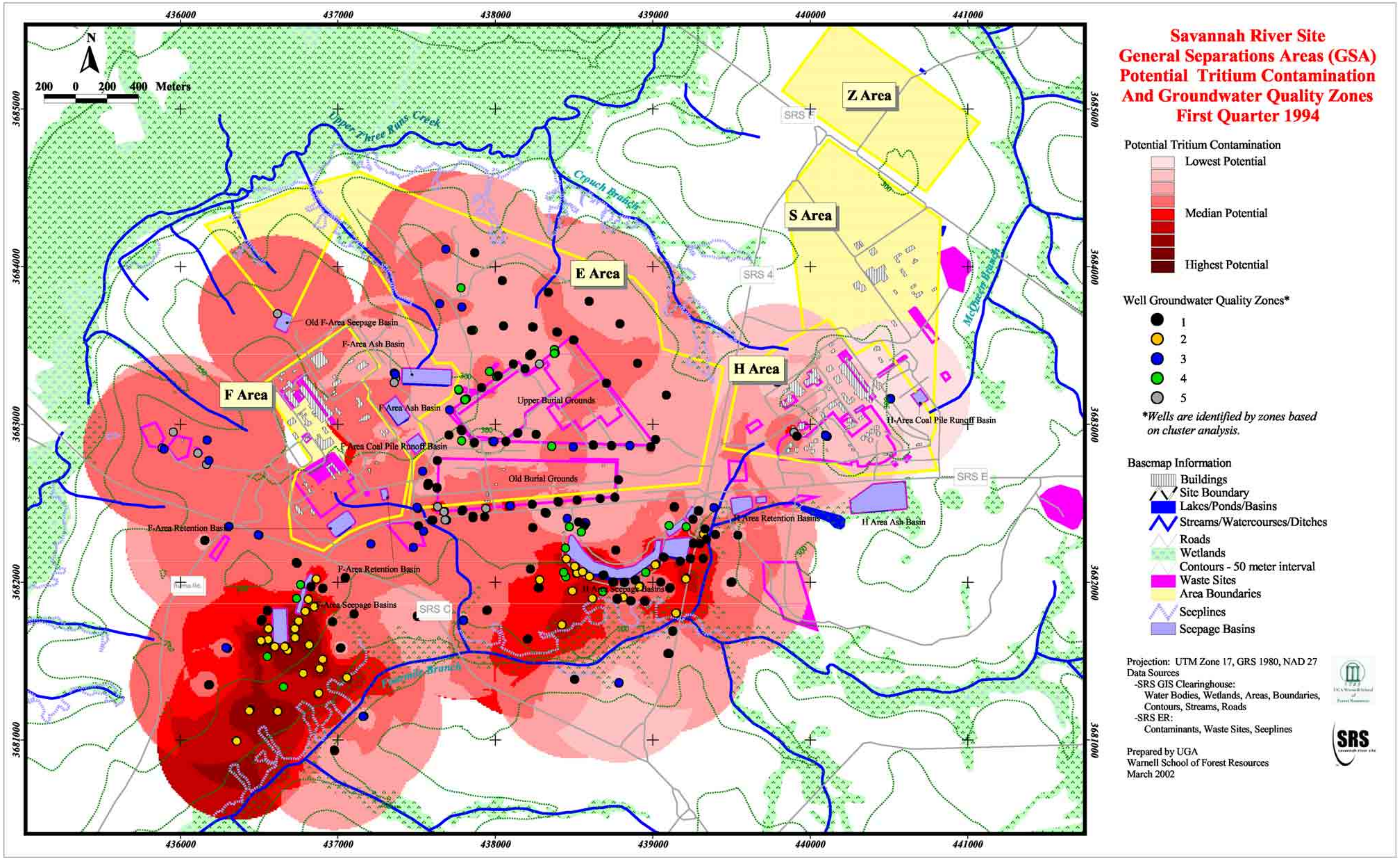


Figure 6.18: Tritium Contamination Potential for First Quarter 1994 with Aquifer Zone Overlay, GSA.

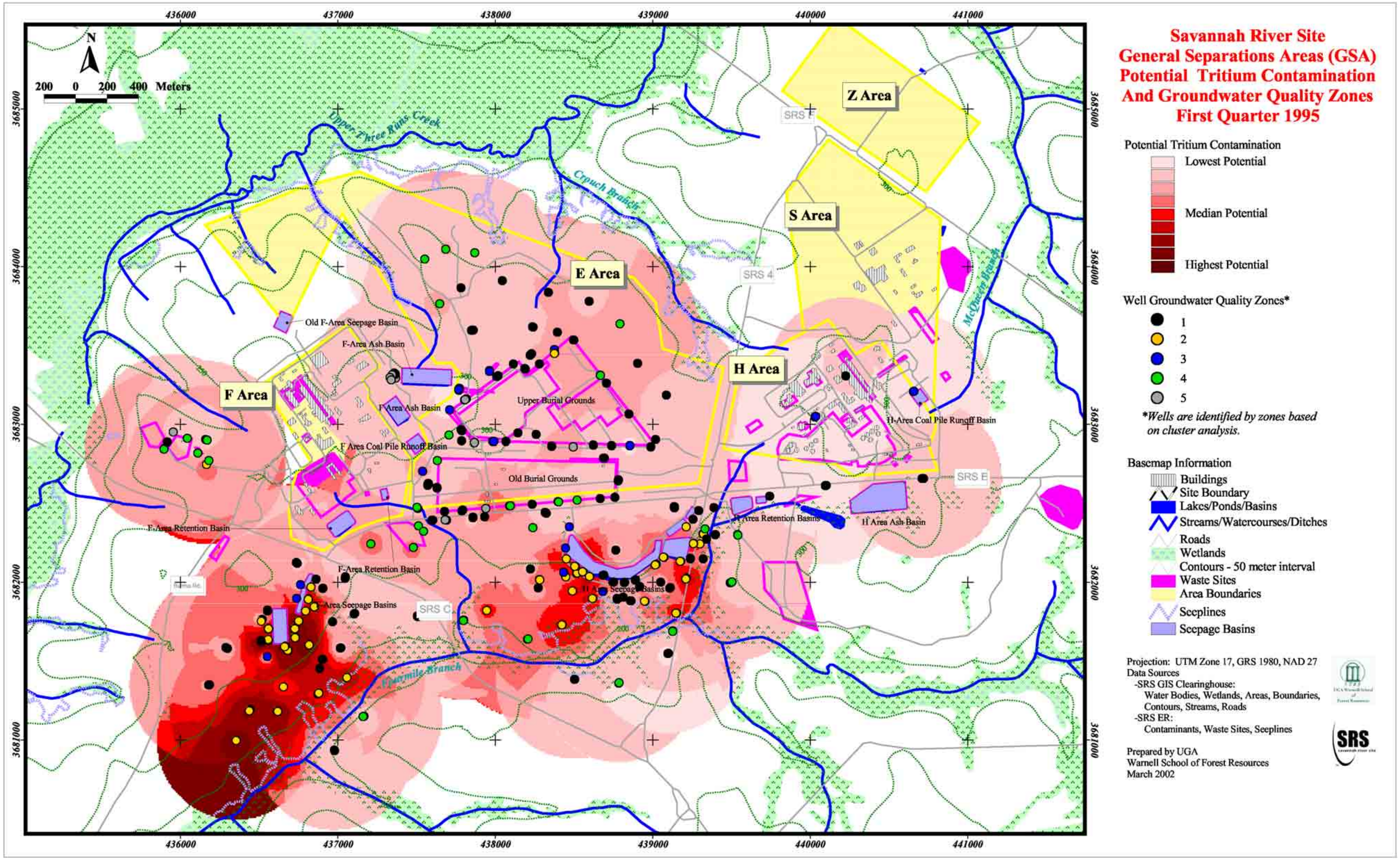


Figure 6.19: Tritium Contamination Potential for First Quarter 1995 with Aquifer Zone Overlay, GSA.

CHAPTER 7

SUMMARY AND CONCLUSIONS

Federal and state regulations mandate the characterization and remediation of groundwater contaminants released as the result of over 50 years of nuclear defense related materials production at the Savannah River Site. Ongoing efforts to describe the extent of contamination at SRS have been slowed by the complex hydrogeology of the Upper Atlantic Coastal Plain region. As part of these efforts, researchers have generated detailed hydrostratigraphic maps, and groundwater flow and contaminant transport models for portions of SRS. They also maintain and sample an extensive network of groundwater monitoring wells; observations are stored in a huge geochemical database, representing a wellspring of historical contaminant and groundwater quality information.

The research presented in this thesis is designed to increase the understanding of contaminant transport and groundwater flow at the Savannah River Site. The two methodologies described herein are completely built around contaminant and geochemical field observations. Our intent is to provide a foundation for future more detailed groundwater geochemical studies at the Savannah River Site.

First, we investigated and developed a methodology for mapping tritium and trichloroethylene contamination concentrations at monitoring well locations. We generated basemaps depicting 1999 contaminant concentrations for all of the facilities Areas at the Savannah River Site. The basemaps established the spatial extents, scales, and symbologies most appropriate for depicting groundwater characteristics in two dimensions. Tritium and trichloroethylene contaminant concentrations from 1999 were plotted on the basemaps and revealed that most contamination at SRS was limited to small portions of the site near reactors and disposal and manufacturing facilities. Trichloroethylene contamination was primarily located at the A/M area marked by metals fabrication and other industrial facilities. Tritium contamination was heaviest at the GSA, where industrial and radioactive materials were processed and wastes disposed. These basemaps were created to efficiently incorporate and represent future groundwater data.

Second, we developed a methodology for mapping groundwater contamination using the concept of aquifer water quality signatures. This methodology was comprised of two key statistical analyses of thirteen geochemical variables over six different quarters. For each quarter, we used a principal components analysis to group analyte and field parameter variables by four separate principal components. We identified the two components most highly correlated with the contaminant variables, tritium and tetrachloroethylene. We then interpolated and mapped factor scores for these two components to depict zones of contamination potential. As a partial validation for our methodology, contamination potential maps of 1993-1995 geochemical data compared favorably to contaminant concentration overlays from 1999.

We also performed a hierarchical cluster analysis on the factor scores from all four principal components. This cluster analysis separated monitoring wells by groundwater quality zone. A quarterly comparison of cluster analysis results revealed that cluster membership for some wells changed from one quarter to the next, perhaps indicating water from a shallow flow regime. Cluster membership for the majority of wells remained stable, suggesting that these wells were screened in deeper aquifer zones with less variable geochemistry. Further study is necessary to determine the sensitivity of cluster analysis to hydrostratigraphy.

In conclusion, the mapping methods described in this thesis provide a novel, yet practical approach to mapping groundwater geochemistry and contamination at SRS. Maps of tritium and trichloroethylene concentrations for 1999 show the extent of contamination at SRS. In addition, preliminary results suggest that PCA and cluster analysis can be used to infer zones of similar groundwater chemistry at SRS, and that our mapping methods merit a more intensive application.

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APPENDIX I

REPORT: MAP REPRESENTATION OF POINT CONTAMINANT DATA AT SRS

Introduction

In this appendix we describe methods for mapping analyte concentrations derived from the extensive quarterly ground water well monitoring program undertaken by workers at the Savannah River Site. Scripts and shapefiles were developed within an ArcView based Geographic Information System to produce ANSI D and E sized paper maps depicting tritium and trichloroethylene contamination at SRS Areas during 1999. These maps suggest that most contamination at SRS is located near production facilities and that outlying areas have groundwater with relatively low concentrations of tritium and trichloroethylene.

The Savannah River Site (SRS) has an established history of groundwater contamination resulting from almost 50 years of special nuclear materials production in support of the nation’s nuclear defense program (Bollinger, 1999). To comply with federal and state regulations, Department of Energy orders, Westinghouse Savannah River Company policies and procedures, and best management practices, groundwater from over 1000 wells across SRS is monitored for a large suite of radioactive and industrial contaminants. Data from this monitoring program have been stored in the extensive Geochemical Information Management System Database (GIMS) in tabular format. To better establish spatial relationships among analyte concentration data, an engineer at WSRC, Jim Bollinger, created an ArcView Geographic Information Systems (GIS) Interface to the GIMS Database in 1998 (Bollinger, 1999). The ArcView Interface to GIMS generates geospatially referenced layers of specific analyte concentrations for groundwater monitoring wells across SRS (Bollinger, 1999).

The work described in this appendix utilizes GIS analyte layers from the ArcView Interface to GIMS as well as GIS coverages of SRS infrastructure and natural features to explore the best possible methods for displaying complex information regarding groundwater contamination at the Savannah River Site. This work is intended to aid in the interpretation of GIMS analyte data and provide a basic foundation for generating a historical record of ground water quality at SRS. A key requirement of this project was the utilization of readily available software and computer resources to reduce expenses and training time for future groundwater mapping efforts at SRS. Using the popular ArcView GIS Software Package version 3.2 on Windows NT-based computers, we produced digital and paper format maps for 1999 analyte concentrations of tritium and trichloroethylene covering all SRS areas.

During this project we studied methods for representing data from different hydrostratigraphic units, both as single point, color-coded map features and as contours. However, given the complex hydrostratigraphy at SRS and ArcView's limited interpolation options, the maps produced for this project lump concentration information for all hydrostratigraphic units. Stemming from this experimentation, a simple, direct method for displaying data in bivariate fashion at single point locations is outlined here. We also generated scripts in ArcView's Avenue language for calculating quarterly changes in analyte concentrations, and for the effective display of closely grouped wells on paper maps. This project establishes the sizes, scales, and aerial extents of basemaps that best communicate levels of contamination for different areas at SRS. Groundwater concentration levels of two of the most reliably measured analytes, tritium and trichloroethylene, were mapped for year 1999 sampling quarters and show the approximate areal extent of contamination at SRS. These maps are intended to be used as basemaps for the display of analyte concentrations from other time periods.

Exploration of Map Display Options

We explored several methods for mapping analyte data produced by the ArcView Interface to GIMS. At first, interpolation between analyte values from wells located within a specific aquifer unit seemed the best way to represent contamination levels for portions of the site where no wells exist. We experimented with ArcView's built in interpolation functions, including Spline, Inverse Distance Weighting, and also a third-party Kriging function. Given the high range in values of the analyte data and the relatively low density of the data points, we were unable to generate satisfactory interpolation/contouring results that could be validated by existing knowledge of the site's complex hydrostratigraphy. In addition, well-to-aquifer relationships at SRS are inferred from a stratigraphic model in many locations; creating contours based on analyte measurements is an inexact science at best (Bollinger, 1999).

We also attempted to graphically map changes in analyte concentrations from one quarter to the next using ArcView point shapefiles generated by the ArcView GIMS interface. To represent these changes we imported the tables for shapefiles from two different quarters (we discovered that the most analytes are measured only twice a year) into a Microsoft Excel spreadsheet. We then matched the well names from each of the two imported tables and subtracted corresponding analyte values. We exported the new table containing subtracted analyte values back to ArcView for display purposes. We used a bivariate legend for each well point location—each point was color-coded (red, yellow, green) based on the relative change from one quarter to the next and then the same point was sized relative to all concentrations mapped. Such maps represent both yearly changes in and the magnitude of the analyte concentration at each well location measured. Because this exercise proved to be labor intensive, we learned the ArcView Avenue scripting language, an object oriented code similar to C. Using Avenue, we wrote scripts that automated the process of formatting and subtracting quarterly analyte values for map display.

Method for Bivariate Display in ArcView

For representing historical changes in groundwater contamination at SRS, a bivariate legend is particularly appropriate because it allows each point location on a map to represent two different variables, in a clear, uncluttered fashion. Each ground water monitoring well is mapped, and concentrations of specific analytes are represented by dots colored according to regulatory compliance (i.e., red for points above safety limits, yellow for points very close to limits, and green for points well below limits). The second variable, change in concentration from the previous quarter, is then represented by the size of each dot. While ArcView does not support bivariate legends ‘out of the box,’ add on scripts implement this functionality. The scripts included with this report allow use of a bivariate legend (“wells.bivariate_legend”).

The “wells.bivariate_legend” script allows the user to specify a field to be symbolized based on a color scheme and a second field to be symbolized based on graduated size. The script then generates a legend for the shapefile representing each possible color scheme/size range combination. The drawback to this method is that the resulting legend is quite complex and difficult to fit onto a paper map. This method is most useful for working within ArcView View documents to locate heavily contaminated wells that exhibit large changes in analyte concentration over time.

As an alternative, a very simple ‘scriptless’ procedure for creating a bivariate legend is to place two of the same point shapefiles on top of one another. Each point in the bottom shapefile must be larger than the largest point in the shapefile on top. In this manner, the bottom shapefile can be colored to represent regulatory compliance, while the top shapefile can cover a range of sizes based on historical changes. The steps for this procedure in ArcView are as follows:

1. Copy and then paste the shapefile theme containing a two variable table into the view.
2. Using the Theme→Properties menu, rename the two themes according to the variables each will represent.
3. For the theme that will remain on the bottom, choose a field and represent it with a color

coded legend from the Legend Editor pop-up window. Set a relatively large size for the points using the Marker Palette box (shift-click to select more than one classified point).

4. Again, from the Marker Palette box, classify the values for the theme that will remain on top using either a size range or a second color scheme. If a size range is used, be sure that the largest possible point will not obscure the underlying theme.

Some experimentation with point sizes is necessary, depending on the size and scale of the paper maps desired. For the example in Figure A1 we used a point size of 24 for the circles representing absolute concentrations (the graduated color legend was supplied by John Reed, WSRC). The range in point sizes for the graduated triangles is 4 to 18. We have found that these point sizes are well-suited to large-scale maps (approximately 1:8,000 to 1:12,000).

Installing the ArcView Extensions and Projects

The scripts written for this project are supplied on the accompanying data CD. The following steps outline the installation of the ArcView extensions containing these scripts. Install the extensions located in the *srs-mapping/Install these Extensions* subdirectory:

1. Copy the two extensions ‘Extents.avx’ and ‘wells.avx’.
2. Paste them into the *c:\esri\av_gis30\arcview\ext32* directory.
3. Open the ArcView application, and then create a new Project.
4. Under the File-->Extensions menu, select the "Named Extents" and the "SRS Well Data Tools" extensions.

With the extensions installed, import the project files located in the Projects subdirectory to the new file system:

If you have access to your C Drive you can simply copy the entire *srs-mapping* folder (minus the large *extras* subdirectory) directly into your *c:* directory and skip the import steps outlined below.

Otherwise:

1. Copy all the shapefiles in the *gisdata* subdirectory into a new local directory on your machine. Write down the path to this directory.
2. From a new View, find the Well Data Tools menu, and select the 'Change Paths for ArcView Projects' option.
3. Browse to the Projects subdirectory on this CD and select any or all of the ArcView project files you want to import.
4. Enter the pathname of the directory where you want to save your imported project files.
5. Enter the new pathname where all themes for the project are stored on your file system (See Step 1). For example, if you would like to save your GIS shapefiles in a directory called *\srs-mapping\gisdata* on the C drive, enter:

   c:\srs-mapping\gisdata

   Remember not to forget the final backslash, as it is required by the script.
6. Allow the script to run--it may take up to an hour if selected several projects need to be imported.

Open the newly imported projects from your local directory.

Tools for Calculating Differences Among Analyte Sampling Events

To show quarterly changes in groundwater contamination at SRS, we developed a series of tools to format shapefile data from the ArcView GIMS interface. These tools are packaged as an extension, and can be installed by following the directions in the next section of this appendix. From the ArcView application the tools can be accessed either through the View→Well Data Tools menu or through an iconic tool located in the View menu bar (Figure A2). The tools were written using the ArcView version 3.2 Avenue scripting language.

With these tools the user can compile several single quarter shapefiles containing analyte values into one multi-quarter shapefile (“wells.compileFields”). Users can click on the point locations for wells from these compiled shapefiles to bring up a bar-graph history of contamination (“wells.histogram”). The tools also calculate differences between analyte measurements from quarter to quarter(“wells.calcChanges”). Finally, the tools provide access to the bivariate legend functionality described in the previous section (“wells.bivariate_legend”). Table A1 summarizes the function and scripting for all the tools described in this report.

To familiarize users with these tools, a sample ArcView tutorial session is described below:

1. Open the ArcView 3.2 application and choose to start working on a new Project.

2. Load all of the shapefiles located in the *\srs-mapping\Tutorial* folder into a new View. These shapefiles were created by the ArcView Interface to GIMS and contain sitewide tritium concentrations for single quarters in 1998 and 1999. Most of the Well Data Tools will only work with files generated by the ArcView Interface.

3. Install the *wells.avx* ArcView extension if you have not already done so. (This procedure is outlined in the “Installing the ArcView Extensions and Projects” section of this appendix.)

4. From the Well Data Tools Menu, choose “1. Select Type of Concentration Data” and specify the field you want to use to summarize concentration data. For this exercise, choose “*U_max_res*”.

5. Again from the Well Data Tools Menu, choose “2. Compile Concentration Fields”. Select the shapefiles containing the analyte concentration data you want to tabulate into a single shapefile. For this example, select all of the shapefiles. Specify a name and location for the output shapefile, *test.shp*, for example.

6. Load the shapefile you just generated into the view and make it active. Click on the Tables icon in the View Document to examine the table for this theme. Note that data from each of the parent shapefiles is tabulated in corresponding fields by year and quarter.

7. Return to the View and zoom in two or three times on any group of wells. Click on the Chart Concentration History icon and then use its arrow pointer to select a well. A chart of the concentration history by quarter for that well will appear. Click on other wells to examine their concentration histories. Note that some wells may not have been monitored during certain quarters.

8. Make the View active again and from the “Well Data Tools” menu select the “3. Calculate Concentration Changes” option. Click on Yes, and load the shapefile containing the compiled concentration fields (*test.shp)*. The script will run and generate a new theme called *Conc-Change <Filename>*. Examine the table for this theme. Analyte values from each quarter have been subtracted from the values for the next subsequent quarter. Negative values indicate that a concentration decreased from the previous quarter and positive values indicate an increase. Blank values are present when no measurements were taken for a well in a particular quarter.

9. With the *Conc-Change <filename>* theme active select the “4. Symbolize Concentrations and Changes” option to generate a bivariate legend to display a quarterly change and the current concentration simultaneously. Choose the *Y99q4-99q2* field to display in color and the *Y99q4* field to display in graduated size. Specify a color ramp and a size range. The script will create a new legend for the theme based on these two fields.

Because the analyte measurements have a very high range of results, colors and sizes of points are difficult to distinguish, particularly when displaying data from the entire site. This method of bivariate mapping is more useful when analyte values are normally distributed and are examined in smaller groups within a single aquifer. The application here is more suited to singling out wells exhibiting relatively extreme levels of contamination and sharp changes through time. The source code for all scripts described in this section can be examined in the *srs-mapping/Projects/wells.apr* ArcView Project file located on the CD.

4.6 Script for Grouping Well Clusters

When mapping SRS analyte values at any scales smaller than 1:2000, point graphics that represent closely spaced well locations begin to overlap. Many wells at SRS are installed as part of clusters drilled to varying depths; often wells within these clusters are spaced only a few meters apart. In order to represent tightly clustered wells on smaller scale maps without overlap, we developed a procedure to group wells located within a user-specified radius. The highest analyte value recorded for a given quarter within each group of wells is attributed to the entire group, ensuring that higher value analyte measurements are not obscured by overlying point graphics representing lower measurements (Figure A3). This procedure is automated as a script, “wells.findclusters” that adds grouping information to the attribute table of a shapefile generated by the ArcView Interface to GIMS.

GIS Coverages for Infrastructure and Natural Features

Many of the GIS layers we used to represent infrastructure and natural features for SRS are distributed by the SRS GIS Data Clearinghouse, freely available at the internet address: http://www.srs.gov. Other data sources include the State of South Carolina GIS Data Clearinghouse, and national data packaged by ESRI with ArcView. Appendix II describes each coverage we used during the mapping process, and any modifications we performed.
Most shapefiles used in this project are in the Universal Transverse Mercator Projection, Spheroid GRS1980, Datum NAD 27, Zone 17. Units for these coverages are meters. The locator maps

depicting the Southeast were generated using ESRI's prepackaged national shapefiles, projected in Decimal Degrees. Appendix I also describes the projection information and source of each coverage.

For many shapefiles the changes were minor; we simply clipped the coverages to the boundaries of SRS. A few shapefiles required more extensive manipulations. Topographic contours for SRS were only available in 10 meter interval format *(contours-clip.shp)*. To improve map readability, we reduced these contours to 50 meter intervals, first by importing the shapefile coverage into ESRI's Arc/Info GIS package and then by generating a Grid-based digital elevation model using the 'topogrid' command. We exported this model back into ArcView format where we created the 50 meter topographic contour shapefile (*srscont50m.shp*) with the View→Surface→Create Contours option available as part of ESRI's Spatial Analyst Extension. To create the shapefile containing the extents of each area visible on paper maps (*extent.shp*) we wrote an Avenue script that converted the visible extent from each ArcView Layout Document into a polygon appended to the *extent.shp* file.

Map Products

Using the methods, scripts, and coverages described in the preceding sections, we developed paper maps for the Savannah River Site. These maps are intended for use as a base to display other analyte concentrations. To demonstrate the utility of these basemaps, we used 1999 concentration data for tritium and trichloroethlyene concentrations to generate two layouts for each area at SRS for a total of 20 maps. The maps are saved in Adobe Acrobat PDF format on the CD prepared for this report and can be viewed electronically or reprinted to any desired paper size (note that map scales change when maps are enlarged or reduced). Table A2 provides a listing of maps, areas covered, and corresponding ArcView project and PDF files.

To create the basemaps we first built View documents in ArcView Projects by loading in the aforementioned shapefiles of infrastructure and natural features. We then loaded in shapefiles containing analyte values for each quarter in 1999. We used the Find Clusters Tool described above to group wells located within a 20 meter radius of one another. Wells grouped together were represented by triangles, while ‘neighborless’ wells were symbolized by dots. The analyte measurements for both tritium and trichloroethlyene were displayed with colored legends supplied by John Reed. Figure A4 depicts these two legends.

Because quarterly analyte measurements were sparse for most areas, we chose to display all four 1999 quarters on the same maps. Thus, the maps provide more of a yearly perspective on tritium and trichloroethylene concentrations in ground water at SRS. We labeled selected features from shapefiles in the View, including roads, contour intervals, waste site names, streams, and lakes. Most of this work was performed by hand because ArcView’s automated labeling option often overlapped labels or obscured analyte points.

We then created Layout documents based on these views. For each Layout document we first specified the layout size as either ANSI D (22 inches by 34 inches) or ANSI E (34 inches by 44 inches) allowing 0.5 inches for top, bottom, left, and right margins. We filled each empty layout with information from a View and specified an appropriate scale. Finding a scale to represent each area was a trial and error process, and we often switched from the Layout documents back to the View documents in order to properly position the visible area in the View. Once we arrived at a satisfactory extent in the View that afforded the maximum visible area on a paper layout, we used the third-party *Saved Extents* add-on extension (*extents.avx*) to save the extent of the View. Thus when repositioning or rescaling the view for labeling or other purposes, we would not lose the best extent for printing from the layout documents. We also saved the layout extents to the shapefile (*extents.shp)*.

Legends for each map were first generated by ArcView’s Layout Legend Tool and then heavily modified to provide effective, meaningful map keys. Two legends and title bars were developed for each Project File—one for trichloroethylene and one for tritium. In each Layout, the ‘extra’ legend/title bar group is stored in the white space beside the full map. Instead of having to repeat the entire process of legend creation, users can simply swap out legend/title bars when building new maps for the same SRS Areas.

Universal Transverse Mercator grids were overlayed on each Layout using ESRI's *Grids and Graticules* extension. We also fitted neatlines around legend-title bar groups as well as around the entire layout.

Finally, we rendered each layout using ESRI's *ArcPress* extension for printing on a Hewlett Packard 755CM inkjet plotter. *ArcPress* was used to rasterize each layout using desktop computer resources because the map sizes were too large for the HP 755CM to convert Postscript information directly.

Conclusions

The procedures and files outlined in this appendix should facilitate the creation of maps to aid in the historical interpretation of ground water quality data at SRS. The maps produced for this project effectively depict 1999 tritium and trichloroethlyene concentrations at well locations across the SRS. They suggest that contamination is limited to locations immediately surrounding SRS facilities involved in the production and disposal of nuclear and industrial materials, the General Separations Area and the Administrative and Manufacturing Area. In contrast to the contaminated ground water in these areas, the maps clearly show levels of contamination below State and Federal standards for wells in outlying areas.

While the point-based maps produced for this project can effectively communicate general trends in contamination at SRS, a method for interpolating analyte concentrations between wells still needs to be developed. Expert contouring of concentration levels by hand is a time-consuming process that requires a thorough knowledge of the SRS hydrogeology. Such contouring may be automated if wells can be reliably matched with aquifers and their flow directions.

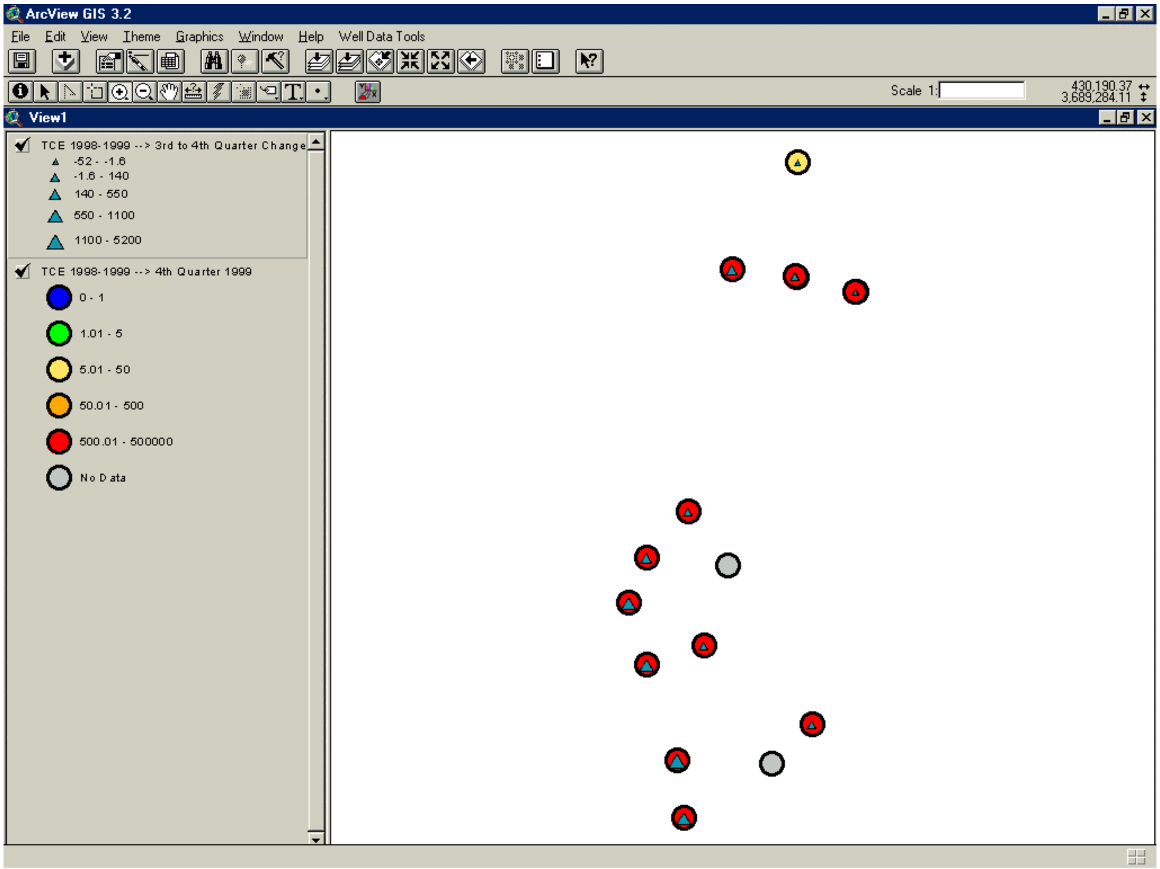

Figure A1: Scriptless method for creating a bivariate legend. The two themes loaded into ArcView View document are identical; data from two different fields are represented on the map. Graduated size triangles depicting changes over a quarter are overlaid atop circles representing the absolute concentration of trichloroethylene for the fourth quarter, 1999.

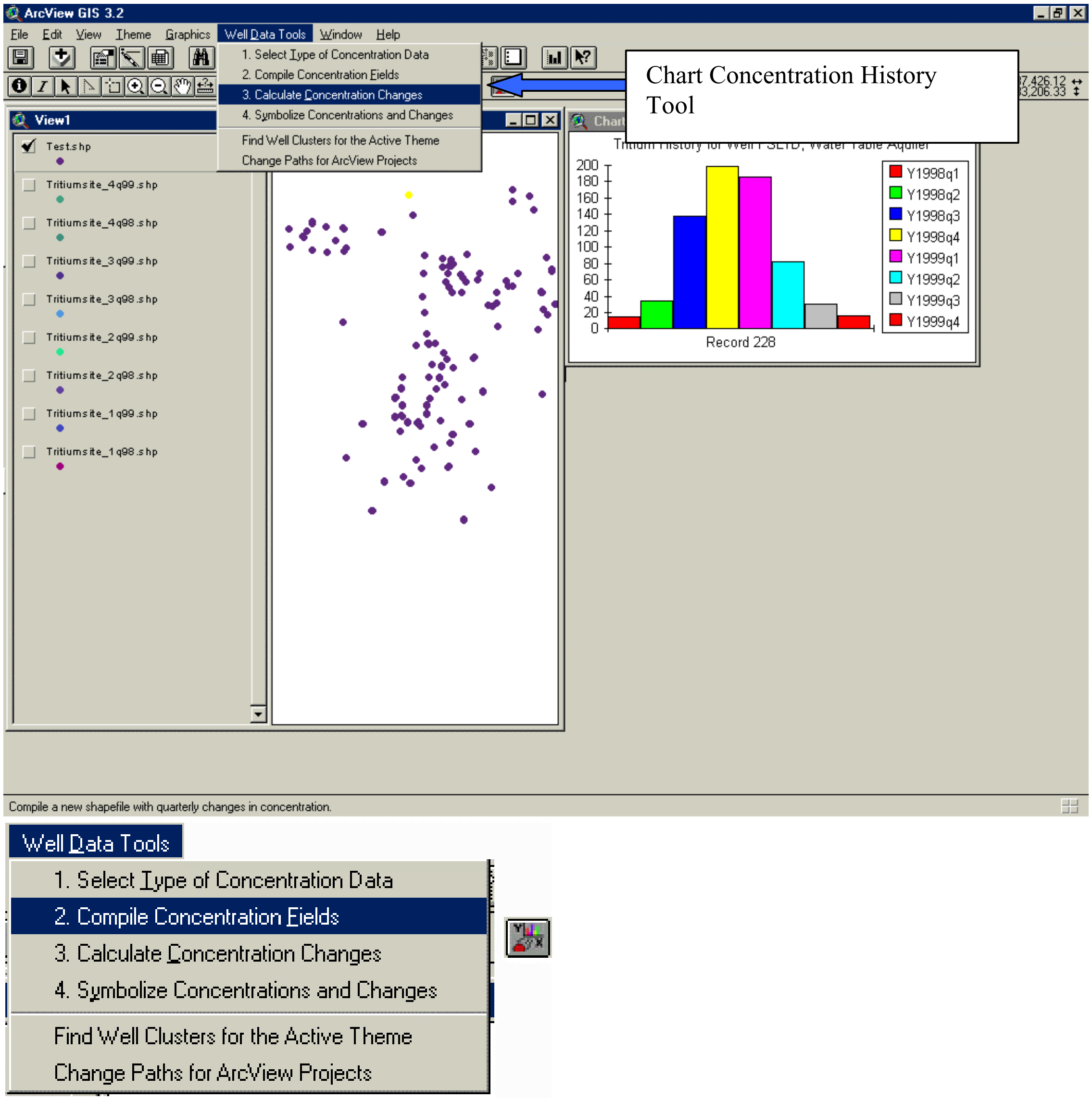

Chart Concentration History Tool

Compile a new shapefile with quarterly changes in concentration.

Figure A2: Screenshot and Zoomed View of Well Data Tools including Bar Chart of Tritium History for 1998-1999.

Tool Name	Script Name	Access	Function
1. Select Type of Concentration Data	wells.SelFields	View→Wells Menu	Allows the user to select which field should be used for analyte values.
2.Compile Concentration Data	wells.CompileFields	"	Places fields from several single quarter analyte shapefiles into a single new shapefile.
3.Calculate Concentration Changes	wells.calcChanges	"	Subtracts analyte values from subsequent quarters. Operates on output from the wells.CompileFields script.
4.Symbolize Concentrations and Changes	wells.bivariate_legend	"	Allows the user to display two different variables at the same point location (size and color).
Find Well Clusters for the Active Theme	wells.findClusters	"	Groups wells by a user-specified radius to a single point and attributes it with the highest analyte value in the group.
Change Paths for ArcView Projects	wells.ChangePaths	"	Ports multiple ArcView projects to other file systems.
Chart Concentration History	wells.histogram	View→Tool Icon	Allows the user to click on a well to display analyte concentration history as a bar chart. Requires a shapefile generated by the Compile Concentration Data tool.

Table A1: Summary of Well Data Tools developed for mapping ground water contamination at SRS.

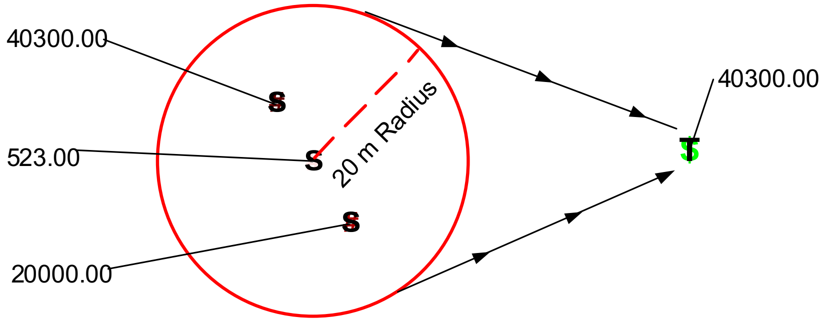

Figure A3: Procedure for grouping wells. The points representing wells (shaded red circles) will be too close together for mapping at small scales. They are grouped together as a single point (green triangle) and the single point is attributed with the highest analyte value recorded in the group.

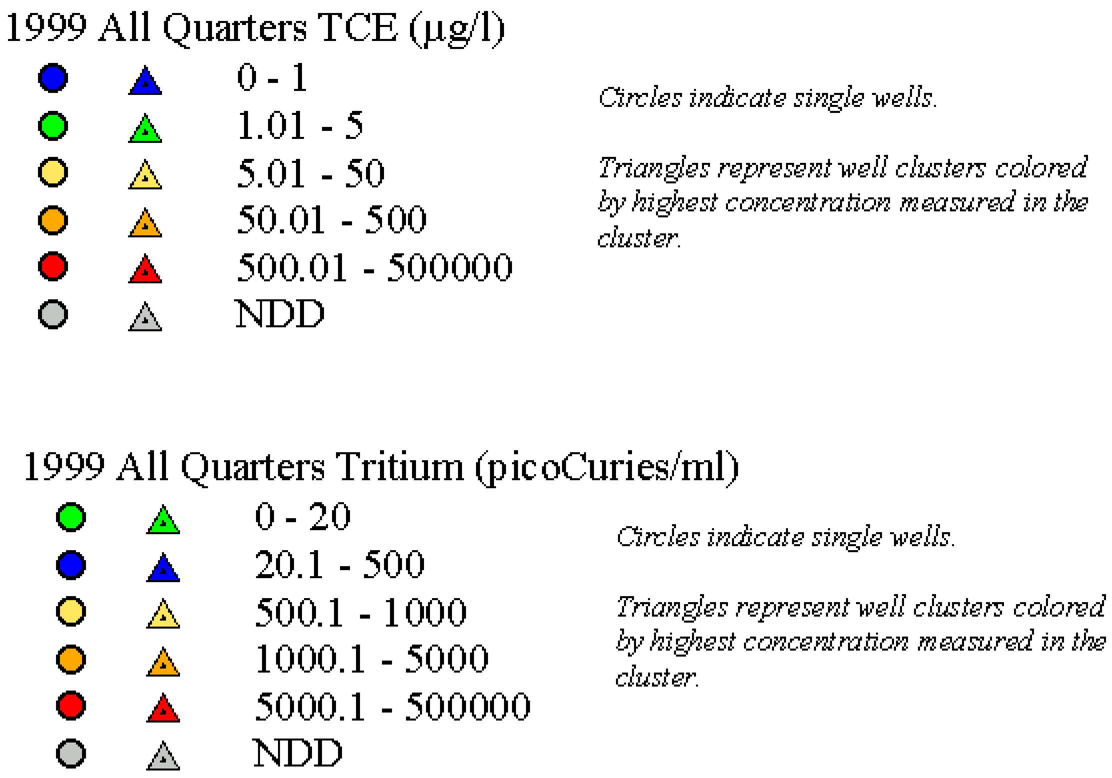

Figure A4: Standard Legends used for the display of trichloroethylene and tritium concentrations. The ranges and color schemes for these legends were supplied by John Reed, WSRC.

SRS Area	Project File	Map Size	Scale	Area (hectares)	PDF Files
Entire Site	*basemap.apr*	E: 34" X 44"	1:50000	80341	*basemap.pdf*
AM Area	*am_areas.apr*	D: 22" X 34"	1:12000	4227	*AMallQ99TCE.pdf,* *AMallQ99Trit.pdf*
B Area and Landfill	*b_landfill.apr*	D: 22" X 34"	1:12000	4227	*BallQ99trit.pdf,* *BallQ99tce.pdf*
C Reactor and N Area	*centralshops.apr*	D: 22" X 34"	1:8000	2060	*CNallQ99TCE.pdf,* *CNallQ99Trit.pdf*
DTX Area	*dtx.apr*	D: 22" X 34"	1:12000	4636	*DTXallQ99TCE.pdf,* *DTXallQ99Trir.pdf*
General Separations Area	*gsa.apr*	D: 22" X 34"	1:10000	3219	*GSAallQ99TCE.pdf,* *GSAallQ99trit.pdf*
K Reactor	*k_reactor.apr*	D: 22" X 34"	1:8000	2060	*KRallQ99tce.pdf,* *KRallQ99trit.pdf*
P Reactor	*p_reactor.apr*	D: 22" X 34"	1:8000	2060	*PRallQ99tce.pdf,* *PRallQ99trit.pdf*
R Reactor and Par Pond	*r_reactor.apr*	D: 22" X 34"	1:18000	10431	*RPARallQ99tce.pdf,* *RPARallQ99trit.pdf*
L Reactor	*l_reactor.apr*	D: 22" X 34"	1:8000	2060	*LRallQ99tce.pdf,* *LRallQ99trit.pdf*

Table A2: SRS Areas, Associated ArcView Project files, and Map information

APPENDIX II

GIS COVERAGES FOR SAVANNAH RIVER SITE BASEMAPS

Key to Codes for Projections:

Projection 1
Universal Transverse Mercator
Zone: 17
Spheroid: GRS 1980
North American Datum 1927
Units: Meters

Projection 2/Coordinate System
Decimal Degrees

Key to Codes for Sources:

1 = SRS GIS Data Clearinghouse
2 = Modified SRS GIS Data Clearinghouse Shapefile
3 = Generated by ArcView Interface to the GIMS Database
4 = Modified ArcView Interface to GIMS Database Shapefile
5 = ESRI Shapefile
6 = Modified ESRI Shapefile
7 = SRS ER
8 = Hand Digitized by John Reed, SRS
9 = Compiled by Jim Bollinger, SRS
10 = Silas Mathes, UGA School of Forestry
11 = State of South Carolina GIS Data Clearinghouse
12 = Modified State of South Carolina GIS Data Clearinghouse

Shapefile	Projection Code	Creator Code	Date Created	Description/Function:
allsecitiesutm.shp	1	6	1/11/2001	Point Shapefile of Southeastern Cities/Used for locator map.
Areas.shp	1	1	4/6/2000	Polygon Shapefile of Areas at SRS/Used to show the extents of Areas at SRS.
Basins.shp	1	2	8/7/2000	Polygon Shapefile Derived from waterbodies.shp/Used to show seepage basins.
Bldgs-clip.shp	1	2	8/1/2000	Polygon Shapefile of SRS Buildings clipped to the site boundaries.
boundline.shp	1	2	7/28/2000	PolyLine Shapefile of SRS Boundary without rail right of way.
Bounds2.shp	1	2	7/27/2000	Polygon Shapefile of SRS Boundary without rail right of way.
Bounds-clip.shp	1	2	6/13/2000	Polygon Shapefile of SRS Boundary with rail right of way.
Buildngs.shp	1	1	4/17/1997	Polygon Shapefile of all Buildings in SRS Vicinity.
contours-clip.shp	1	2	8/1/2000	Polyline Shapefile of SRS contours at 10 m interval. Clipped to site boundaries.
Erwu_ply.shp	1	7	7/5/2000	Polygon Shapefile of ER waste unit boundaries.
Erwu_pt.shp	1	7	7/5/2000	Point Shapefile of ER waste units.
extents.shp	1	10	2/27/2001	Polygon Shapefile of Visible Extents for each Area on a D-sized map.
fmcseepline.shp	1	8	11/12/1999	Polyline Shapefile of Seepline South of GSA.
hydropolys.shp	1	12	7/28/2000	Polygon Shapefile of all Permanent Waterbodies at SRS.
largesecities.shp	2	6	8/3/2000	Point Shapefile of Major Southeastern Cities/Used for locator map.
majorroads.shp	2	6	8/3/2000	Polyline Shapefile of Major Southeastern Roads/Used for locator map.
Roads-clip.shp	1	2	6/13/2000	Polyline Shapefile of SRS Roads clipped to SRS boundaries.
savannahriver2.shp	1	2	7/27/2000	Polyline Shapefile of the Savannah River Segment Bordering SRS.
savbuffer.shp	1	2	7/27/2000	Polygon Shapefile of the Savannah River Segment Bordering SRS buffered to a width of 200 meters. For map display purposes.
Savriver.shp	1	2	7/27/2000	Polyline Shapefile of the Savannah River Segment Bordering SRS.
secities.shp	2	6	8/3/2000	Point Shapefile of Southeastern Cities/Used for locator map.

Shapefile	Projection Code	Creator Code	Date Created	Description/Function:
secitiesutm.shp	1	6	1/11/2001	Point Shapefile of Southeastern Cities/Used for locator map.
serdsutm.shp	1	6	1/11/2001	Polyline Shapefile of Major Southeastern Roads/Used for locator map.
sestatesutm.shp	1	6	1/11/2001	Polyline Shapefile of Southeastern State Boundaries/Used for locator map.
simpleroads.shp	1	12	7/28/2000	Polyline Shapefile of roads from State of SC clipped to SRS boundaries.
southeast.shp	2	6	8/3/2000	Polygon Shapefile of Southeastern States.
Srscont50m.shp	1	2	8/2/2000	Polyline Shapefile of SRS contours at 50 m interval. Derived from the SRS 10m contours.
srsstreams-clip.shp	1	2	8/5/2000	Polyline Shapefile of Streams from SRS STREAMS.SHP Coverage, clipped to SRS boundaries.
STREAMS.SHP	1	1	3/21/1997	Polyline Shapefile of Streams from SRS GIS Data Clearinghouse.
Streams-clip.shp	1	12	8/3/2000	Polyline Shapefile of Streams from State of SC. Clipped to SRS boundaries.
tcesite_2q98.shp	1	3	7/25/2000	Point Shapefile of sitewide TCE sampling, 2Q 98
tcesite_3q98.shp	1	3	7/25/2000	Point Shapefile of sitewide TCE sampling, 3Q 98
tcesite_1q99.shp	1	3	7/25/2000	Point Shapefile of sitewide TCE sampling, 1Q 99
tcesite_2q99.shp	1	3	7/25/2000	Point Shapefile of sitewide TCE sampling, 2Q 99
tce1q99cluster.shp	1	4	2/19/2001	Point Shapefile of groups of wells within 20 meter radii, sitewide TCE sampling, 1Q99
tce1q99single.shp	1	4	2/19/2001	Point Shapefile of wells more than 20 meters apart, sitewide TCE sampling, 1Q99
tce2q99cluster.shp	1	4	2/19/2001	Point Shapefile of groups of wells within 20 meter radii, sitewide TCE sampling, 2Q99
tce2q99single.shp	1	4	2/19/2001	Point Shapefile of wells more than 20 meters apart, sitewide TCE sampling, 2Q99
tce3q99cluster.shp	1	4	2/19/2001	Point Shapefile of groups of wells within 20 meter radii, sitewide TCE sampling, 3Q99
tce3q99single.shp	1	4	2/19/2001	Point Shapefile of wells more than 20 meters apart, sitewide TCE sampling, 3Q99
tce4q99cluster.shp	1	4	2/19/2001	Point Shapefile of groups of wells within 20 meter radii, sitewide TCE sampling, 4Q99
tce4q99single.shp	1	4	2/19/2001	Point Shapefile of wells more than 20 meters apart, sitewide TCE sampling, 4Q99
tcesite_4q99.shp	1	3	7/25/2000	Point Shapefile of sitewide TCE sampling, 4Q99

Shapefile	Projection Code	Creator Code	Date Created	Description/Function:
tcesite_4q98.shp	1	3	7/25/2000	Point Shapefile of sitewide TCE sampling, 4Q98
tcesite_3q99.shp	1	3	7/25/2000	Point Shapefile of sitewide TCE sampling, 3Q 99
tcesite_1q98.shp	1	3	7/25/2000	Point Shapefile of sitewide TCE sampling, 1Q 98
tritiumsite_4q99.shp	1	3	7/25/2000	Point Shapefile of sitewide Tritium sampling, 4Q99
tritiumsite_4q98.shp	1	3	7/25/2000	Point Shapefile of sitewide Tritium sampling, 4Q98
tritiumsite_3q99.shp	1	3	7/25/2000	Point Shapefile of sitewide Tritium sampling, 3Q99
tritiumsite_3q98.shp	1	3	7/25/2000	Point Shapefile of sitewide Tritium sampling, 3Q98
trit1q99cluster.shp	1	4	2/27/2001	Point Shapefile of groups of wells within 20 meter radii, sitewide Tritium sampling, 1Q99
trit1q99single.shp	1	4	2/27/2001	Point Shapefile of wells more than 20 meters apart, sitewide Tritium sampling, 1Q99
trit2q99cluster.shp	1	4	2/27/2001	Point Shapefile of groups of wells within 20 meter radii, sitewide Tritium sampling, 2Q99
trit2q99single.shp	1	4	2/27/2001	Point Shapefile of wells more than 20 meters apart, sitewide Tritium sampling, 2Q99
trit3q99cluster.shp	1	4	2/27/2001	Point Shapefile of groups of wells within 20 meter radii, sitewide Tritium sampling, 3Q99
trit3q99single.shp	1	4	2/27/2001	Point Shapefile of wells more than 20 meters apart, sitewide Tritium sampling, 3Q99
trit4q99cluster.shp	1	4	2/27/2001	Point Shapefile of groups of wells within 20 meter radii, sitewide Tritium sampling, 4Q99
trit4q99single.shp	1	4	2/27/2001	Point Shapefile of wells more than 20 meters apart, sitewide Tritium sampling, 4Q99
tritiumsite_1q98.shp	1	3	7/25/2000	Point Shapefile of sitewide Tritium sampling, 1Q98
tritiumsite_1q99.shp	1	3	7/25/2000	Point Shapefile of sitewide Tritium sampling, 1Q99
tritiumsite_2q98.shp	1	3	7/25/2000	Point Shapefile of sitewide Tritium sampling, 2Q98
tritiumsite_2q99.shp	1	3	7/25/2000	Point Shapefile of sitewide Tritium sampling, 2Q99
utrseepline.shp	1	8	11/12/1999	Polyline Shapefile of seepline North of GSA
wastes.shp	1	1	2/9/2001	Polygon Shapefile of ER waste unit boundaries with names shortened for improved map display.

Shapefile	Projection Code	Creator Code	Date Created	Description/Function:
wastesites_ed.shp	1	2	8/5/2000	Polygon Shapefile of ER waste unit boundaries clipped to SRS boundaries.
WATERBDS.SHP	1	2	1/16/1997	Polygon shapefile of water bodies from the SRS GIS Data Clearinghouse.
waterbds-clip.shp	1	2	8/3/2000	Polygon shapefile of water bodies clipped to the SRS Boundaries.
WETLANDS.SHP	1	1	4/20/1997	Polygon shapefile of wetlands from the SRS GIS Data Clearinghouse.
wetlandsbkg.shp	1	2	2/15/2001	Polygon shapefile of wetlands clipped to SRS Boundaries.
allwells.shp	1	9	8/5/2001	Point shapefile of all monitoring wells at SRS.