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Management Plan for the Oak Ridge Reservation Hydrology and Geology Study Groundwater Data Base

B. K. Thompson

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Energy Systems Environmental Restoration Program
ORNL Environmental Restoration Program

Management Plan for the Oak Ridge Reservation Hydrology and Geology Study Groundwater Data Base

B. K. Thompson

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EXECUTIVE SUMMARY

The Oak Ridge Reservation Hydrology and Geology Study (ORRHAGS) Groundwater Data Base has been compiled to consolidate groundwater data from the three U.S. Department of Energy facilities located on the Oak Ridge Reservation: the Oak Ridge K-25 Site, the Oak Ridge National Laboratory, and the Oak Ridge Y-12 Plant. Each of these facilities maintains its own groundwater and well construction data bases. Data were extracted from the existing data bases, converted to a consistent format, and integrated into the ORRHAGS Groundwater Data Base structures. This data base management plan documents the development and maintenance of the ORRHAGS Groundwater Data Base and contains information on data base objectives; roles and responsibilities of the personnel involved; and flow, updating, and storage of the data.

1. INTRODUCTION

The Oak Ridge Reservation Hydrology and Geology Study (ORRHAGS) Groundwater Data Base has been compiled to consolidate groundwater data from the three U.S. Department of Energy (DOE) facilities located on the Oak Ridge Reservation (ORR): the Oak Ridge K-25 Site, the Oak Ridge National Laboratory (ORNL), and the Oak Ridge Y-12 Plant. Each of these facilities maintains its own groundwater and well construction data bases. Data were extracted from the existing data bases, converted to a consistent format, and integrated into the ORRHAGS Groundwater Data Base structures. The ORRHAGS Groundwater Data Base, now in its first version, includes results of groundwater chemical analyses, field parameters measured during sample collection, water level measurements, information on hydrogeologic parameters, general well information, and well construction data for ~2500 wells throughout the ORR.

This data base management plan documents the development and maintenance of the ORRHAGS Groundwater Data Base and contains information on data base objectives; roles and responsibilities of the personnel involved; and flow, updating, and storage of the data. The ORRHAGS data base structure, conventions, and utilization are documented in the ORRHAGS Groundwater Data Base Dictionary (Thompson 1993).

The K-25 Site data extracted for the first version of the ORRHAGS Groundwater Data Base include groundwater information dating from 1987 to 1989. The data were compiled by the K-25 Site Groundwater Protection Program. The data base also includes well construction information dating from 1986 to 1989, compiled by Geraghty and Miller, Inc. (1989). Any external reference, publication, or release of the K-25 Site data must be cleared by the K-25 Site Groundwater Protection Program Manager's Office, which is part of the K-25 Site Environmental Management Department.

The ORNL data extracted for the first version of the ORRHAGS Groundwater Data Base include groundwater information dating from 1985 to 1989 and well construction information dating from 1949 to 1990. All ORNL data were compiled by the ORNL Environmental Restoration Program. Any external reference, publication, or release of ORNL data must be cleared by the ORNL Groundwater Protection Program Manager's Office, which is part of the ORNL Environmental Restoration Program.

The Y-12 Plant data extracted for the first version of the ORRHAGS Groundwater Data Base include groundwater information dating from 1986 to 1989 compiled by the Y-12 Plant Environmental Management Department and well construction information dating from 1943 to 1991 (King et al. 1991). Any external reference, release, or publication of Y-12 Plant data must be cleared by the Y-12 Plant Groundwater Protection Program Manager's Office, which is managed by the Y-12 Plant Environmental Management Department.

2. OBJECTIVES FOR THE DATA BASE

Groundwater data and well construction information have been, and continue to be, collected, stored, and reported independently by each of the three facilities on the ORR. Because the facilities operate independently, the data structures, formats, and software vary from site to site. The ORRHAGS Groundwater Data Base consolidates groundwater data and well construction information in a consistent format and structure that can be used with many software packages under different operating systems for geoscience analyses and interpretation. The purpose of the ORRHAGS Groundwater Data Base is to provide data to earth scientists for use in conducting geologic and hydrogeologic research.

The groundwater data and well construction information found in the ORRHAGS Groundwater Data Base will be used for a variety of hydrogeologic research applications and other purposes. Examples of research uses of the ORRHAGS groundwater data include examination of interwell stratigraphic, lithologic, and hydraulic relationships; flow systems; geologic units or regimes; and contaminant transport. Although the ORRHAGS Groundwater Data Base was developed to support reservation-wide research activities, groups involved in other activities (e.g., investigation of remedial action alternatives) may choose to access the ORRHAGS Groundwater Data because of its compatibility with geoscience applications.

3. ROLES AND RESPONSIBILITIES

Creation of the first version of the ORRHAGS Groundwater Data Base involved (1) designing the ORRHAGS data base structure, (2) accessing and transferring data from the site data bases, (3) examining the site data base structures and contents, (4) matching the site data to the ORRHAGS Groundwater Data Base fields, (5) creating SAS* programs to translate the site data into the ORRHAGS data format, (6) transferring the data to the ORRHAGS structure in dBASE IV,† and (7) appending the data from each plant to create Version 1 of the ORRHAGS Groundwater Data Base.

As the site data bases receive new data, new information will be added to the ORRHAGS Groundwater Data Base to create subsequent versions. In some cases historical data that have already been transferred to the ORRHAGS Groundwater Data Base may be modified in the site data bases. In the site data base files, if there are numerous changes, if the changes cannot be identified, or if new data cannot be identified, then those data files will be regenerated and replaced. Creation of subsequent versions of the ORRHAGS Groundwater Data Base will involve (1) accessing and transferring new data, changed data, or data that must be replaced from the site data bases; (2) checking for changes to the site data base structures and contents; (3) changing entries in the previous version of the ORRHAGS Groundwater Data Base to reflect changes in the site data; (4) extracting ORRHAGS data that must be replaced; (5) modifying the ORRHAGS Groundwater Data Base structure to accommodate new or previously excluded information; (6) modifying the SAS programs to include changes in the site or the ORRHAGS data base structures or contents; (7) transferring the data to the ORRHAGS structure in dBASE IV; and (8) appending the new data from each plant to the previous version or the modified previous version of the ORRHAGS Groundwater Data Base files.

3.1 RESPONSIBILITIES OF THE DATA BASE ADMINISTRATOR

The ORRHAGS Groundwater Data Base Administrator is responsible for (1) overseeing the project, (2) designing and modifying the ORRHAGS Groundwater Data Base structure, (3) matching the site data to the ORRHAGS Groundwater Data Base fields, (4) creating the final ORRHAGS Groundwater Data Base files in dBASE IV, (5) maintaining the ORRHAGS Groundwater Data Base files on the personal computer (PC), (6) documenting changes made to the ORRHAGS dBASE IV files, (7) preparing the ORRHAGS Groundwater Data Base Dictionary, and (8) preparing the ORRHAGS Groundwater Data Base Management Plan.

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*SAS is the registered trademark of SAS Institute, Inc., Cary, North Carolina.

†dBASE IV is the registered trademark of Ashton-Tate Corporation, Torrance, California.

3.2 RESPONSIBILITIES OF THE PROGRAMMER

H&R Technical Associates, Inc., of Oak Ridge, Tennessee, was contracted to create the SAS programs that transform the chemical and well data into data files in the ORRHAGS Groundwater Data Base structures. Because of budgetary constraints, the ORRHAGS Groundwater Data Base Administrator compiled the well data from the K-25 Site and the Y-12 Plant into the ORRHAGS Groundwater Data Base structure for the first version. H&R Technical Associates is responsible for (1) accessing and transferring data from the site data bases, (2) understanding the structure and contents of the site data bases, (3) transforming data into the ORRHAGS Groundwater Data Base format by creating SAS program modules, (4) providing the intermediate files to the ORRHAGS Data Base Administrator in dBASE IV, (5) maintaining and updating the SAS programs, and (6) maintaining transferred data files.

3.3 ROLES OF THE GROUNDWATER COORDINATORS AND OTHER DATA BASE ADMINISTRATORS

Each groundwater program on the ORR has a groundwater coordinator. It is the responsibility of each site groundwater coordinator to retain control over the compilation, publication, and release of the groundwater data and well construction information for that site. Access to the ORRHAGS groundwater data by non-ORRHAGS researchers must be approved by the groundwater coordinator for that site.

The groundwater coordinators and the data base administrators for each site determine when data are finalized and, therefore, available to be appended to the ORRHAGS Groundwater Data Base. The ORRHAGS Groundwater Data Base will be updated annually; however, a full year of data may not always be available each year from each site.

A component of the Federal Facility Agreement (FFA) between the DOE Oak Ridge Field Office, the Environmental Protection Agency (EPA), and the Tennessee Department of Environment and Conservation requires the development of a consolidated data base containing all the environmental data generated at DOE facilities managed by Martin Marietta Energy Systems, Inc. In addition to the three facilities at Oak Ridge, Tennessee, Energy Systems manages gaseous diffusion plants at Paducah, Kentucky, and at Portsmouth, Ohio. The Oak Ridge Environmental Information System (OREIS) is responsible for the development and the maintenance of this consolidated environmental data base. Unlike the ORRHAGS Groundwater Data Base, OREIS is a compliance data base that includes data other than groundwater data and well construction information and also compiles data from the two facilities outside the ORR. The OREIS data base is still in the testing phase. After the OREIS program becomes operational, ORRHAGS may access OREIS data directly, or ORRHAGS may continue to collect and restructure data from the three Oak Ridge sites or from OREIS.

4. FLOW OF THE DATA

4.1 GROUNDWATER DATA FLOW

The ORRHAGS Data Base Administrator requested access to finalized groundwater data from all three existing site groundwater data bases. After permission to access the data was granted, the data were made available by the Data Base Administrator at each site. The data were transferred from each site, stored on an IBM 3090 mainframe computer at ORNL, and restructured as necessary.

All site data were stored in mainframe or PC SAS data sets. SAS programs were written to create data files that could be imported into the ORRHAGS dBASE IV structures. To introduce consistency in the data, the SAS programs matched the site chemical names to ORRHAGS field names; performed unit conversions; standardized formats for character, numeric, and date fields (Table 1); and made missing value substitutions (Table 2). The site data were screened to verify that the missing numeric value substitution of 9999999.0000 was not a valid numeric value. The SAS programs produced 30 data files, corresponding to the following 10 ORRHAGS data base file structures for each site: acid extractables (ACID); anions (ANION); base/neutral extractables (BASE); field parameters (FIELD); metals (METAL)—that is, cations; miscellaneous parameters (MISC); polychlorinated biphenyls (PCB); pesticides (PEST); radionuclides (RAD); and volatile organic compounds (VOC). Every record in these files contains the following key fields: (1) the facility that installed the well (PLANT), (2) the well name (WELL), (3) the date a groundwater sample was collected (DATE_SAM), (4) the logical field representing whether or not it was a filtered sample (FILTER_Q), and (5) the logical field representing whether or not it was a duplicate sample (DUP_Q). Additional information on the fields contained in each ORRHAGS Groundwater Data Base file can be found in the ORRHAGS Groundwater Data Base Dictionary (Thompson 1993).

The generated data files were transferred from the IBM 3090 to the STC VAX at ORNL, downloaded to a PC via the Kermit file transfer utility, read into the ORRHAGS data base file structures, copied or backed up to floppy disks, and then delivered to the ORRHAGS Data Base Administrator.

Table 1. Standard formats

Field type	Format
Character	Capital letters
Date	Two-digit month, two-digit day, two-digit year: MM/DD/YY
Numeric	Maximum of 16 places with 4 decimal places (Numbers too large or too small are represented in exponential notation.)

Table 2. Missing value substitutions

Missing values	Substitution
Numeric	9999999.0000
Date	January 1, 1900: 01/01/00
Missing day and month	
Well construction	January 1 of the given year: 01/01/YY
Well destruction	December 31 of the given year: 12/31/YY

4.2 SITE-SPECIFIC GROUNDWATER DATA FLOW

Data in the K-25 Site data base are stored on a PC in SAS data sets. The appropriate data were extracted, uploaded to the ORNL STC VAX as SAS transport files via Kermit or via SAS, and copied onto the IBM 3090 mainframe at ORNL for analysis. The structure of the K-25 Site data base consists of multiple files in which the data are organized by remedial action site. The related files contain one record for each analytical result. Because the related files in ORRHAGS contain one record for each sample, it was necessary to convert the K-25 Site data to a sample-based structure.

Specific conductance and pH are measured in both the field and the laboratory and are stored in separate ORRHAGS data files. It was possible to reconstruct where measurements of specific conductance and pH were taken for ORNL and Y-12 data. However, these data from the K-25 Site were not included because the locations at which measurements were taken could not be reconstructed from the information available.

Data in the ORNL data base are stored on the IBM 3090 mainframe computer at ORNL in SAS data sets. The appropriate data were extracted from these data sets and transformed from an analysis-per-record structure to a sample-per-record structure; the original fields were then matched to the ORRHAGS fields. Copies of the files were made available to ORRHAGS for processing. The ORNL data base structure consists of multiple files in which data are organized by individual research projects. The ORNL Environmental Restoration Program data base staff assisted in matching fields from each study to fields in the ORRHAGS data structures.

Data in the Y-12 Plant data base are stored on the IBM 3090 mainframe computer at ORNL in SAS data sets. The structure of the Y-12 Plant data base is similar to that of the ORRHAGS data base. The Y-12 Plant data base consists of multiple files in which data are organized by sample year. Laboratory qualifiers are stored in a qualifier field or fields in the K-25 Site, ORNL, and ORRHAGS data bases. However, the Y-12 Plant stores most of the laboratory qualifiers as "special missing values" in SAS. These special missing values are stored in the same field as the analytical results. A small number of the laboratory qualifiers are stored differently (i.e., in different files) and were not reconstructed.

4.3 WELL CONSTRUCTION DATA FLOW

The ORRHAGS Data Base Administrator requested access to well construction data from all three existing site data bases. After permission to assess the data was granted, the data were made available by the Data Base Administrator at each site. Well data were extracted from existing data files: one file for the K-25 Site, eight files for ORNL, and one file for the Y-12 Plant. The ORNL well construction information in the site data base files is stored on the IBM 3090 in SAS data sets. The GEN and WCON data files for ORNL were transferred from the IBM 3090 to the STC VAX at ORNL, downloaded to a PC via the Kermit file transfer utility, read into the ORRHAGS dBASE IV file structures, copied or backed up to floppy disks, and then delivered to the ORRHAGS Data Base Administrator. Well construction data in the K-25 Site and Y-12 Plant data bases are stored in non-SAS files. The non-SAS data files for these two sites were converted into PC SAS data sets before being restructured into the ORRHAGS Groundwater Data Base structure by the ORRHAGS Groundwater Data Base Administrator.

To introduce consistency in the data, SAS programs were created to match the site well fields to the ORRHAGS well fields. The SAS programs also performed unit conversions; format standardizations for character, numeric, and date fields (see Table 1); character field manipulations; and missing value substitutions (see Table 2). The site data were screened to verify that the missing numeric value substitution of 9999999.0000 was not a valid numeric value. SAS programs produced two data files for the ORNL data: general well data (GEN) and well construction data (WCON). Every record in these files contains the following key fields: (1) the site that installed the well (PLANT) and (2) the well name (WELL). Additional information on the fields contained in each ORRHAGS Groundwater Data Base file can be found in the ORRHAGS Groundwater Data Base Dictionary (Thompson 1993).

The GEN and WCON files for the K-25 Site and the Y-12 Plant were created from finalized SAS data sets via the SAS procedure PROC DBF. PROC DBF automatically creates a dBASE IV file from a SAS data set. Length and format statements are used to create a finalized SAS data set that has the same structure as the ORRHAGS data base files. The SAS DBF procedure can reproduce the structure of the ORRHAGS data base files, except for a logic field format. After the dBASE IV files are created, fields that should be logic fields are converted from character to logic. This conversion does not alter the contents of the field; it simply changes the format of the field.

More wells exist on the ORR than are routinely sampled. Therefore, the GEN and WCON files contain information about more wells than do the chemistry files. A field called CHMDAT in the GEN file contains a list of the groundwater data files that contain data for each well.

4.4 SITE-SPECIFIC WELL DATA FLOW

Well construction data in the K-25 Site data base are stored in a DOS-based Lotus 1-2-3* file. These data were transposed in Lotus, exported as a text file, and imported into a PC SAS data set for processing. The SAS DBF procedure was used to create the GEN and WCON files.

Well construction data in the ORNL data base are stored on the IBM 3090 at ORNL in eight SAS data sets organized by well type. The SAS programs that processed this data accessed the ORNL well files directly on the IBM 3090.

Well construction data in the Y-12 Plant data base are stored in a MacIntosh-based FileMaker Pro† data file. The data were converted to a SYLK file format, read into the Microsoft Excel‡ software package, converted to a dBASE IV file format, and then converted into a PC SAS data set via the SAS DBF procedure before becoming available to ORRHAGS for processing. The SAS DBF procedure was used to create the GEN and WCON files.

4.5 INTERMEDIATE FILE PROCESSING

SAS programs were developed to restructure the site data so that the data structure would match that of the ORRHAGS Groundwater Data Base. Data files that had been downloaded from the mainframe computer and read into the dBASE IV file structures or the dBASE IV files created via PROC DBF in SAS were called intermediate files. The naming convention under which intermediate files are stored is as follows: a prefix indicating the site from which the data came (i.e., K for K-25 data, X for ORNL data, and Y for Y-12 data), the standard file name, and a suffix consisting of an underscore and an intermediate version number. For example, the first intermediate acid file from Y-12 was stored with the name YACID_1.DBF.

The data were converted to ORRHAGS format as they became available. The Y-12 Plant data were processed first; the ORNL data, next; and K-25 Site data, last. Examination of ORNL data required the modification of the ORRHAGS Groundwater Data Base structure designed for the Y-12 Plant data; similarly, examination of the K-25 Site groundwater data required modification of the ORRHAGS Groundwater Data Base structure designed for ORNL and the Y-12 Plant. The ORRHAGS data base structure and contents were modified and corrected after some intermediate files were created. It was sometimes easier to modify or correct the intermediate file than to revise a SAS program and generate a new intermediate file.

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*Lotus 1-2-3 is the registered trademark of Lotus Development Corporation, Cambridge, Massachusetts.

†Filemaker Pro is the registered trademark of Claris Corporation, Santa Clara, California.

‡Microsoft Excel is a product of the Microsoft Corporation, Redmond, Washington.

In general, intermediate files were changed by (1) making a copy of the current intermediate file, (2) changing the copy, (3) checking to ensure that the changes were made appropriately, (4) replacing the previous intermediate file with the modified intermediate file, (5) recording the change, and (6) documenting any comparison procedure results. The ORRHAGS Data Base Administrator maintains all of the documentation for changes to the intermediate files. Changes to the intermediate files were made in either dBASE IV or PC SAS. Simple changes to the ORRHAGS data base structure (e.g., changing a variable name) were processed in dBASE IV, and the version number of the intermediate file remained the same. However, when changes were made to an intermediate file in PC SAS, the version number of the intermediate file was increased by one.

The ORRHAGS Groundwater Data Base Administrator has the sole authority to change data in the ORRHAGS intermediate data files. Changes to the intermediate files for the first version of the ORRHAGS data base files are documented on an ORRHAGS data base entry change form or on an ORRHAGS data base structure modifications form. The ORRHAGS change form lists the date, the name of the file, the key variables, the changed field, the original incorrect value, the new corrected value, and notes (Fig. 1). The ORRHAGS modification form lists the date, the name of the file, the field, and a description of the modification (Fig. 2). The SAS programs were modified to reflect changes in the ORRHAGS data base structure even though the change may have been made at the intermediate level.

There are 36 intermediate ORRHAGS dBASE IV files. There are three files, one from each plant, with the following ORRHAGS data base structures: ACID, ANION, BASE, FIELD, GEN, METAL, MISC, PCB, PEST, RAD, VOC, and WCON. For example, three of the intermediate files have the ACID structure: one from the K-25 Site, one from ORNL, and one from the Y-12 Plant. The final 12 ORRHAGS data base files contain each of the intermediate files with the same structure. Final files are stored with the following naming convention: the standard file names followed by an underscore and the final version number (i.e., *filename*_1.DBF). The final file names for Version 1 are ACID_1.DBF, ANION_1.DBF, BASE_1.DBF, FIELD_1.DBF, GEN_1.DBF, METAL_1.DBF, MISC_1.DBF, PCB_1.DBF, PEST_1.DBF, RAD_1.DBF, VOC_1.DBF, and WCON_1.DBF.

Date: 3/27/92

File: VER1_0\KFIELD_1.DBF

Plant	Well	Sample Date	Dup	Filter	Variable	Change from	Change to
K-25	UNW-002	11/19/87	F	F	DOXY_1	0.0000	9999999.0000
K-25	UNW-002	11/19/87	F	F	DOXY_1_C	NA	

Notes: Not measured value. NA stands for NOT APPLICABLE. Values changed in dBASE IV browse mode. The original and changed file were compared in SAS before replacement.

Fig. 1. ORRHAGS entry change form.

Date	File name	Variable	Modification
11/30/91	VER1_0\KACID_1.DBF	SOURCE	Changed name of SOURCE variable to SRC_ACID

Fig. 2. ORRHAGS modification form.

5. UPDATES TO THE DATA BASE

A new version of the ORRHAGS data base will be generated annually by the ORRHAGS administrator and programmer. A subsequent version will include the previous version's data (with any necessary corrections or substitutions), newly finalized groundwater data, and newly recorded wells. The rate at which new groundwater data are finalized varies and is determined by the groundwater coordinators and/or the site data base administrators. Well data will be reviewed annually, and data for any wells not in the current version of the ORRHAGS data base will be added. The transfer of new data from the three site data bases may not be identical to the data transfer for Version 1. However, any variation of the previous data transfer methods will be documented by the ORRHAGS Data Base Administrator. The subsequent versions of the finalized data base files will have the same file names as the previous finalized data base files, except that the version number will be increased by one. When new data are transferred to ORRHAGS, any known modifications to the previously transferred data will be requested. The same basic procedures used to change intermediate files will be used to change the previously finalized files. Modified finalized files will be renamed by adding a letter to the end of the finalized file name, beginning with the letter A (i.e., *filename*_1A.DBF). If the changes are too extensive, the data may need to be retransferred and replaced. However, because the groundwater sample data incorporated into the ORRHAGS data base are finalized, regenerating previously transferred groundwater sample data should not always be necessary.

It is possible that additional parameters may be measured in the laboratory or that previously excluded parameters may become important to ORRHAGS researchers. The ORRHAGS Data Base Administrator, in consultation with researchers, will decide if the inclusion of newly measured parameters or previously excluded parameters is necessary in subsequent versions of the ORRHAGS Groundwater Data Base. To include additional parameters in the data base, the ORRHAGS Groundwater Data Base structure must be modified. First, a copy will be made of an ORRHAGS data base file. A variable will then be added to the data base structure and the change documented on an ORRHAGS entry change form or an ORRHAGS modification form. If the variable is a newly measured parameter, a missing value should be stored in this variable for all previous records; however, if the variable is a previously excluded parameter, previously existing results will be merged by matching on the key variables to the existing file.

6. STORAGE OF THE DATA BASE

Three copies of the finalized ORRHAGS Groundwater Data Base files are stored on write-protected Bernoulli disks in dBASE IV format. Two copies are stored in the ORRHAGS Data Base Administrator's office, and one copy is stored off-site. These official copies are never used for direct processing of the data. Copies are always made to other disks before data queries, updates, or modifications are performed.

Most of the finalized data base files are too large to fit on a 1.2-MB floppy disk. Files can be transferred on a 44-MB Bernoulli disk. Requests for data from the ORRHAGS data base are currently handled on a case-by-case basis. Data release to users will generally involve a memorandum of agreement for subsequent review of planned publication or release of data acquired. Data requests should be sent to the ORRHAGS Data Base Administrator.

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