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Effectively Using Groundwater Geochemistry Data: A GIS Approach

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James S. Bollinger

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ABSTRACT

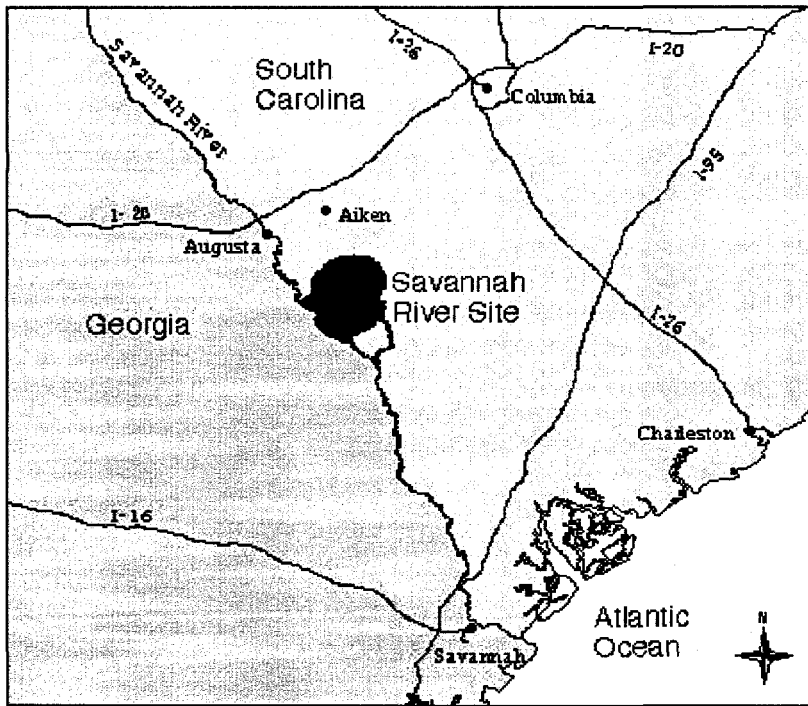
The Savannah River Site (SRS) has accumulated a wealth of groundwater geochemistry data during the past two decades from a large network of monitoring wells. These data, archived in an Oracle database, have been accessible only in quarterly reports or a spreadsheet format. An ArcView extension has been developed to extract the data using a simple interface. The data are filtered, processed, and returned as an ArcView theme, permitting rapid analysis and evaluation of contaminated areas.

Typically, these data must be analyzed by hydrostratigraphic unit to be useful. Unfortunately, a compendium of well screen-versus-aquifer relationships for groundwater monitoring wells at SRS has not been available, making the geochemical data difficult to use and analyze. Therefore, a 3-D hydrostratigraphic model has been developed in geographic information systems (GIS) and used in conjunction with well construction data to determine the location of well screen zones within the SRS vertical hydrostratigraphy. This information has been incorporated into the ArcView extension so that geochemical data can be analyzed and displayed in ArcView by hydrostratigraphic unit.

INTRODUCTION

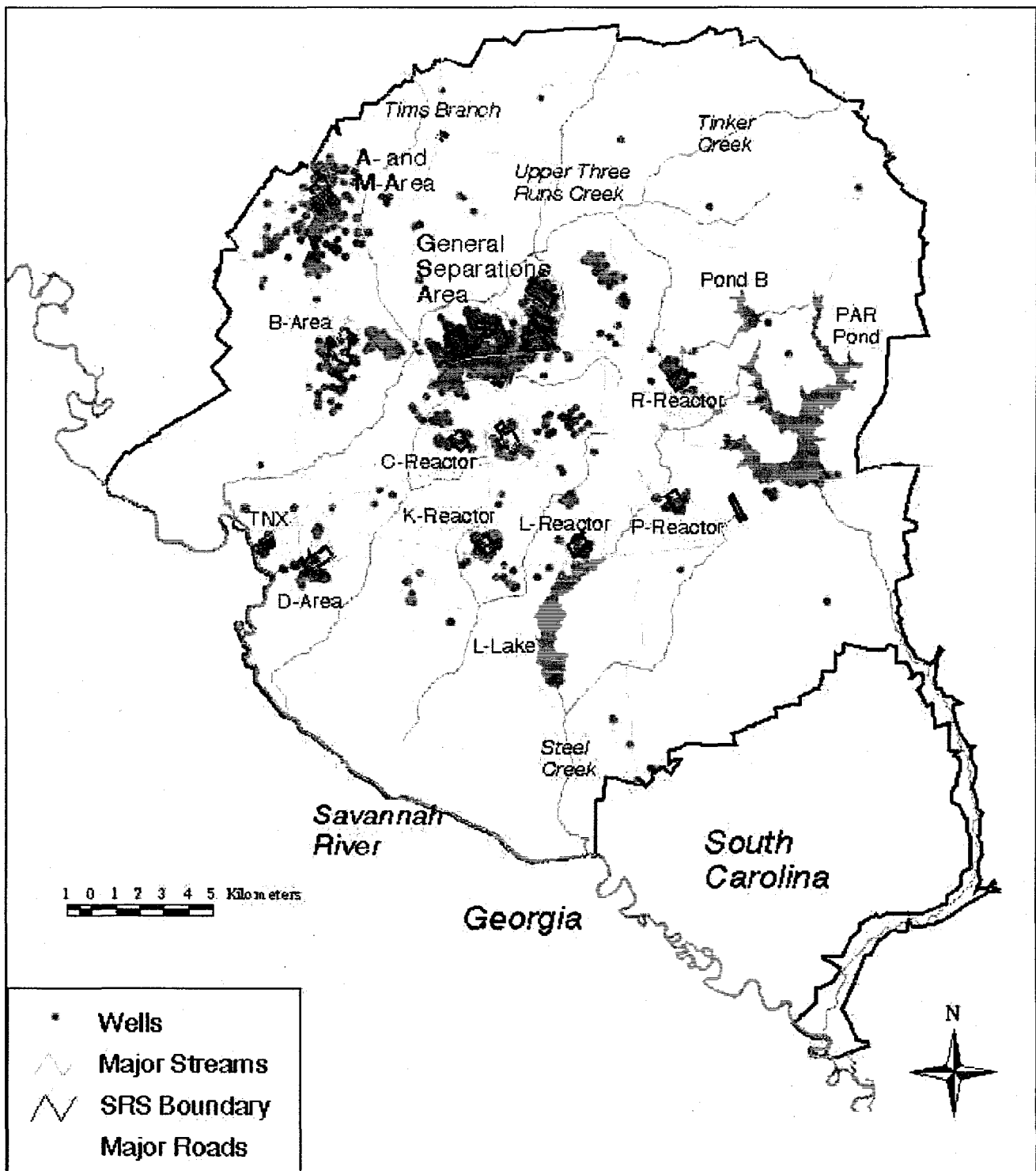
For more than 40 years, SRS produced materials for the U.S. Department of Energy (DOE) to support the nation's nuclear weapons stockpile and nondefense programs. Construction began on the site, located in South Carolina along the Savannah River (figure 1), early in 1951. In less than five years, all major facilities—five reactors, two chemical separations facilities, laboratory and test reactor facilities, a heavy water extraction plant, a nuclear fuel and target fabrication facility, and waste management facilities—had been completed. Construction of these facilities on the 310-square-mile site represented the largest single construction job ever undertaken in the United States at the time (WSRC, 1994).

Figure 1. Regional Location of the Savannah River Site



Production of nuclear materials for more than 40 years has resulted in significant groundwater contamination. Contaminants in site aquifers consists primarily of organic solvents, heavy metals, and various radionuclides. Because of this contamination, an extensive groundwater monitoring program, comprised of approximately 2,000 groundwater monitoring wells, has been in place to show compliance with federal, state, and local regulations, as well as with DOE orders. Groundwater well locations at SRS are illustrated in figure 2. This program also monitors the effects of SRS operations on onsite and offsite resources and on human health (WSRC, 1995). Groundwater geochemistry data from the monitoring program are used extensively to evaluate the effectiveness of environmental restoration programs and to determine future groundwater cleanup needs. The groundwater geochemistry data are stored in an Oracle relational database referred to as the geochemical information management system (GIMS).

Figure 2. Location of Groundwater Wells at SRS



GIMS data have been accessible only in hard-copy and spreadsheet form, making GIS use of the data difficult. In addition, GIMS data contain duplicate sample result records for many of the monitoring wells in a given sampling period. These duplicate records consist of split and replicate sample results taken from the same well that are sent to different analytical laboratories for quality assurance purposes. Prior to use in GIS, these duplicate records must be identified and combined into a single record per well.

Each sample result also is attributed with field and result qualifiers that describe (1) the field conditions

when the groundwater sample was taken and (2) the quality of the laboratory analytical results. These qualifiers must be interpreted carefully for the data to be used appropriately. Meaningful analysis of the groundwater geochemistry data also requires that the data be examined by hydrostratigraphic unit. Unfortunately, a compendium of SRS well-versus-aquifer relationships did not exist at the start of this project, so wells screened in a particular aquifer unit had to be identified and sorted manually.

The overall process of interpreting the field and result qualifiers, identifying and averaging duplicate analytical results, sorting the wells by aquifer unit, and posting the sample results on a map—is arduous and prone to human error. GIS software therefore was used to automate this process so that GIMS data could be extracted, processed, and displayed directly as a geographic theme using the Environmental Systems and Research Institute's ArcView desktop software. Developing the ArcView extension to provide automated GIS access to GIMS data was the first step toward improving GIS use of those data. The second step involved using GIS to determine where monitoring well screen zones were located within the SRS vertical hydrostratigraphy so that GIMS data could be displayed and analyzed in ArcView by hydrostratigraphic unit.

As a result of this two-step process, an ArcView extension has been developed that

- retrieves the requisite data from GIMS
- screens the data based on the field and result qualifiers
- converts the analytical or field parameter results into consistent units
- locates wells with duplicate records and computes an average result value for these wells
- adds an attribute indicating the aquifer unit where each well is screened
- returns the requested data as an ArcView point theme

The user then can easily display GIMS data by aquifer unit and perform analyses that were not feasible prior to the development of this software extension.

GIMS DATABASE DESCRIPTION

SRS groundwater monitoring wells are clustered near facilities such as the General Separations Area (GSA), where nuclear materials were chemically separated and processed, and the M-Area metallurgical facility, where nuclear fuel rods and other reactor components were fabricated. Groundwater contaminants present in the GSA are primarily tritium, heavy metals, and other radionuclide products resulting from the nuclear fuel chemical separation process. Contaminants underlying the M-Area facility consist mainly of organic degreasers such as trichloroethylene, which were used in the nuclear fuel manufacturing and machining processes.

When a particular groundwater monitoring well is sampled, field parameters such as groundwater temperature, depth to water, specific conductivity, pH, and turbidity are measured. Groundwater samples then are collected and analyzed for many different chemical analytes, including various organics, heavy metals, and radionuclides. Well sampling schedules vary from monthly to biannually depending on the purpose and location of the particular monitoring well; however, most wells are sampled quarterly. Multiple samples are collected at some groundwater monitoring wells for quality assurance purposes. These duplicate samples are sent to different laboratories so that analytical results from the laboratories can be compared. Blank samples, containing only distilled water, and spike samples, containing a known concentration of a particular analyte, also are prepared and sent for analysis. The blank sample results are used to determine whether field or laboratory contamination is present, and the spike samples are prepared to determine laboratory precision and accuracy. All of the duplicate, blank, and spike analytical results are entered into the GIMS database.

Analytical and field parameter results are annotated with qualifiers indicating the conditions present when the field measurements and subsequent laboratory analyses were performed. These qualifiers—included in GIMS—are critically important to assessing the quality of each result value.

GIS ACCESS TO SRS GEOCHEMISTRY DATA

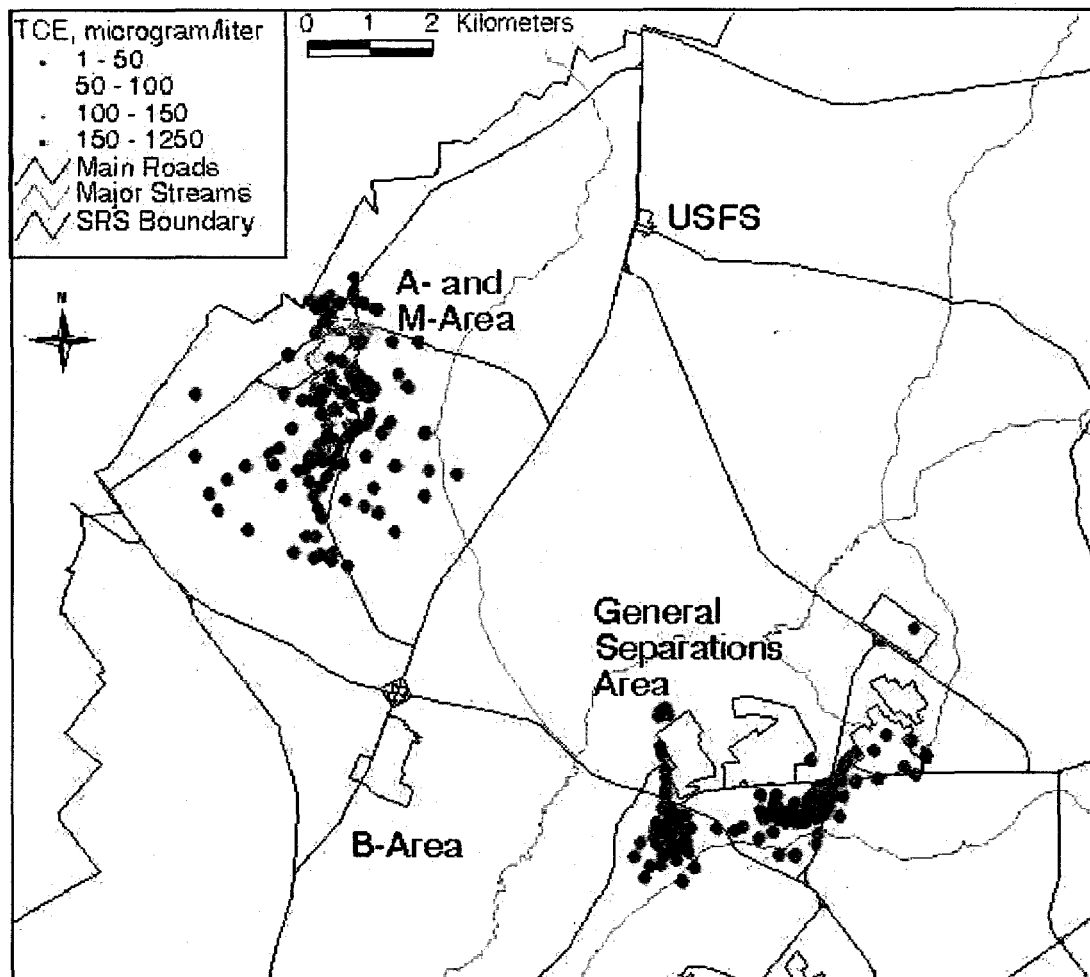
An ArcView application has been written to provide SRS users with GIS access to the GIMS Oracle database. This software application was written in Avenue, an object-oriented programming language that provides the capability to develop customized ArcView applications. The application consists of a number of Avenue scripts and ArcView tables that have been compiled into an ArcView extension. ArcView extensions provide users with considerable flexibility because they can be loaded into an existing ArcView project when needed, and then unloaded at any time.

When the extension is run, a number of sequential message boxes are displayed prompting the user for information about the type of GIMS data desired. This user-supplied information includes (1) specific analyte or field parameter, (2) coordinate system for the ArcView shape file that will be created as a result of the GIMS query, (3) hydrostratigraphic model to be used in attributing each well with a corresponding aquifer unit, and (4) year and quarter of interest. This information first is incorporated into a Standard Query Language (SQL) string using Avenue string processing requests, then submitted to the system using the Avenue SQL connect object. The SQL request then is routed to a remote Unix database server using Oracle SQL*Net software, and the requested data is returned to ArcView as a virtual table. The SQL processing is handled by two subscripts—one for field parameter data and one for analyte data. Separate subscripts were required because of differences in the GIMS table structure for analytical versus field parameter data.

The GIMS data then is filtered to remove (1) blank and spike sample results and (2) data with a qualifier flag indicating that the sample result was rejected for quality assurance purposes. Note that all analytical results are placed in GIMS, including rejected results. Rejected results are included in GIMS to document that the analysis was performed as required for regulatory compliance. The analytical results next are converted into consistent measurement units.

Analytical-result values must be compared with the practical quantitation limit (PQL) to determine whether the result is below the method detection limit (MDL). The MDL is the lowest reasonably accurate concentration of an analyte or radionuclide that can be reproducibly detected for a given analytical method. These comparisons are performed in an Avenue subscript by calculating the analyte-specific PQL, comparing the analyte result to the PQL, and appending an appropriate data qualifier attribute to the result if it is below the PQL. Several additional filtering steps then are performed to ensure that the analytical or field parameter data meet regulatory compliance standards. Finally, wells with duplicate sample results are identified, and the duplicate results are averaged. The filtered and processed data then are used to create an ArcView point theme in the coordinate system chosen by the user, and the point theme is added to the active View and classified by average analyte concentration. An example of a typical GIMS query result is illustrated in figure 3. Additional attributes provided with the ArcView shape file include the well name, well coordinates, number of duplicate results averaged, maximum result for a given well, average minimum detection limit, qualifiers associated with the sample result, sample date, and aquifer unit. The aquifer attribute gives the user the ability to display GIMS data by aquifer unit.

Figure 3. Query Results for Trichloroethylene in the A-Area/M-Area (First Quarter, 1997)

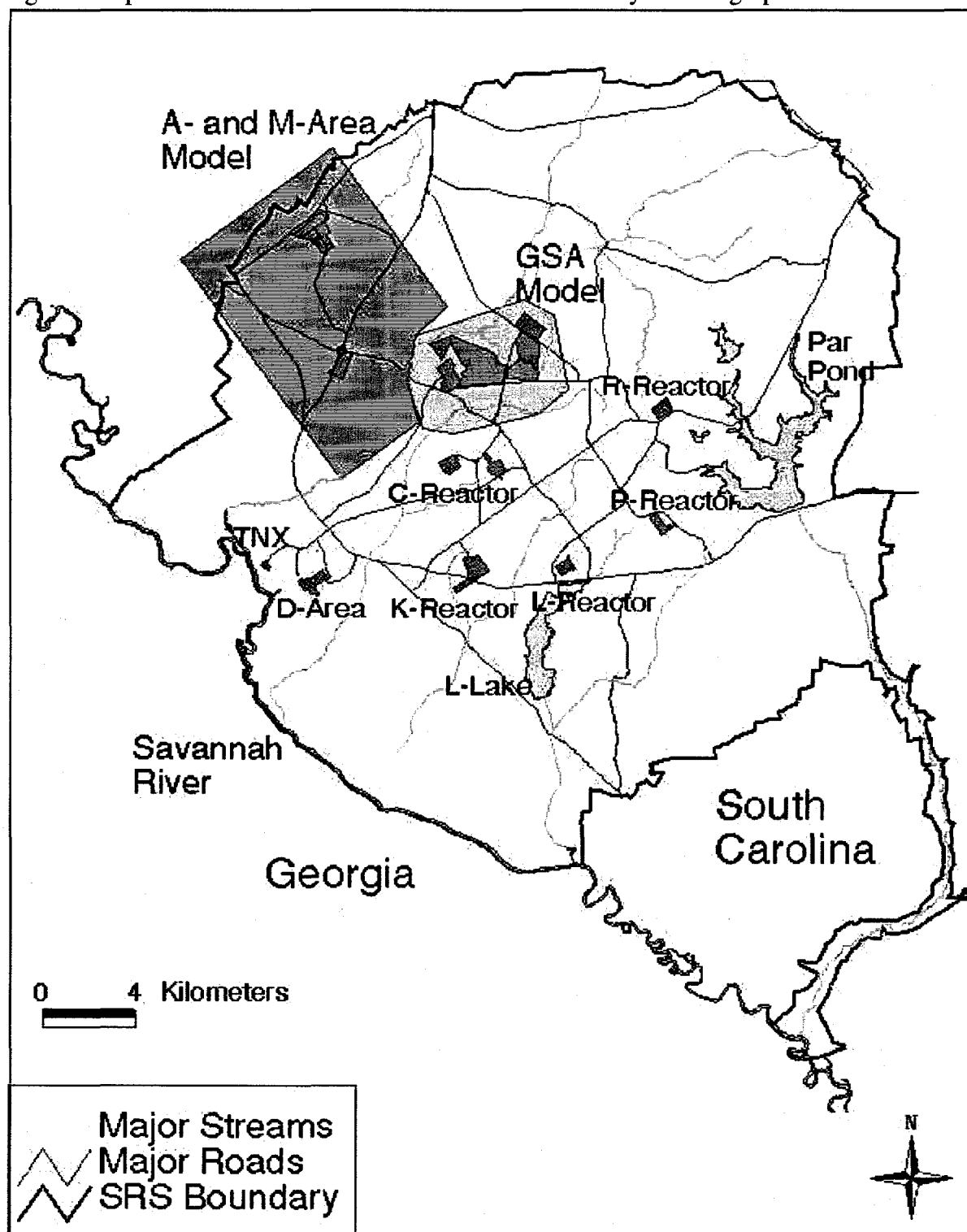


LOCATING WELL SCREEN ZONES WITHIN THE SRS VERTICAL HYDROSTRATIGRAPHY

Development of the ArcView GIMS extension was the first step in providing GIS users and other professionals easy access to GIMS data. The utility of this application would, however, be quite limited if the data could not be displayed and analyzed by hydrostratigraphic unit. Well construction records containing the screened hydrostratigraphic unit for a particular well typically are held by the organization or professional responsible for the well installation. Unfortunately, these records have not been compiled into a single source of information delineating the aquifer unit in which each well is screened. It was recognized early in this task that gathering and compiling this information from many different organizations and individuals to determine the screened aquifer unit for each well would be a monumental undertaking.

As an alternative, GIS technology was used to develop three 3-D hydrostratigraphic models for SRS. These models then were used in conjunction with available well screen zone elevations to determine the hydrostratigraphic unit in which each SRS well is finished. The 3-D hydrostratigraphic models are based on lithostratigraphic sections constructed from drill-core descriptions and geophysical logs (Aadland, 1995). The lithologic units within each model domain were correlated and assigned to specific hydrostratigraphic units on the basis of the hydrologic properties exhibited by the various lithofacies. Figure 4 illustrates the geographic extent of the three hydrostratigraphic models. The three models include (1) a regional model that covers all of SRS, (2) an A-Area/M-Area model for the SRS technical and administrative area, and (3) a GSA model for the SRS general separations area.

Figure 4. Spatial Extent of the A-Area/M-Area and GSA Hydrostratigraphic Models



The regional hydrostratigraphic model was developed by Aadland (1995) and was used to develop a regional groundwater flow model of SRS and the surrounding area. Flach and Harris (1997) and Jackson

and Looney (1996), respectively, developed the A-Area/M-Area and GSA hydrostratigraphic models for use in detailed groundwater flow and transport models of these respective areas. Figure 5 illustrates the hydrostratigraphic nomenclature used for the three models. The availability of a large number of geophysical logs and drill-core descriptions in the A-Area/M-Area and the GSA facilitated the development of the detailed hydrostratigraphic models for these areas. The regional model does not include as much detail in the vertical hydrostratigraphy, as can be seen in figure 5, because of the limited number of geophysical logs and drill-core descriptions available for many areas of SRS. Note that the regional model geographically covers both the A-Area/M-Area and the GSA. All three models were used to develop the well screen versus aquifer relationships because the A-Area/M-Area and GSA models break out the vertical hydrostratigraphy in more detail than the regional model. Thus, users have a choice as to which model they utilize, depending on their particular application and need.

Aadland (1995) performed an extensive evaluation of the regional hydrostratigraphy surrounding SRS. The site is located in the Atlantic Coastal Plain physiographic province, near the updip edge of the Atlantic Coastal Plain sequence, and is underlain by a seaward-dipping wedge of unconsolidated and poorly consolidated sediments. These sediments extend from their contact with crystalline rocks of the Piedmont physiographic province at the Fall Line to the edge of the continental shelf. Coastal plain sediments in South Carolina range from early Late Cretaceous to recent in age. The character of these sediments indicates depositional environments ranging from fluvial through deltaic to shallow marine.

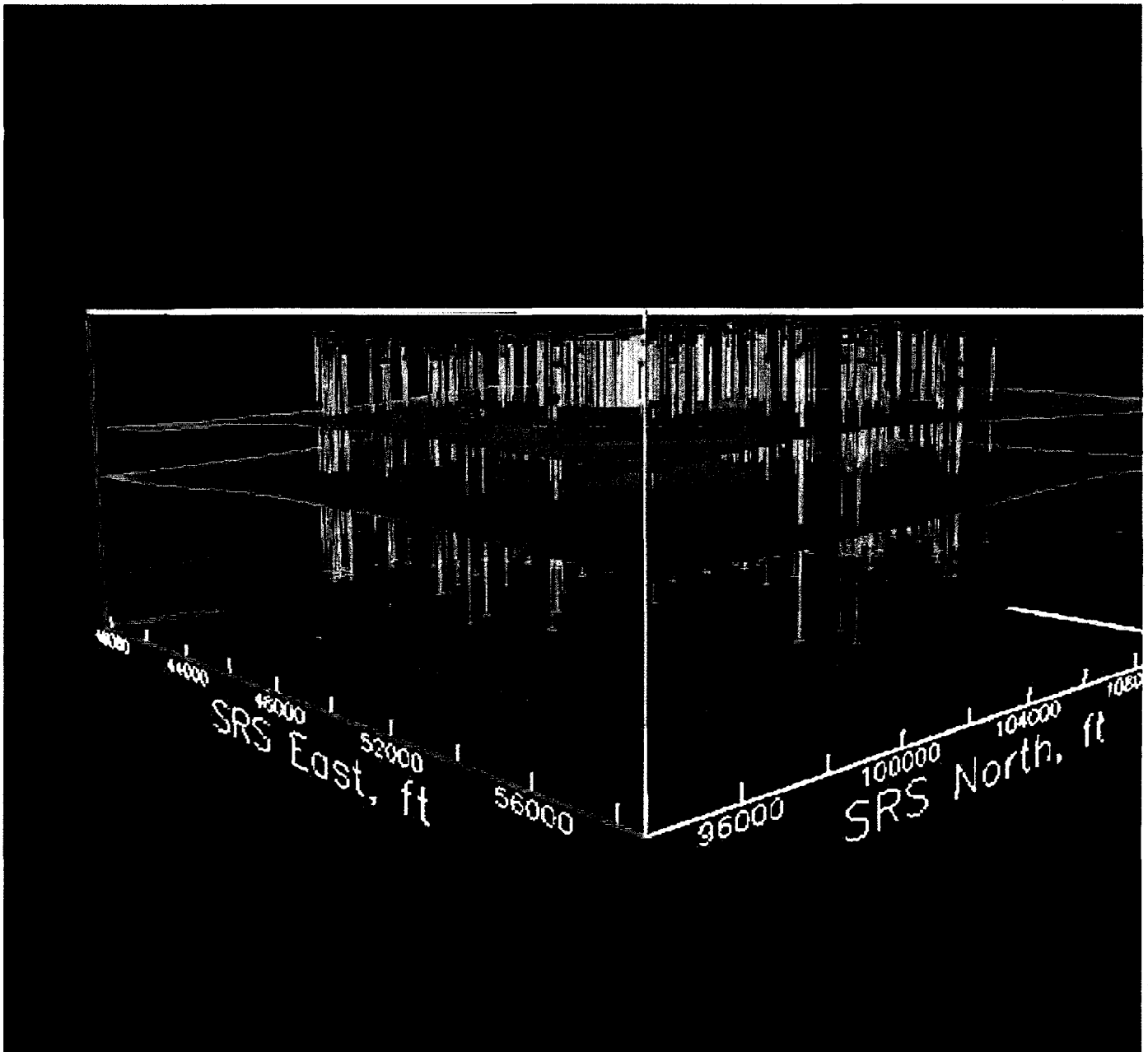
Figure 5. Hydrostratigraphic Model Nomenclature

Geologic Period	A- and M-Area Model	GSA Model	Regional Model
Tertiary	M-Area Aquifer	Upper-Upper Three Runs Aquifer	Water Table Aquifer
		Lower-Upper Three Runs Confining Unit	
		Lower-Upper Three Runs Aquifer	
	Gordon Confining Unit	Gordon Confining Unit	Gordon Confining Unit
	Gordon Aquifer	Gordon Aquifer	Gordon Aquifer
	Upper Confining Unit of Crouch Branch Confining Unit	Crouch Branch Confining Unit	Crouch Branch Confining Unit
	Middle Sand Aquifer of Crouch Branch Confining Unit		
	Lower Confining Unit of Crouch Branch Confining Unit		
Crouch Branch Aquifer	Crouch Branch Aquifer	Crouch Branch Aquifer	
Cretaceous	McQueen Branch Confining Unit	McQueen Branch Confining Unit	McQueen Branch Confining Unit
	McQueen Branch Aquifer	McQueen Branch Aquifer	McQueen Branch Aquifer

The fluvial to marine sedimentary wedge consists of alternating sand and clay with tidal and shelf carbonates common in the downdip Tertiary section. Regional dip is to the southeast, averages about 35 feet per mile on the sub-Cretaceous unconformity, and decreases upward. This variety in depositional conditions has resulted not only in wide differences in lithology across SRS, but in a complex system of transmissive and confining sediment units. Over most of the site, the Coastal Plain sequence is underlain by relatively impermeable crystalline rocks of the Appalachian orogen.

Each of the hydrostratigraphic models described above was represented in Arc/Info as a series of stacked lattices representing the interface between confining zones and aquifer units. The lattices were created based on Arc/Info point coverages with elevation attributes representing these interfaces. Inverse distance weighting (IDW) interpolation was used to develop the lattices for all three hydrostratigraphic models, because the 3-D hydrostratigraphic surfaces are relatively flat and amenable to IDW interpolation algorithms. Residual values for each surface were calculated by taking the difference between the original hydrostratigraphic elevation points and the corresponding points interpolated from the surface lattices. These calculated residuals then were normalized by the maximum elevation change across each hydrostratigraphic surface. The majority of the normalized residual values were less than 0.1 percent of the maximum hydrostratigraphic surface elevation change, indicating that IDW interpolation provides a reasonable surface fit to the data. Three of the hydrostratigraphic surfaces for A-Area/M-Area are illustrated in figure 6. The Arc/Info lattices for these surfaces were imported into EarthVison software by Dynamic Graphics, Inc., to develop the 3-D rendering shown in figure 6.

Figure 6. 3-D Rendering of Three Hydrostratigraphic Surfaces from the A-Area/M-Area Model with Wells Displayed



After the lattice models were completed, well construction information located in an Oracle database was extracted and used to create a point coverage in Arc/Info representing over 2,700 wells across SRS. This set of well data includes groundwater monitoring wells, piezometers, and special wells. Attributes in the well point coverage included the top and bottom elevation of each well screen zone. For each of the three hydrostratigraphic models, Arc/Info GRID was used to interpolate the elevation at each well spatial location from each of the lattices. These elevations were added as attributes to the Arc/Info well point coverage.

ArcView Avenue scripts then were written to compare top and bottom screen elevations with the elevation of the lattices at each well spatial location and to determine the location of the top and bottom screen zones within the vertical hydrostratigraphy. The scripts compare the hydrostratigraphic unit corresponding to the top and bottom screen zones for each well to identify the unit in which the well is screened. In a few cases, the top and bottom screen zones are located in different hydrostratigraphic units. Wells with top and bottom

screen zones located in two different aquifer units are flagged as potentially breaching a confining unit. Wells with screen zones that only partially penetrate an adjacent confining unit are assigned to the aquifer unit containing the remaining portion of the well screen.

ArcView tables for each hydrostratigraphic model were produced by the foregoing analysis. Attributes in each table included the well name, corresponding hydrostratigraphic unit, and a flag identifying each well that potentially breaches a confining unit. The number of wells potentially breaching a confining unit for each of the three models was: 17 out of 775 wells for A-Area/M-Area, 40 out of 1,087 wells for the GSA, and 100 out of 2,707 wells for the regional model. Note that most of the potentially breaching wells in the regional hydrostratigraphic model are located to the south of A-Area/M-Area, where several of the confining units are known to be quite thin or nonexistent. The absence of these confining units cannot be represented by the lattice model because the lattices simulate continuous surfaces. Taking into consideration this information, only 45 out of the 2,707 wells may actually breach a confining unit, as indicated by the regional hydrostratigraphic model. The geophysical log of each well identified as potentially breaching a confining unit eventually will be examined to determine whether the well should be removed from service.

The validity of the well screen-versus-aquifer relationships developed above depends on the accuracy of the hydrostratigraphic models and the goodness-of-fit of the Arc/Info lattice surfaces to each of the models. The lattices were verified to have provided a good fit to the data by the examination of the normalized residuals described previously. Two comparisons were made to determine the overall validity of the well screen-versus-aquifer relationships: (1) the well-versus-aquifer relationships derived from the regional model (which covers the same geographic area as the GSA and A-Area/M-Area models) were compared with those derived from the GSA and A-Area/M-Area models as a check for consistency, and (2) the well-versus-aquifer relationships from the regional, GSA, and A-Area/M-Area models were compared with Resource Conservation and Recovery Act (RCRA) Part B permit aquifer designations for a select group of wells.

Comparisons of aquifer designations from the GSA and regional models indicated that the aquifer designations are in agreement for 1,037 of the 1,087 wells considered. Results of the A-Area/M-Area model comparison with the regional model indicated that aquifer designations for 700 out of 775 wells considered were in agreement. More than 90 percent of the A-Area/M-Area aquifer designations agree with the regional model, and 95 percent of the aquifer identifiers in the GSA and regional model are in agreement. These comparison results indicate a reasonable degree of consistency between the regional versus GSA models and the regional versus A-Area/M-Area models. It should be noted that the three hydrostratigraphic models were developed by different groups of geologists and hydrogeologists. Finally, these comparison results indicate that the regional model provides a reasonable representation of the local hydrogeology in the GSA and A-Area/M-Area, despite the fact that this model is limited to some degree in vertical resolution because of the relative paucity of geophysical data over large regions of the site.

Finally, comparisons of the well-versus-aquifer relationships for the three hydrostratigraphic models were made with 846 groundwater monitoring wells with aquifer designations contained in the SRS RCRA Part B permit. The following is a summary of the comparison results: (1) 359 out of 401 aquifer identifiers were in agreement for the A-Area/M-Area model versus the RCRA aquifer identifiers; (2) 384 out of 391 aquifer designations were in agreement for the GSA model versus the RCRA aquifer designations; and (3) 776 out of 846 aquifer designations were in agreement for the GSA model versus the RCRA aquifer designations. In all three cases, better than 90 percent agreement exists between the three hydrostratigraphic model-derived and RCRA aquifer designations. Many of the cases where the RCRA and model designations are in disagreement occur for wells that are indicated by the hydrostratigraphic models to be screened in confining units.

The preceding comparison results indicate that the aquifer designations based on the GIS analysis are in very good agreement with existing data and provide a reliable basis for examining GIMS data by hydrostratigraphic unit. The three tables of aquifer information produced as a result of the foregoing analysis were incorporated into the ArcView GIMS extension described previously so that GIMS data can be accessed quickly and displayed by hydrostratigraphic unit.

CONCLUSIONS

Accessing GIMS data, processing and filtering the data, and importing the results into ArcView or Arc/Info used to be a very time-intensive task, requiring more than a day for a single analytical or field parameter result. Moreover, GIMS data previously were accessed and processed using spreadsheets, and guesswork was involved in interpreting data qualifiers and sorting the data by hydrostratigraphic unit. This resulted in costly, time-consuming errors in data interpretation and related analyses. The same data now can be retrieved and automatically processed using the new ArcView GIMS extension in about one minute, providing immediate access to geochemistry data. Thus, the guesswork previously involved in filtering GIMS data and categorizing the data by hydrostratigraphic unit has been eliminated—fundamentally changing the way GIMS data are accessed and used by the environmental community at SRS.

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