PNL-3528

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Status Report on SIRS: Sorption Information Retrieval System

D. D. Hostetler
R. J. Serne
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November 1980

Prepared for the
Office of Nuclear Waste Isolation
U.S. Department of Energy
under Contract DE-AC06-76RLO 1830

Pacific Northwest Laboratory
Operated for the U.S. Department of Energy
by Battelle Memorial Institute

Battelle

PNL-3528

PACIFIC NORTHWEST LABORATORY
operated by
BATTELLE
for the
UNITED STATES DEPARTMENT OF ENERGY
Under Contract DE-AC06-76RLO 1830

Printed in the United States of America
Available from
National Technical Information Service
United States Department of Commerce
5285 Port Royal Road
Springfield, Virginia 22151

Price: Printed Copy $______*; Microfiche $3.00

*Pages	NTIS Selling Price
001-025	$4.00
026-050	$4.50
051-075	$5.25
076-100	$6.00
101-125	$6.50
126-150	$7.25
151-175	$8.00
176-200	$9.00
201-225	$9.25
226-250	$9.50
251-275	$10.75
276-300	$11.00

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SUMMARY

Two major uses were identified for the Sorption Information Retrieval System: 1) to aid geochemists in the elucidation of sorption mechanisms and 2) to aid safety assessment modelers in selection of Kds for any given scenerio. Other benefits such as providing an auditable vehicle for the Kd selection were also discussed.

The SIRS hardware and software were discussed in detail. In order to provide a permanent data storage bank, the capability of rapid and selective retrieval, the capability to perform statistical analyses and to allow user interaction as well as versatile hard copy output, several software programs were constructed on a PDP 11/55 minicomputer. Software described include: 1) data input, 2) data subsetting, 3) statistical analysis and 4) auxiliary programs. Examples of the data selection processes, sample statistical analysis and data output are shown.

Currently, SIRS is operational with a data base containing 2000 Kd experiments performed in FY 1977 and 1978. Plans to install backlogged data are described. Recommendations to merge SIRS with a DOE developing software system Analysis of Large Data Sets (ALDS) are discussed. ALDS will provide a greatly enhanced statistical and analytical capability over SIRS. ALDS is the first large scale scientific data base management system to be developed by DOE. It is a multimillion dollar effort presently being implemented at PNL on sophisticated hardware not available to WRIT. The ALDS software will be much more easily transferred to other organizations as it is much less machine dependent than SIRS. Within 1 1/2 years, it is envisioned that ALDS will be capable of taking over all aspects of SIRS especially in the area of selection of Kds for safety assessments. Provided that the Kd data bank can be transferred from ALDS to SIRS, some usuage of SIRS by WRIT geochemists is contemplated in the area of sorption mechanism identification because SIRS does offer the convenience of high user-interaction.

From an operational standpoint, SIRS has achieved its original design goals of providing a highly interactive system for rapid data retrieval and analysis. The data base (both installed and backlogged) includes Kd values

for a large number of radionuclides occurring in radioactive wastes originating from the commercial nuclear power industry. Kd values determined to date span, several groundwater compositions, and a wide variety of rock types and minerals. The data system not only includes Kd values, but also background information on the experiments themselves. This will allow the potential user to retrieve not only the Kd values of interest but also sufficient information to evaluate the accuracy and usefulness of the data.

The real-time cross correlation or comparison of most sorption experimental parameters possible with SIRS provides unique analytical utility. Enhanced data availability and analysis permits a much increased data perusal by geochemists. Old hypotheses concerning sorption chemistry can be verified and thoroughly documented, or new trends may be discovered and new theories tested.

The need for increased quality assurance procedures to address data input was identified in anticipation of DOE's pursuit of repository licensing exercises. Preliminary plans are described in Appendix D.

ACKNOWLEDGMENTS

This work was supported by the Waste Rock Interactions Technology (WRIT) Program being conducted by Pacific Northwest Laboratory. This program is sponsored by the Office of Nuclear Waste Isolation, which is managed by Battelle Memorial Institute under Contract DE-AC06-76RLO 1830 with the Department of Energy.

We gratefully acknowledge the assistance of Cathy Washburne and Lynn Degrave who coded and key punched the sorption data to facilitate its installation into the computer.

Finally, the advice and assistance of Dennis Friedrichs on all software aspects was appreciated.

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FIGURES

INTRODUCTION

Radioactive waste products result from commercial nuclear power production, and require isolation from the biosphere for thousands of years. Current plans of the Department of Energy (DOE) call for final management of these wastes by isolation in deep continental geologic formations. The wastes are expected to be kept in isolation as a result of chemical, thermal, and mechanical stability of the waste package systems and geologic repositories.

The Department of Energy, through the National Waste Terminal Storage (NWTS) program, is developing nuclear waste isolation systems in geologic formations that prevent unsafe radionuclide concentrations from entering the biosphere. In order to assess the safety of geologic repositories, capability to address the following factors is needed: 1) geologic and repository stability, 2) magnitude and the direction of possible transport media flow, 3) concentration, nature and retardation of species of the radionuclides in the transport fluid, and 4) biological uptake of radionuclides by food chains.

The Waste/Rock Interactions Technology (WRIT) program is specifically designed to address the needs of item (3) above. To accomplish this goal, the WRIT program will develop the necessary data and predictive capability on the release and subsequent geochemical interactions of radionuclides with engineered barriers and natural geologic media. The major products of the planned research in the WRIT program are: 1) the generation of defensible, reproducible data on leaching, sorption, and nuclide-release processes through the use of scientifically-acceptable methodologies, and 2) the development of credible models of leaching, sorption, and release processes based on underlying theory and experimental observation that can be used in consequence analysis.

The use of these models, in concert with other models (transport model, release scenario stability model, dose model) that are being developed under the Assessment of the Effectiveness of Geologic Isolation Systems (AEGIS) and WIPAP programs, will result in a suite of models capable of assessing the safety of geologic repositories.

Preliminary analysis has shown that by using geologic selection criteria for selecting a repository site, the probability of a repository breach and resulting hazard to man is very low. In the event that the repository is breached by intruding groundwater, radioactive waste will be leached after some time and radionuclides brought into solution. A very important barrier to radionuclide movement is retardation due to the interaction between radionuclides and natural geologic media and engineered barriers. The most common quantification of this retardation is through the use of the adsorption distribution coefficient, Kd.

In most instances, Kd is sensitive to the surface area, mineral composition, amorphous oxide, and organic content of the rock or sediment and the pH, Eh, and chemical composition of the carrier solution. The Kd can also be dependent on the species of nuclide present, its concentration and hydrodynamics of the geohydrologic system. The interactions which occur as soluble radionuclides percolate through geomedia are presented in Figure 1.

Therefore, to properly identify, interpret, or utilize a Kd value for any nuclide a large amount of supplementary information is necessary. For these two reasons, the importance of sorption in the determination of safety assessment and the large amount of information needed to interpret the applicability of a given Kd to a particular case, a tool which aids in the storage and analysis of large amounts of data has been created. The tool, SIRS: Sorption Information Retrieval System is a computer software package which stores all the Kd and supplementary data, which sorts through the data upon command to select only those data with potential application to the scenario under study and which can perform simple statistical calculations and figure plotting to allow correlations to be identified.

The ensuing text will delineate the uses of the computerized storage, retrieval and analysis system of radionuclide sorption-desorption data by geologic media, both for applications in nuclear waste repository safety assessments and for interpretation of basic research on nuclear waste/rock interactions.

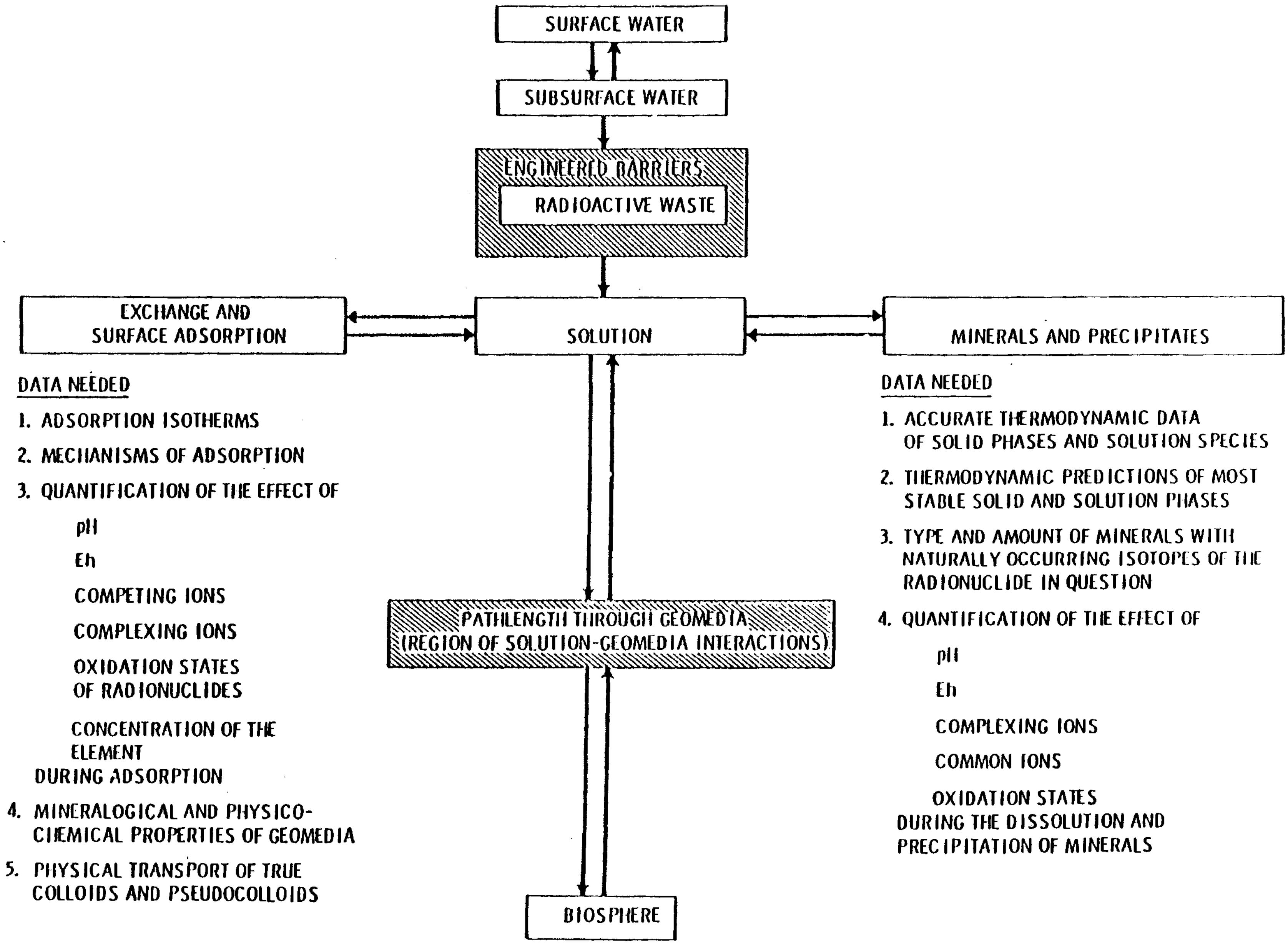

FIGURE 1. Radionuclide Interaction in Geologic Media

This document constitutes the second status report on the develoment of SIRS. The first document, PNL-3139 Status of Sorption Information Retrieval System, by D. D. Hostetler, R. J. Serne and A. Brandstetter was published in September 1979. At that time, the software for data input and data retrieval and display were completed but not debugged. The present document delineates progress made to date on actual implementation of SIRS and recaps progress reported in PNL-3139 to assure that the reader can understand SIRS from this document alone.

It is contemplated that one more document will be necessary to fully document SIRS, to illustrate by example its usefulness and to provide a user's manual.

SORPTION INFORMATION RETRIEVAL SYSTEM PURPOSE

Several of the needs and potential uses of a computerized sorption information system were briefly described in the introduction. In this section, a few more uses of the system will be described.

There are two basic uses for the computerized system: safety assessment uses and mechanism identification uses. As mentioned, the WRIT program supplies input data such as the sorption-desorption values to the organizations performing the overall safety assessments. Because nuclide retardation by rocks and sediments is a key contributor to the natural processes which protect mankind from rapid contact with buried wastes and because the physicochemical processes which contribute to the retardation are several and appear quite complicated, a great deal of interest and importance has been placed on the usage of Kds. As our understanding of the physics and chemistry of sorption is not complete, some controversy is present. The importance of retardation in the overall safety assessment calculations exacerbates the controversy. To increase the confidence in the retardation numbers used in safety assessments, two efforts are underway within the WRIT program. One effort is to identify the basic physicochemical processes controlling sorption-desorption and the other is to select Kd values for each given safety assessment scenario very carefully based upon close simulation within the laboratory of actual real world physicochemical environments.

Along this latter vein, extensive supporting information (characteristics of the geologic media/groundwater system) is necessary to properly characterize a sorption experiment. Without this ancillary information, predictive, extrapolative, and interpolative activities cannot be performed objectively. In the ideal case, all the parameters listed below would be determined; in real instances as many of the parameters as economically, logistically and technically feasible should be measured.

Numerous characterizations should be performed on geologic media and pore waters to allow calculations of migration rates or Kds. The characterizations can be broken into two broad categories: physical or hydrologic, and geochemical. A list of characterizations and their relative importance follows. The relative importance is based on the assumption that insufficient time and funds will be available to perform the complete characterization. If only partial geochemical characterization is possible, emphasis should be on the first seven items. For the physical and hydrologic characteristics, Items 4, 5 and 6 or 7 are most important.

Important Geochemical Characterizations

1. Qualitative and quantitative mineralogy including primary and secondary crystalline materials, amorphous coatings, etc., determined primarily by X-ray diffraction, chemical treatment techniques, and petrographic examination. Calcium carbonate content and hydrous oxide content (amorphous and crystalline) as well as aluminosilicate contents are most important. Scanning electron microscopy and microprobes can be used to determine microstructural mineralogy. These techniques can be very important in assessing the differences between mineralogy and weathering environments of cracks and fractures from the bulk rock material.
2. Cation-exchange capacity
3. Pore water pH, Eh
4. Pore water major cation content (Na, Ca, Mg, k)
5. Pore water major anion content (Cl, HCO_3, CO_3, SO_4, NO_3)
6. Pore water SiO_2
7. Organic content of geologic material.

Less Important Geochemical Characterizations

1. Anion exchange capacity
2. Distribution of major cations on exchange sites
3. Pore water organic content especially potential ligands (humic, fulvic acids)
4. Pore water minor constituents especially naturally occurring isotopes of important waste nuclides (Sr, Cs, I, U, Ra) and chemically similar elements (Ba, Rb, Br).

For geologic environments that are presently devoid of water a saturated water extract should be prepared which then is used in place of the above mentioned pore water.

Important Physical or Hydrologic Characterizations

1. Hydraulic conductivity
2. Percentage saturation
3. Permeability
4. Water velocities
5. Surface area and particle size distribution (unconsolidated materials)
6. Porosity
7. Percentage fractures of fissures (consolidated material)
8. In situ temperature

One of the main purposes of SIRS is to store all of this supporting information in a convenient and permanent fashion. In addition to being capable of permanent storage, SIRS must rapidly be capable of retrieving all types of data for selected types of rocks/waters for any particular scenario of interest to safety assessors. The advantages of computerized storage and retrieval from the safety assessment viewpoint include: 1) the minimum space requirements and permanence of data storage compared to hand transcription, 2) rapid selection and retrieval of data subsets compared to human selection, 3) ease in transfering total selected data to other users via magnetic tape, 4) ease of updating or correcting data previously stored, 5) capability for non-technical or at least non-geochemist persons to facilitate selection, 6) auditability of selection process and 7) delineation of a standard data collection format. The latter three advantages deserve some explanation.

The data bank is set up such that the operator is lead through the selection procedure step by step. The data bank is usuable by nontechnical or non-geochemists. We want the data information-retrieval system to be usable by modelers without necessitating a lot of technical interpretation. If a modeler needs Kds for a particular scenario, the information-retrieval system will inquire about the type of scenario and after the operator inputs on the keyboard, the computer will go select possible choices and display them along with any other basic details requested. Also having a set protocol or written procedure for selection makes it possible to audit the selection of data used. In the future, a quality assurance program with respect to the data input into the computer data base will be implemented such that quality as well as selection procedures can be audited. These audit aspects will become quite important during the formal licensing process.

The use of SIRS should greatly improve the traceability of selected Kd values over present procedures which rely on the judgement of a few select geochemists. In addition, the SIRS system could be used effectively as a management tool to check on the status of ongoing work to ascertain what labs are producing data on what rock types. Via this check, it would be possible to identify gaps in data collection or over emphasis on certain media, nuclides etc.

Finally, the delineation of a standard data reporting format should provide impetus to experimenters to collect the important ancillary information and to standardize the reporting of results. Much of the past confusion and controversy over Kds has occurred because experimenters did not appreciate the need for careful and complete characterization of the rock/water/nuclide system or careful documentation of experimental details. Thus, the use and comparison of partially undefined Kd values has lead to imprecise predictions of nuclide migration and unfavorable agreement between lab and field results or between different experimenters who erroneously assummed that they were dealing with identical systems. Although it is beyond the scope of this document to explore the status and our understanding of experimental sorption procedures the interested reader is referred to Relyea et al. (1980), Brandstetter et al. (1980) and Burkholder et al. (1979).

This latter point has also helped improve the experimental design of laboratory sorption tests and with the increased system characterization has allowed the investigation of sorption mechanisms. To aid in mechanisms identification, SIRS includes simple statistical routines which allow means, and standard deviations to be calcuated as well as curve fitting or regression to be performed on one variable such as Kd versus another variable such as pH. An important aspect of SIRS along this data analysis line is its user-interactive capability. This provides several modes of operational freedom for the user, because he can readily examine or modify much of the model logic and input data. This capability allows the user to test the effects that modified logic or data will have on the simulation run results. In this way, logic or data that gives erroneous results can be quickly identified and corrected. The high degree of interaction allows the experimenter to sit at the keyboard and search for interesting trends between the variables and rapidly check hypotheses in hopes of elucidating the controlling mechanisms. The present concept and standard data format of the WRIT Sorption Information Retrieval System are presented in Appendix A. The standard formats delineate all the currently required information on rock, groundwater and nuclide characteristics and experimental methodology. Data base organization is generally represented by Appendix A and is hierarchical in nature.

The computer can search on any of the seven main categories decribed in Appendix A and subset the data automatically. For example, for a listing of all Kd data for basalt geomedia, the computer will subset all basalt data. To compare Kds from a salt brine across all rock types, all brine information will be subsetted, etc. The computer system sorting capability is also linked to statistical programs such that subsetted data can be statistically analyzed. After data subsetting and analysis, the results can be displayed on a cathode ray tube (CRT) or hard copies can be produced. In this fashion, means, standard deviations, covariances, or other pertinent statistical parameters for Kd can be obtained as a function of minerals, surface area, cation exchange capacity, groundwater composition, etc.

With proper experimental design and media/water characterization, statistical methods can be used to relate the dependent variable (migration rate or Kd) to independent variables (rock type, solution type, etc.). Although the derived relationships do not prove cause-and-effect, they do allow prediction of trends. Thus, from Kd data on a finite number of rock, mineral, and water types, estimates can be made of Kd values for other rocks and water environments not directly studied, if certain precautions are observed. In addition, the data base can help provide: 1) a formulation of geochemical criteria useful for ranking the ability of media to isolate nuclear wastes, and 2) a delineation of the more important variables that should be studied in greater detail in mechanism studies.

SIRS SYSTEM HARDWARE AND SOFTWARE DESCRIPTION

The purpose of SIRS is to aid in the storage, retrieval and analysis of large amounts of experimental data. Rapid selection and retrieval of stored sorption data will help in two efforts: 1) sorption mechanism identification (basic research) and 2) mass transport calculations in safety assessment applications. The major design considerations identified prior to creation of SIRS were:

- hardware availability
- rapid accessibility
- user interaction
- simple statistical analysis capability
- various output capabilities especially graphical.

In addition, four important considerations were necessary in designing SIRS software. First, software should be modular to promote overlaying capability. Overlaying memory would be necessary to improve data processing capability by allowing larger data arrays in core and minimizing disk I/O. Second, data base characteristics such as array sizes, data categories, record lengths, etc., should be variables declared by an initializing program. This flexibility to alter data base characteristics will reduce the need for future software modification. Third, a random access data file structure was needed in which data records could be easily located (i.e. the locations could be calculated rapidly to reduce costs). Fourth, interactive graphics was necessary to allow theoretical and experimental geochemists to view sorption data in an efficient, understandable fashion, thus promoting the analytical utility of SIRS. Finally, all design considerations previously mentioned needed to be implemented with available computer hardware strengths and weaknesses in mind.

The current hardware configuration available to SIRS can be seen in Figure 2. The DEC PDP 11/55 minicomputer system satisfied the above design considerations. The 11/55 is a very high speed, interactive system configured for data collection, reduction, analysis and retrieval. Important components of this system used by SIRS are one 4.8 megabyte fixed disk, a 2.4 megabyte

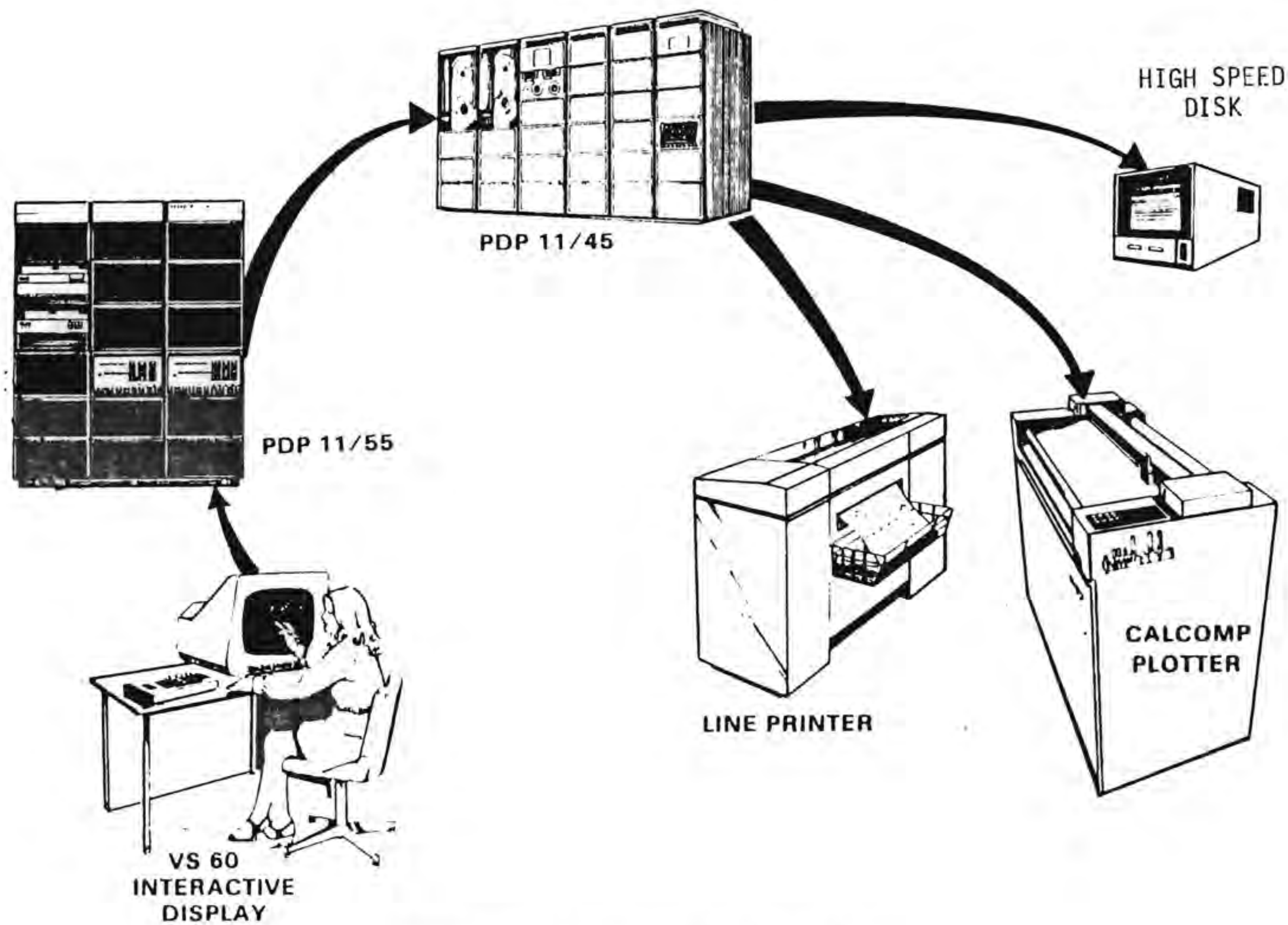

FIGURE 2. Computer Configuration

removable cartridge disk, a 300 megabyte disk drive with removable pack, a DEC VS-60 refresh vector scope with light pen, a line printer, and three-pen plotter. The availability of over 300 megabytes of dedicated, on-line, rotating storage provides the important ability to sacrifice storage space for more rapid data access. The light-pen-sensitive CRT gives enhanced user control of data base software and allows rapid display of analysis results. Plots of data points, graphs, histograms, curve fits etc., are possible on the CRT. In addition, histograms, graphs, covariance matrices, experimental data, etc., can be directed to either a Calcomp plotter or lineprinter for hard copy output.

At the inception of SIRS, the PDP 11/55 was readily accessible to the PNL experimenters and safety assessment modelers. Simple statisitcal packages based on subroutines within International Mathematical and Statistical Library (IMSL) are available.

The disadvantages of the system result directly from its strengths. The hardware configuration is probably unique and much of the system level software has been developed by PNL scientists. Programming in such an environment is generally more complicated and time consuming, though performance can be considerably enhanced. The data base software developed on this system is not transportable or readily adaptable to other computers. Also, the facility is a "hands-on" interactive tool not amenable to off-site use. At SIRS inception in the fall of 1978, data base use was anticipated only by PNL geoscientists and safety assessment modelers, hence the decision to proceed with development on the 11/55 system. Since the initial efforts, several events have occurred which have exacerbated the disadvantages of the SIRS system.

In February of 1979, a group of European scientists visted PNL and were briefed on the SIRS concept. It became apparent to all present that an international Kd data bank would be quite useful. In addition, the attributes of SIRS to help identify sorption mechanisms appealed to several experimenters. Finally, the Office of Nuclear Waste Isolation (ONWI) recognized that computer model transferability to other agencies such as the NRC would be of great benefit during model verification and validation. The Europeans also have recently

(August 1980) requested that any cooperative sorption-retrieval system be compatible with computer facilities of the Nuclear Energy Agency (NEA) at Saclay, France. Future directions to accommodate these events and findings since SIRS has become operational are discussed later in the recommendations section.

With the described PDP 11/55 hardware and the experimental data format described in Appendix A, a detailed initial design of the data base software was performed. Two factors predominantly influenced data base design: 1) data characteristics and 2) data analysis methods. Data characteristics are the nature of the data itself; record lengths, data types, number of records, data interrelationships, etc. Data analysis methods are the ways which data will be processed such as types of statistical tests, data subsetting and data output formats. Data characteristics and data analysis techniques affect each other and thus affect software design.

DATA CHARACTERISTICS

Important considerations regarding data characteristics are logical data grouping, data interrelationships, and types of data. These factors directly influence data storage methods and data identification. Simple, efficient data storage methods and data identification schemes are necessary to minimize software development time, simplify software modification, minimize data processing time, and promote data base understanding.

The most consistent data grouping is the experiment itself. Although Kd is the focal point, all data characterization on a sorption experiment is important. Geochemists intend to define relationships among important variables using SIRS to compare different experimental results. Definition of these relationships should lead to a better understanding of sorption chemistry and the Kd measurement. A fully characterized sorption experiment has approximately 100 parameters describing it. Experimenters generally record something less than the maximum number. Figure 3 shows the major parameters necessary to fully characterize a sorption experiment. The description of each parameter is broken into several levels. For example, the first level descriptor "Reference' is divided into five descriptors at the next level-'Name', 'Lab',

Reference	Exp. Details	Geologic Matter	Aqueous Phase (Begin)	Aqueous Phase (End)	Nuclide	Adsorption-Function
A. Name	A. Method	A. Name	A. Macro	A. Macro	A. Iso	A. Kd
B. Lab	B. State	B. Origin	B. Trace	B. Trace	B. Conc	B. Units
C. Source	C. Ratio	C. Total			C. Spe	C. Dir
D. Quality	D. Time	D. Mineral			D. Add	D. Num
E. Time	E. Temp	E. CO_3			E. Loading	
	F. ATM	F. OX				
	G. SEP	G. CEC				
	H. Analyze	H. AEC				
	I. Rad	I. SA				

FIGURE 3. Sorption Experiment Organization

'Source', 'Quality', and 'Date'. These descriptors can be divided also, but Figure 3 shows only the first two levels of data descriptors for illustration. Data descrptors will also be referred to as data categories. Within SIRS, data categories exist to the fourth level, with each succeeding level being logically related to the previous ones. Appendix A contains a complete description of all existing experimental parameters.

The organizational structure of sorption experimental data as illustrated in Figure 3 lends itself to a hierarchical data base approach. Hierarchical data bases relate data consisting of several levels of descriptors or categories. In hierarchical structures or "trees", each main category branches out or subdivides into several other categories designated as lower level. Conversely, each end point of data can be completely characterized or described by proceeding back through (up) the hierarchy.

A hierarchical structure fits the logical organization of the sorption experimental data and provides acceptable organization for anticipated data analysis techniques. Precise combinations of experimental parameters compared during analysis cannot be identified a priori. The main purpose of SIRS is to allow the capability to compare a variety of variables from many experiments. This cross-comparison capability coupled with a sufficiently large data set will enable the geochemists to define major relationships and important variables.

In light of the goal of extensive cross-comparison of data, a simple and flexible method of uniquely identifying each data point for computation purposes was necessary. The hierarchical structure was readily adapted to an indexing system which accomplished this. Each data category at the first level in Figure 3, 'Reference', 'Experimental Details', 'Geologic Media', 'Aqueous Phase', etc., were assigned a number from 1 to N1 (N1 being the total number of data categories at that level). Each level 1 category is subsequently broken into N2 categories at the next level, level 2. This process proceeds until all levels of data categories have identifying indices.

As mentioned at present, SIRS has a maximum of four levels of data categories. Thus, a unique identifier consisting of four indices can be associated with each data category. This association of numbers and data category descriptors is necessary for efficient computer processing of experimental data. Figure 4 shows how the 'Experimental Details' category of Figure 3 would be divided into its data categories at all four levels. Also, each data category has its associated four number index. For example, the four number index 2,1,0,0 identifies the level 2 category 'Method'. 'Method' can be further divided at level 3, one division being 'Batch'. 'Batch' unique identifying index is 2,1,1,0. Appendix B contains the indices of all presently available data categories. The indexing method is flexible and can accommodate changes in the number and content of the data categories. As SIRS operation continues, data categories will undoubtedly be added, deleted, or changed.

The last major concern for experimental data characteristics is data type. Experimental data is found in three forms: as a number, a descriptive label, or a comment. Each data point will generally be a number or a label, but sometimes pertinent comments are attached by an experimenter to a data point. For example, the descriptor 'PNL' could be a label indicating which organization performed a reference experiment. The number 7.0 could represent a measure of pH. In addition, either of these type data points could have additional information specific to that number or label. The comment data type handles this additional information. By using numbers, labels, and comments, most experimental information can be transmitted from the laboratory to the computerized data base. Individual categories of the data tree or hierarchy are represented as labels or as ranges of numbers. Numeric data are divided into a finite number of ranges. Otherwise, there would be an infinite number of data categories for numeric data. An example range might be '7.0 to 8.0' for pH or '0 to 15 ml' for sample volume (as seen in Figure 4 at level 4).

The indexing system provides a simple, flexible way of uniquely identifying individual data points. The identifying indices for each data category are consistent with the hierarchical data structure. The data base capability of handling the three types of information--numeric, label, and comments--permits maximum transmission of experimental data for subsequent analysis by SIRS users. Experimental data is grouped logically by experiment consistent with analysis goals. A more detailed description of data formatting and data input can be found in Appendices B and C.

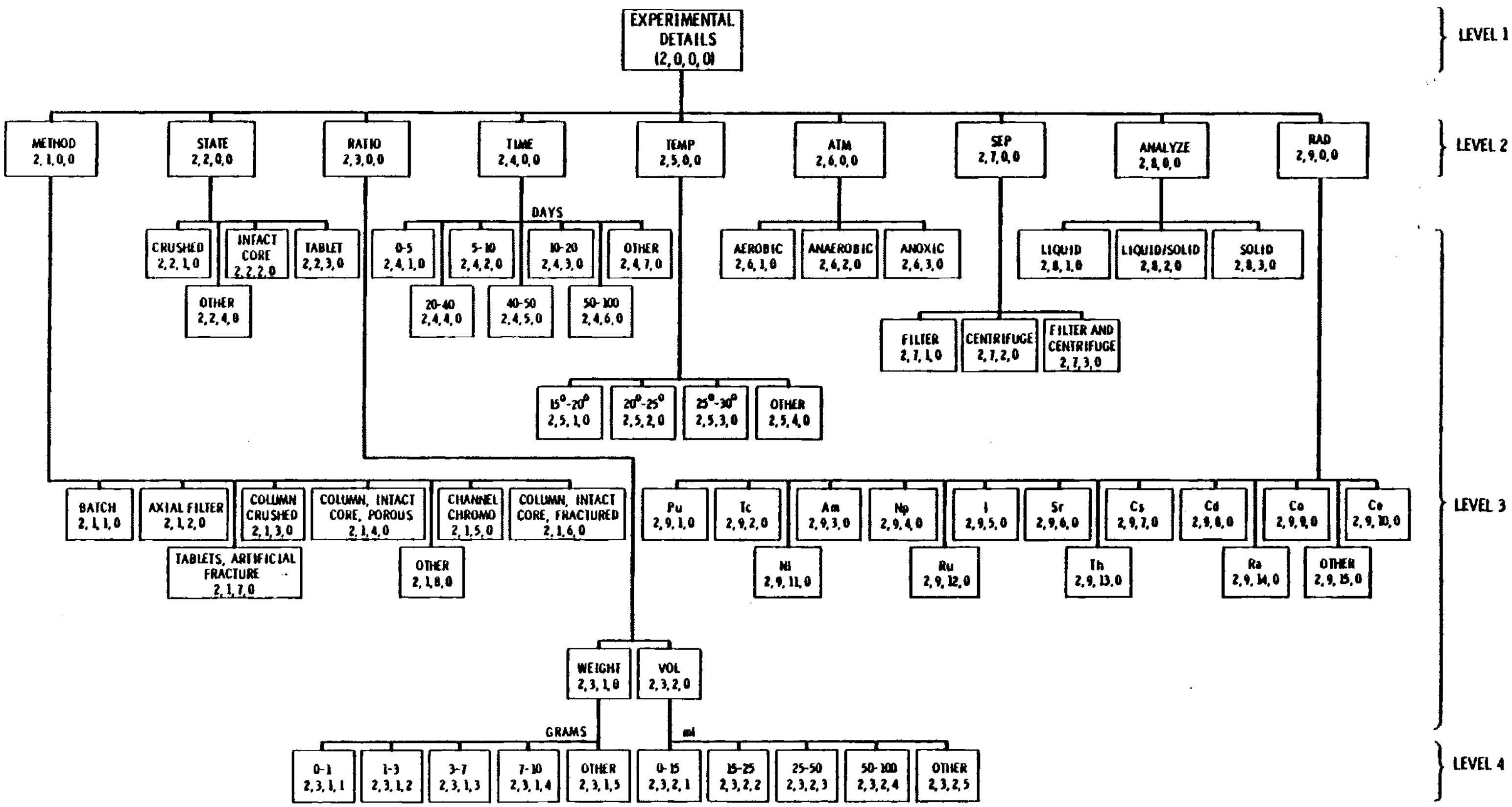

FIGURE 4. Example of Hierarchial Tree

DATA HANDLING AND ANALYSIS TECHNIQUES

To date, the primary users of SIRS are PNL experimental geochemists. Extensive data subsetting capability, rapid data retrieval, simple statistical analysis, and interactive graphic output are the features necessary to best serve the experimental geochemists' purposes. For the safety assessment modelers, rapid data retrieval and simple statistical analysis should prove to be the most important attributes. The previous section described the characteristics of sorption experimental data and its hierarchical organization. Data identification methods were developed while considering data storage and data processing needs. General data manipulation techniques will be discussed in this section.

SIRS software can be divided into three general groups: 1) data input, 2) analysis, and 3) auxiliary computer routines. Data input programs establish data base characteristics, check raw experimental data, pre-process experimental data, and provide limited data editing capability. Analysis routines provide user subsetting ability, statistical analysis and hard copy graphics. Auxiliary programs perform desired data base user functions but are not integral parts of data base software. An example would be the inventory program which calculates decay products resulting from nuclear power reactor wastes used by the safety assessment modelers. Other auxiliary programs will undoubtedly be established as data base use proceeds and specific user needs become defined.

Data Input Software

The data input routines serve the vital functions of creating the data files and assuring data integrity. These routines are not the highly interactive analysis programs available to the geochemist data base user, instead they constitute accounting and storage programs.

Experimental data are first recorded on 80/80 sheets in a format consistent with the established indexing method (see Appendices B and C). These data are then entered by teletype or card reader to computer disk files.

Next, the raw data are processed by an input computer program that checks for any inconsistencies or errors. For instance, numeric information is checked against allowable ranges of that data. Also, maximum record lengths encountered are checked and recorded.

Since a dominant function of SIRS is data subsetting, it is important that subsetting be as efficient as possible. Disk space is not a constraint, but data retrieval speeds are. Consequently, a certain amount of pre-processing helps by calculating location pointers for certain data subsets and storing these in disk files. Individual data categories were chosen as the smallest subsets for which location pointers were generated. Data base user subsetting simply takes these pre-processed pointers and creates larger subsets of the sorption experimental data. For example, a user might desire to analyze the subset of experimental data involving basalt as the geologic media and cesium as the radioisotope. The locations of sorption experiments with basalt and cesium data would be readily available in disk files generated previously, thus drastically reducing real-time processing but using more disk resource. This practice is often called generating 'inverted tables'. The actual random disk storage of sorption experimental data and the generation of location pointers for individual data categories are the key to the data input routines.

The last function performed by data input programs is checking the input data. Input data to be checked can be either the experimental data itself or any supporting data such as the data categories (labels and numeric ranges), data category descriptions, units, or data types. All supporting information is stored in disk files originating from the initialization of the data base characteristics. The data base initializing program is used once for data base initial definition and can be used later for altering data base characteristics. These characteristics consist of indexing dimensions, file sizes, file names, permissible record lengths, etc. After declaring these parameters, all data categories, descriptions, units, and data types are stored on disk for subsequent access by the analysis routines. A more complete description of these data files and parameters is found in Appendix C.

Data Analysis Software

Data analysis codes perform two functions: 1) data subsetting and 2) statistical analysis. Data subsetting is accomplished by the light-pen selection of the data categories desired for analysis. Statistical analysis consists of a graphic display of sorption data in various combinations. At present, only simple curve fitting and basic statistics are possible with SIRS. These two routines (subsetting and analysis) compose the highly interactive user-oriented portion of SIRS. No data can be altered by analysis programs. Experimental data can only be subsetted, analyzed, and output in various formats.

Data subsettng is simply light-pen selection of desired data categories, which can be easily understood by allowing the user to select and view portions of the data hierarchy. To initialize the data analysis, one would select either 'Data Subsetting' or 'Statistical Analysis' using the light pen and touching the appropriate choice. Figure 5 portrays the CRT screen at this initializing stage. For example, let us assume that the user has selected 'Data Subsetting' and wishes to select a particular subset of the whole data bank. As an analogy, consider the subdivision of data categories within the hierarchy to be branches of a tree. Starting at the lowest level or base of a data tree, a user can proceed to any point in the data tree providing the proper branches are taken. Figures 6, 7, 8 and 9 illustrate how a user selected a subset of sorption experimental data consisting of experiments with a certain percent phyllosilicate content. Such a selection is useful to estimate the importance of a certain family of clays (phyllosilicates) on the sorption of radionuclides. Should one find that as the wt% of these clays increases in rock or sediments that many radionuclides exhibit increased sorption, one could state that sites with high phyllosilicate content in the strata which constitute pathways back to the biosphere would be favored. In addition, one might suggest that backfill barriers consist of such clays to increase the total engineered systems sorption potential.

To select phyllosilicates as a selection criteria, the operator moves the light pen from the level 1 star (*) to the category 3 (Geologic Media) star as depicted on Figure 6. Figure 6 is a hard copy display of what is actually

```
Stop Program

DATA BASE ANALYZER
  Data Subsetting
  Statistical Analysis
```

FIGURE 5. Initial Selection Process

```
                                     Stop Program

                                     DATA BASE ANALYZER
                                       Data Subsetting
                                       Statistical Analysis
   1. Reference
   2. Experimental Details
 * 3. Geologic Media                 DATA SUBSETTING
   4. Aqueous Phase (Begin)          ANALYZER OPTIONS:
   5. Aqueous Phase (End)
   6. Nuclide                          Initialize
   7. Adsorption Function
                                       SPECIFY LEVEL
                                        * Level 1
                                          Level 2
                                          Level 3
                                          Level 4

                                       Search Data Base

                                       Display Exp. Data
                                        Next Experiment
                                        Previous Experiment
```

FIGURE 6. CRT Display During Level 1 Selection on Geologic Media

```
                                            Stop Program


                                            DATA BASE ANALYZER
                                              Data Subsetting
1. GEOLOGIC MEDIA
   1. Name
   2. Origin                                DATA SUBSETTING
   3. Total                                 ANALYZER OPTIONS:
 * 4. Mineralogy
   5. CO3                                     Initialize
   6. OX
   7. CEC                                     SPECIFY LEVEL
   8. AEC                                        Level 1
   9. SA                                       * Level 2
                                                 Level 3
                                                 Level 4

                                              Search Data Base

                                              Display Exp. Data
                                               Next Experiment
                                               Previous Experiment
```

FIGURE 7. CRT Display During Level 2 Selection on Mineralogy

```
                                        Stop Program

                                        DATA BASE ANALYZER
                                          Data Subsetting
                                          Statistical Analysis
3. GEOLOGIC MEDIA
   4. MINERALOGY
      1. Tectosilicates                 DATA SUBSETTING
      2. Cyclosilicates                 ANALYZER OPTIONS:
      3. Nesosilicates
      4. Inosilicates                     Initialize
    * 5. Phyllosilicates
      6. Oxides                           SPECIFY LEVEL
      7. Sulfates                            Level 1
      8. Sulfides                            Level 2
      9. Phosphates                        * Level 3
     10. Carbonates                          Level 4
     11. Chlorides
     12. Other                            Search Data Base

                                          Display Exp. Data
                                           Next Experiment
                                           Previous Experiment
```

FIGURE 8. CRT Display on Level 3 Selection on Phyllosilicates

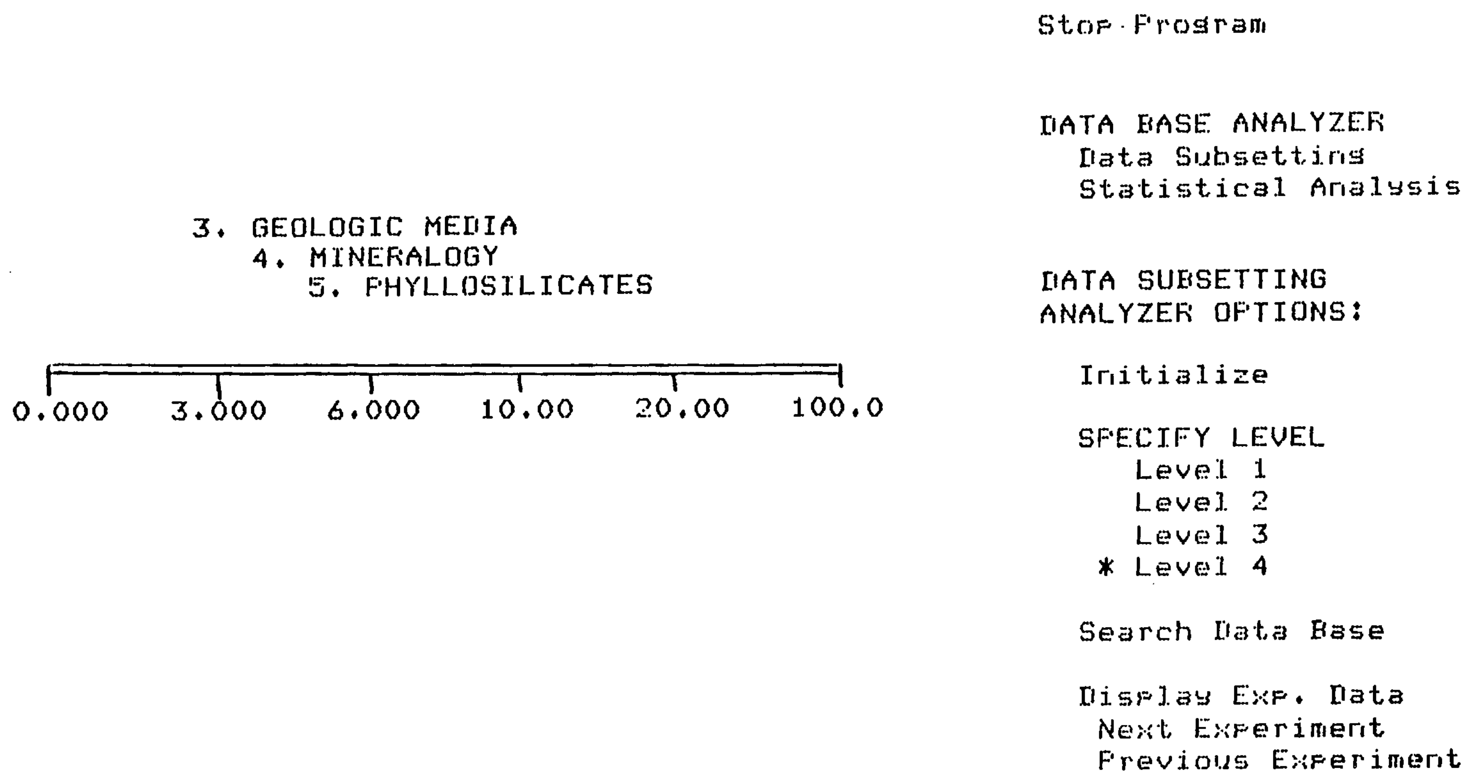

FIGURE 9. CRT Display for Level 4 Selection on % Phyllosilicates

seen on the CRT. After this level 1 selection, the SIRS system will automatically switch to Figure 7. Figure 7 is a hard copy display of the second level hierarchy for Geologic Media. To select on phyllosilicates, the operator simply moves the light pen from the "*" next to level 2 to the category 4 (Mineralogy) star. The SIRS will automatically switch to Figure 8 whereupon the user would move the light pen from the level 3 star to the star in front of category 5 (Phyllosilicates). The CRT will then automatically switch to Figure 9 whereupon the user selects a range of wt% between any other the avilable ranges (0,3,6,10,20,100) by running the light pen from the desired left hand boundary to the desired right hand boundary. In this example, the range 0 to 100% was chosen. If the user wishes to continue defining the selection process such as choosing only a few nuclides or a certain type of groundwater, the light pen would be moved back to level 1 and the process described by Figures 6 through 9 repeated for another level 1 category such as 6 (Nuclide) or 5 Aqueous Phase (End) respectively. Once all the desired selection criteria have been requested, the user initializes the search by moving the light pen "*" to the SEARCH DATA BASE command. The SIRS will then inform the user of how many experiments meet the desired criteria by printing out the following message: [Number of Experiments which meet the chosen criteria: - - -]. The user can then display the selected experiments with all anciliary information one by one on the CRT for review or request hard copy as shown in Appendix A on page A.7. The selection of subsetted data categories can be altered as frequently and often as the user desires. The user can request SIRS to perform simple statistical analysis functions on any particular subset chosen.

Currently, SIRS can perform the following simple statistical and graphical operations:

- calculation of means and standard deviations
- logarithmic transformations
- simple curve fitting (regression) up to the fifth order
- bar graphing
- x-y graphing
- log y-x graphing.

The curve fitting routine solves for the function $y = f(x)$ using either first, second, third, fourth or fifth order terms of x such as:

$$y = a + bx \text{ or } y = a + b x + cx^2$$

or

$$y = a + bx + cx^2 + dx^3 + ex^4 + fx^5$$

The values for the coefficients a, b, c etc. are automatically determined as is the goodness of fit parameter r^2. Upon command, these values are displayed or sent to peripherals for hard copy.

To initiate the analysis, the user would designate 'Statistical Analysis' using the light pen. The CRT screen will automatically display Figure 10. The user would then select one of the options; 'Bar Graph', 'Plot Data', 'Log Plot', 'Graph Data' or 'Curve Fit'. The 'Bar Graph' subroutine determines the simple statistics mean and standard deviation on chosen subsetted data and also allows frequency distributions to be created. Figure 11 is an example bar graph of the number of Kd observations within the installed data base delineated by isotope.

The 'Plot Data' subroutine takes numerical data such as Kd values and creates a two dimensional figure versus another variable such as perhaps solution pH. The 'Log Plot' subroutine is similar to 'Plot Data' except that the variable designated as y is plotted on a logarithmic scale. Figure 12 is a typical two dimensional plot with the Kd Sr on the y axis, and % phyllosilicate on the x axis. The 'Graph Data' and 'Log Graph' subroutines provide only one function, to automatically connect the points within their respective two dimensional scatter plots with a continuous line.

The 'Curve Fit' subroutine is called upon when one wishes to determine the best fit $y = f(x)$ function for two chosen variables.

When one wishes to get a hard copy of any of the above described graphical or statistical representations, one simply activates the 'Hard Copy' subroutine as seen in Figure 10 with the light pen.

```
Stop Program

DATA BASE ANALYZER
  Data Subsetting
  Statistical Analysis

STATISTICAL ANALYSIS
ANALYSIS OPTIONS:

  New Category

  Bar Graph
  Plot Data
  Log Plot
  Graph Data
  Log Graph
  Curve Fit
  Hard Copy
```

FIGURE 10. CRT Display to Initiate Statistical Analysis and Graphics

The combination of subsetting and user-defined comparisons yields definite advantages when working with large experimental data sets. Subsetting takes advantage of preprocessing to minimize run time by limiting the amount of experimental data used for analysis. A wide variety of sorption data is contained in SIRS but it is rarely subject to analysis as a whole. Typically, geochemists work with only portions of the experimental data set hence, subsetting user pre-processed information to reduce data retrieval and analysis times is valuable. User-defined comparisions of subsetted data permit comparison of any experimental data. Though flexible, these comparisons are made at run time (i.e., not pre-processed). Consequently, more processing time is necessary especially as the size of the experimental subset increases. This section has illustrated how data subsetting, statistics and graphic output capabilities can effectively be utilized to perform analysis of experimental data.

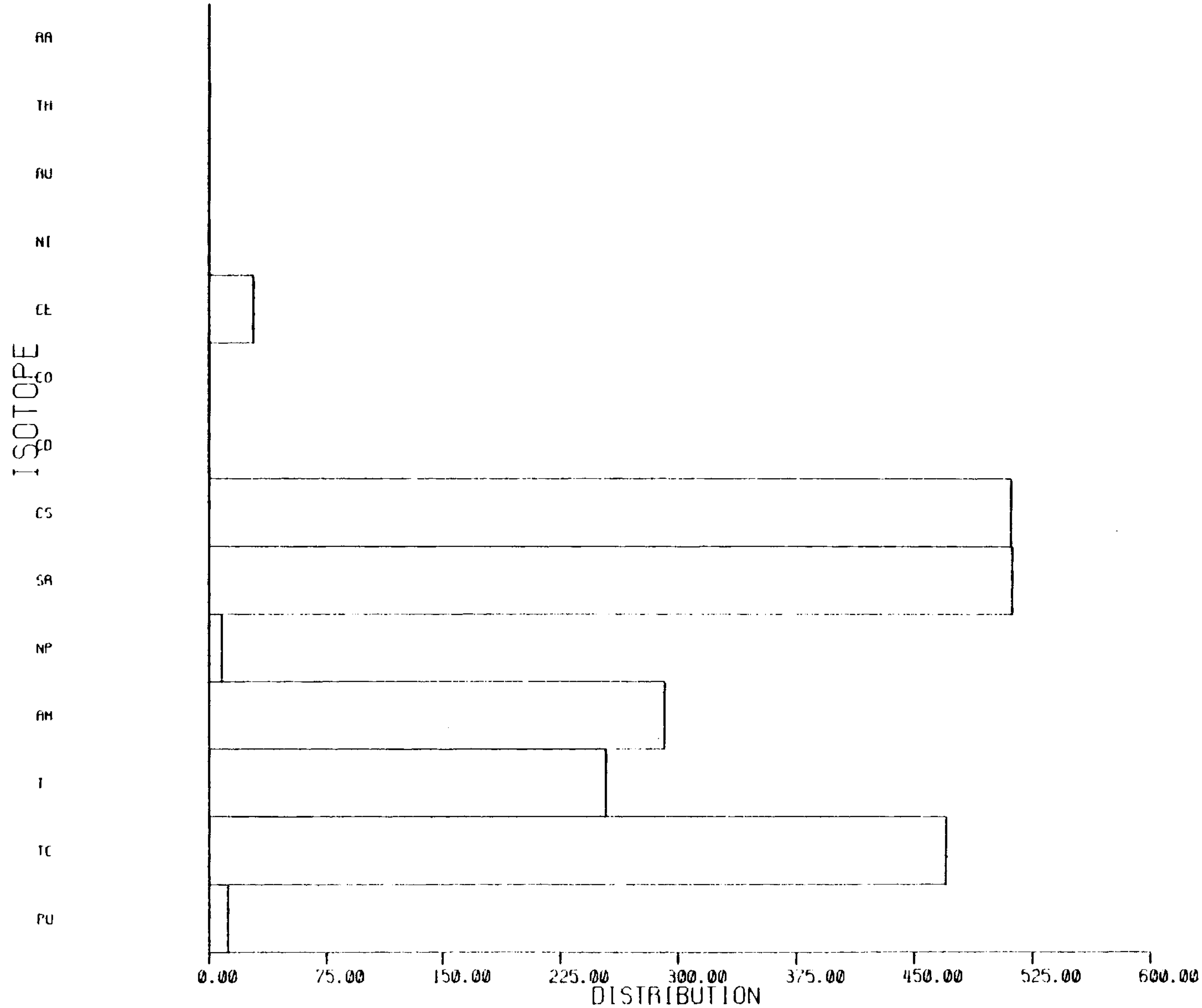

FIGURE 11. Frequency Distribution of Isotopes vs. Number of Kd Values Present in Data Base

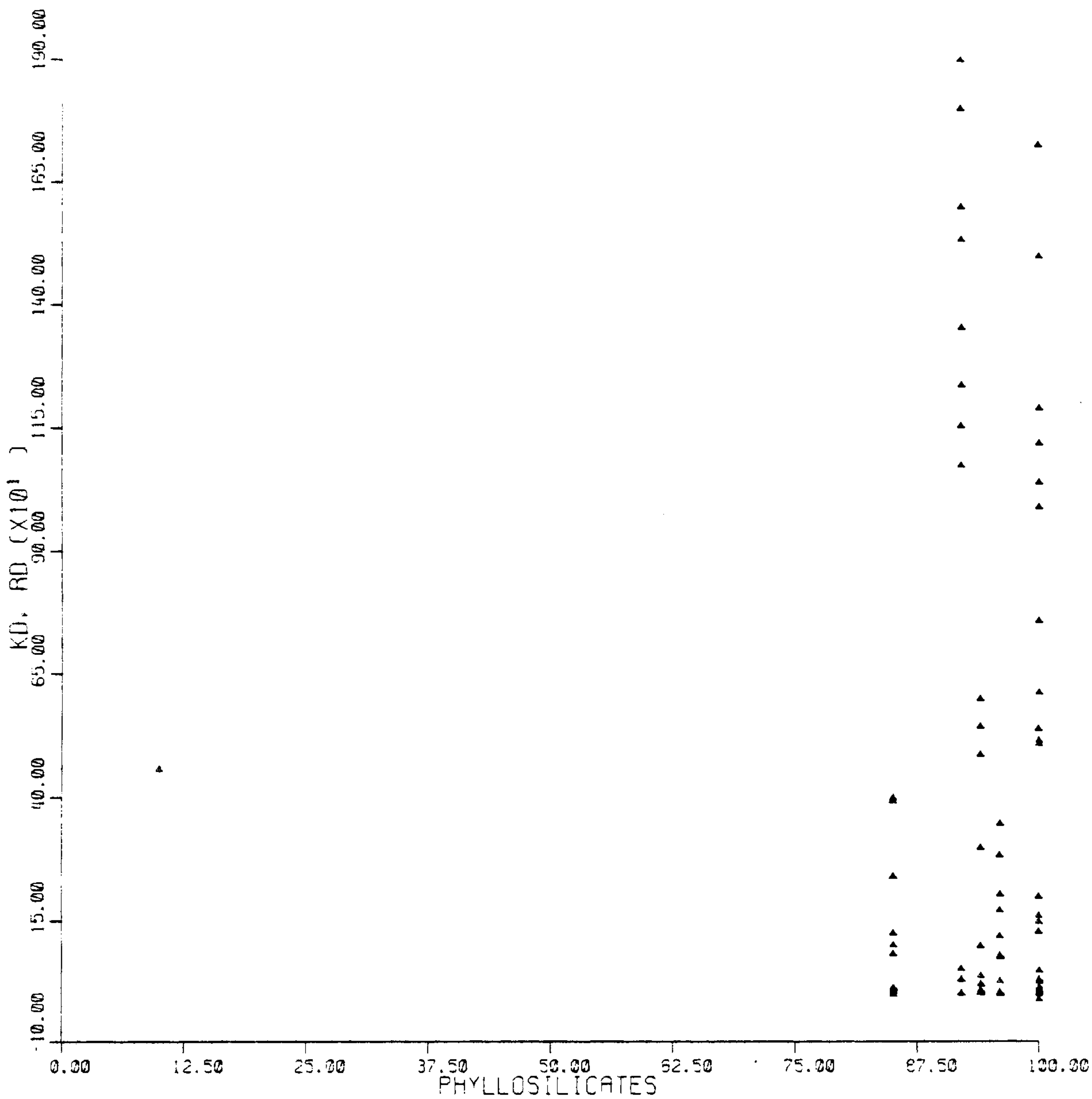

FIGURE 12. Example Scatter Plot

AUXILIARY PROGRAMS

Auxiliary programs are not an integral part of the data base software. Their purpose is to provide a specific capability augmenting data base software. A current example is the inventory program. This program calculates radioisotope waste inventories as a function of time. Safety assessment modelers use this routine to find which radioisotopes are most important at various times after closure of a waste repository. After chossing a starting inventory data file and an elapsed time, the computer routine calculates the remaining radionuclide inventory table up to a million years. Figure 13 shows the cathode ray tube (CRT) output for this program. Modelers can look at Figure 13 and decide which nuclides dominate the inventory versus time and thus select a subset of nuclides to study. They can then extract the pertinent Kd information from the main data base routines for use in contaminant transport and dose modeling. As data base use proceeds, additional auxiliary programs will be identified and developed. These developments can be kept separate from the main data base software, thus making software modification easier. Also, data base software quality assurance will be more easily maintained.

SIRS CURRENT STATUS

As of September 1, 1980, the Sorption Information Retrieval System (SIRS) is operational. The software for data input, data subsetting, simple statistical analyses and data output to various hard copy machinery has been demonstrated on a limited data base.

The current installed data base consists of 2000 laboratory experiments performed at PNL and LASL in FY 1977 and 1978. The available data from the other national laboratories for 1977 and 1978 has been coded and is awaiting installation. The data for 1979 and 1980 has not been formally coded by any of the WISAP/WRIT contractors. Data generated within the United States on other than the WRIT program exists but no provisions have been made to attempt to incorporate these data or to estimate their magnitude or quality. There also exists data from other countries which to date has not been considered for incorporation into SIRS. It is estimated that the backlogged WRIT data will take one year to install and more than triple the data entries.

Given current (FY 1981) funding projections for WRIT, there will be no monies allocted to SIRS refinement or backlogged data entry. Subcontractors will again be required to produce coding forms as shown in Appendix A for all FY 1981 Kd data to facilitate entry into the data base.

ACTIVATION PRODUCT INVENTORY IN REFERENCE ZIRCALOY CLADDING
HULLS AS FUNCTION OF DECAY TIME ALL FUEL CYCLE MODES.

CI/MTHM FOR VARIOUS DECAY PERIODS

RADIONUCLIDE	2.0E+01 YR	1.2E+02 YR	2.4E+02 YR	4.8E+02 YR	9.6E+02 YR	1.9E+03 YR	3.8E+03 YR	7.7E+03 YR	1.5E+04 YR	1.0E+06 YR
C14	6.0E-02	5.9E-02	5.8E-02	5.7E-02	5.3E-02	4.8E-02	3.8E-02	2.4E-02	9.5E-03	
S35										
MN54	1.7E-07									
FE55	6.7E-01									
CO58										
CO60	1.5E+01	3.0E-05								
NI59	3.0E-02	3.0E-02	3.0E-02	3.0E-02	3.0E-02	3.0E-02	2.9E-02	2.8E-02	2.6E-02	5.2E-06
NI63	4.3E+00	2.0E+00	8.2E-01	1.4E-01	3.6E-03	2.6E-08				
ZR93	9.0E-02	9.0E-02	9.0E-02	9.0E-02	9.0E-02	9.0E-02	9.0E-02	8.9E-02	8.9E-02	4.3E-02
ZR95										
NB95										
CD113M	2.7E-03	1.9E-05	5.0E-08							
SN119M	2.7E-08									
SN121M	2.0E-02	1.9E-08								
SN123										
W181										

PERIODS ARE MEASURED FROM REACTOR DISCHARGE

INVENTORY 1

INVENTORY 2

INVENTORY 3

INVENTORY 4

RETURN TO CONTROL

DATA SELECTION

PLOT FILE

PRINT FILE

PAGE FORWARD

PAGE BACKWARD

INVENTORY AFTER 20.Δ YEARS

FIGURE 13. Inventory Setup

A new proposal to DOE headquarters and NEA is being prepared for October 6, 1980 submission. The proposal would allow the existing SIRS system to be hybridized with a more versatile and easily transferable information/ retrieval system, Analysis of Large Data Sets (ALDS) being constructed and implemented for DOE. The proposal would require 1 1/2 to 2 years at a funding level of $150,000/year. Besides making SIRS more versatile and machine independent, the WRIT backlogged data and international experimental data would be installed in the data base (up to 6000 data/yr).

RECOMMENDATIONS

Between the formulation of SIRS in the fall of 1978 and its implementation in the summer of 1980, several events and observations have occurred which lead to the following recommendations.

The initial usage of SIRS as a tool for internal PNL scientists to aid in sorption mechanism identification and Kd selection for safety assessment should be modified to allow others external to PNL such as the Nuclear Energy Agency of Europe and Intera Environmental Consultants, Inc. (a part of ONWI's Waste Isolation Performance Assessment Program) hands on access. The current hardware dependency and highly interactive capabilities of SIRS is not amenable to software transferability.

At the inception of SIRS the chosen hardware, a PDP 11/55 was readily available to WRIT personnel. Since then, a high demand has surfaced for the unique capabilities of the system to aid in the breach scenario generation, boundary geohydrologic conditions generation and site specific data storage and retrieval needed to perform reference site analyses. The demand for the 11/55 system by the AEGIS program has risen to such a level that it is difficult to obtain time to use the system. This is especially critical for the usage of SIRS by experimental geochemists in their pursuit of mechanism identification because their needs currently rate a lower priority. The applications of SIRS for Kd selection for safety assessment still maintains a rather high priority and is given adequate computer time.

After the initial implementation of SIRS, it has become apparent that the system is somewhat inflexible to data input techniques. This results in the need to either demand that the experimenters provide the data in a format more typical of Appendices B and C or that the computer software people expend significant amounts of time restructuring the data by hand. The former demand, that the experimenters transcribe their data in the format of Appendices B and C, has met strong opposition. The protocol is difficult to explain to the experimenter and costly to implement. On the other hand, forcing the computer persons to re-transcribe the data in an amenable fashion has led to additional human errors (incorrect categorizations, misprints and misinterpretations of the geochemistry) and additional costs. Currently, it costs at least $20/data point (one sorption experiment) to get the data installed into the computer with only minimal quality asssurance checking. As this constitutes the major cost by far in implementing SIRS and as little can be done to improve the situation due to machine limitations other alternatives were explored.

It was discovered in early FY 1980 that a new software package called Analysis of Large Data Sets (ALDS) was under development at PNL for the DOE. This multimillion dollar effort to create a versatile software system to sort, to store and to perform sophisticated statistical analyses could very nicely lessen many of the identified shortcomings of SIRS. Some effort has been performed to demonstrate that ALDS can perform all of the basic functions of SIRS excepting a few of the convenient highly interactive (light pen) operations. The preliminary appraisal is that ALDS can perform better all the basic operations and offers many other options and basic tools not a part of SIRS.

Thus, it is recommended that future development work on a sorption information retrieval system be performed via ALDS software philosophy. The existing SIRS will be kept on line for those few instances when the interactive capabilities for PNL geochemists would benefit. Also, some of the added versatility of ALDS may allow "conformed" data to be more cheaply transferred back to the SIRS hardware. In other words, the initial data installation would proceed via the ALDS format requirements (which are less restrictive than current SIRS). Then after ALDS computer generated filing and addressing to binary, the "conformed" Kd data could be switched over to SIRS.

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H. C. Burkholder, J. H. Greenborg, J. A. Stottlemyre, D. J. Bradley, J. R. Raymond and R. J. Serne. 1979. Waste Isolation Safety Assessment Program. Technical Progress Report for FY-77. PNL-2642 Pacific Northwest Laboratory, Richland, Washington.

D. D. Hostetler, R. J. Serne, and A. Brandstetter. 1979. Status of Sorption Information Retrieval System. PNL-3139 Pacific Northwest Laboratory, Richland Washington.

J. F. Relyea, R. J. Serne and D. Rai. 1980. Methods for Determining Radionuclide Retardation Factors: Status Report. PNL-3349. Pacific Northwest Laboratory, Richland, Washington.

APPENDIX A

EXPERIMENT CODING FORMAT

Generic Kd Coding Form
(Revision 1)

Reference	Exp. Details	Geologic Matter	Aqueous Phase (Begin)	Aqueous Phase (End)	Nuclide	Adsorption-Function
A. Name	A. Method	A. Name	A. Macro	A. Macro	A. Iso	A. Kd
B. Lab	B. State	B. Origin	B. Trace	B. Trace	B. Conc	B. Units
C. Source	C. Ratio	C. Total			C. Spe	C. Dir
D. Quality	D. Time	D. Mineral			D. Add	D. Num
E. Time	E. Temp	E. CO_3			E. Loading	
	F. ATM	F. OX				
	G. SEP	G. CEC				
	H. Analyze	H. AEC				
	I. Rad	I. SA				

EXPLANATION OF Kd CODING FORM (REVISION 1)

Category I. Reference

A. Name of Investigator who is reporting results, person who performed experiments, or the person most capable of answering questions on the data. We would like to be able to track each data point back to a knowledgeable person.

B. Lab affiliation of investigator named in A.

C. Source where one could find the results published and described. Please use the following format:

> Author's names, (date), title of paper, journal or lab report and number, publisher where applicable, page number.
>
> If unpublished, use UNP.

D. Quality refers to one's confidence in the data. A critical assessment should be performed which includes identification of limitations, such as lack of certain parameter characterization, unexplained perterbations, etc. For conciseness, we have chosen a five category value system:

1. Excellent quality
2. Above average quality
3. Average quality
4. Below average quality
5. Poor quality

Because this categorization is arbitrary, comments as to why you gave the data are given certain rating are welcome. We would consider the excellent category to include Kd data on which complete characterization of media, solution, and nuclide are available and that have been reproduced several times with good precision.

Average quality would leave some characterization work ill-defined (those which are least important and most costly to determine, have not been reproduced, or have precision no better than ±30%).

Below average data show meager system characterization, little reproducibility, or identified experimental limitations.

E. For quality assurance purposes each data point needs to be dated as to when it was submitted to the computer (calendar year).

Category II. Experimental Details

A. Method refers to batch, axial filter, column, intact core, channel chromatography, etc. For batch add more detail as to whether cold washes and blank corrections were used. For example, use mnemonics such as

BATCH (3W, BC) = batch, three cold washes, with blank tube sorption correction

BATCH (OW) = batch, zero cold washes and no correction.

B. State of geologic media such as crushed 40μm; intact core 2.5 cm dia x 5 cm; tablet 1 cm x 0.5 cm; crushed 30-80μm, etc.

C. Ratio of solids to solution for batch Kd; for columns include pore velocity or column velocity (for example, 1 PV = 1 cm/hr CV = 0.5 cm/hr) and porosity and column bulk density; n = posority; Bd = bulk density

D. Time of contact such as shaking time for batch system or residence time in flow through columns (h) = hours, (d) = days

E. Temp is the temperature of the experiment in °C.

F. ATM is the equilibrating atmosphere air, N_2, Ar, 10% CO_2 - 90% Ar, etc.

G. Sep separation technique; did you use filters (state median pore size) or centrifugation, (include approximate g's)

FIL(.4) = filter 0.4μm

CEN(50) = centrifuged at 50 g's where g = 980 cgs units

H. Count state whether the Kd is determined by counting LIQUIDS only or SOLID and LIQUID

L/L = liquids only

S/L = solid and liquid

I. RAD List other radioisotopes which were run simultaneously in the experiment just in case we determine certain nuclides affect other nuclides.

Example: Sr, Cs, Tc means these isotopes were run together.

Category III. Geologic Media

A. Name Use the generic name of the rock or mineral; basalt, granite, montmorillonite, etc.

B. Origin Geographic description, formation information, etc.

Eleana shale, Sentinel Gap basalt, Argillaceous Shale Wards #404561, etc. For controlled sample rocks that we provided, where in doubt we can add the description.

C. Total Chemical composition as oxides (SiO_2, $Al_2O_3 TiO_2$, FeO, MnO, CaO, MgO, K_2O,Na_2O, P_2O_5, etc) in %.

D. Minerals Present in rock sample, list major ones first, minor ones last; if possible in order of composition (largest first). If there are quantitative estimates add this information as % and tr $\leq$ 5%.

E. CO_3 = carbonate content of rock

F. OX = hydrous Fe, Mn, Al oxides content of rock

G. CEC = cation exchange content of material, units = meq/100g. Specify pH of system (typically pH = 7).

H. AEC = anion exchange content of material, units = meq/100g. Specify pH of system.

I. SA = surface area; use "EG" for ethylene glycol, "BET" for gas adsorption, use units m^2/g, for example, EG(1.3)

Category IV. Aqueous Phase

BEG signifies before tracer adsorption begun, END signifies at the same time as Kd determined.

A. Macro Constituents include:

(1) pH
(2) Eh (units vs S.H.E.)
(3) Na
(4) Ca
(5) K
(6) Mg
(7) Cl^-
(8) HCO_3 $-CO_3$
(9) SO_4
(10) SiO_2

B. Trace constituents include:

(11) NO_3, ppm
(12) Organic carbon
(13) B
(14) Trace metals or anything else measured

Category V. Nuclide

A. ISO Isotope used such as ^{237}Pu, ^{95m}Tc, etc.

B. CONC Concentration added to groundwater in M = molarity. Include any carrier if present.

C. SPE Species or valence state added if known; also if the valence state distribution was determined after equilibration state, such as:

Pu(VI)BEG; Pu(IV)15%, Pu(V)50%, Pu(VI)10%END

means the original spike was 100% Pu(VI), and after shaking the final distribution was as shown.

D. ADD describes how the tracer was added to the groundwater, such as DRY means evaporated to dryness and gw added; WET/PH/3DF0.4 means a small aliquot of liquid tracer was added to the groundwater, the system re-pH'ed to the appropriate value and shaken for 3 days prior to filtration through 0.4μm filters before usage.

DRY/1DC50 means the dried spike was brought back into solution equilibrated for one day, and centrifuged at 50 g's before usage.

E. Loading describes (a) the percent of total exchange capacity of the adsorbent fill with the nuclide of interest or (b) the mass of nuclide adsorbed/mass of adsorbent at the condition when the Kd measurement is performed. This value can be calculated from knowledge of the cation or anion exchange capacity in case (a) and mass balance considerations. One must know the original mass of nuclide used in each experiment.

Category VI. Adsorption Function

A. Kd Place the value for Kd or Rd, whatever you prefer to call it. If a retardation factor is determined in a flow-through column as a function of water velocity, designate by the symbol RF.

Where several measurements were made, also give the standard deviation, such as

75 ± 12 = a Kd

(RF) 60 ± 30 = retardation factor

B. UNITS ml/g or ml/m^2 or LESS = unitless

C. DIRECTION ADS = adsorption direction

DES = desorption direction

A spike addition to a column would be ADS-DES

D. NUM = number of observations used to derive data point, for example 3 = triplicate samples

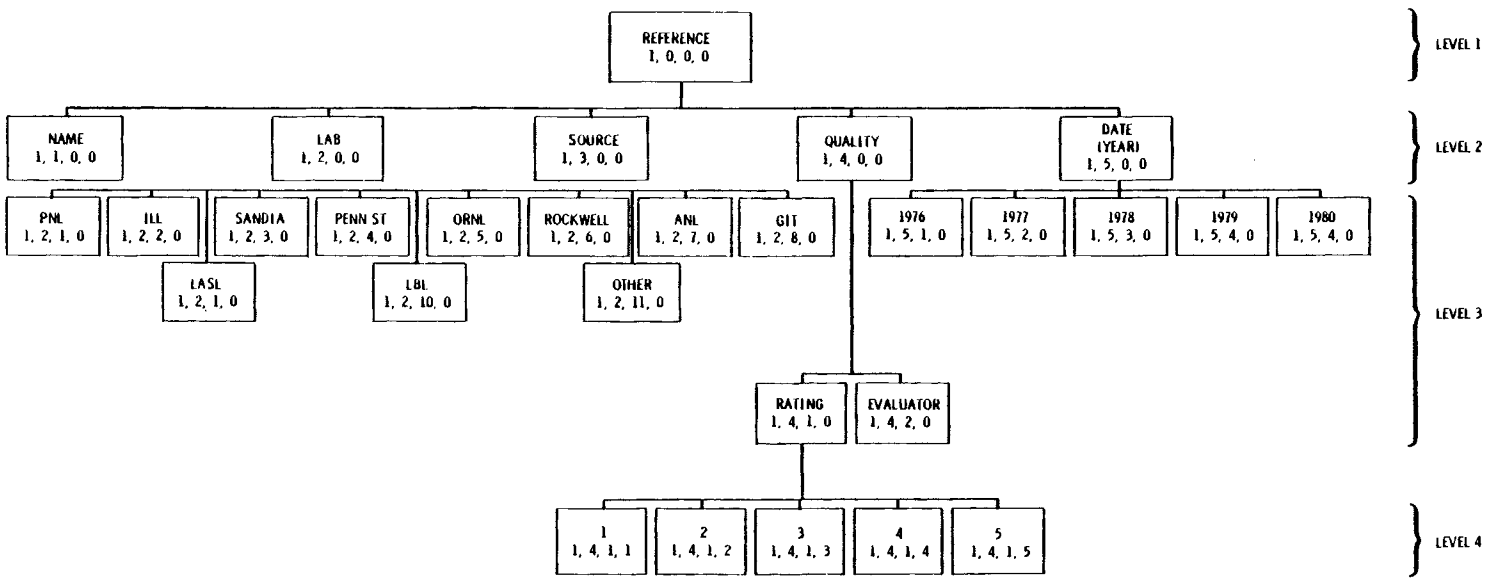
Example of a Batch Kd Experiment by Relyea

PNL Batch Kd for Microcline

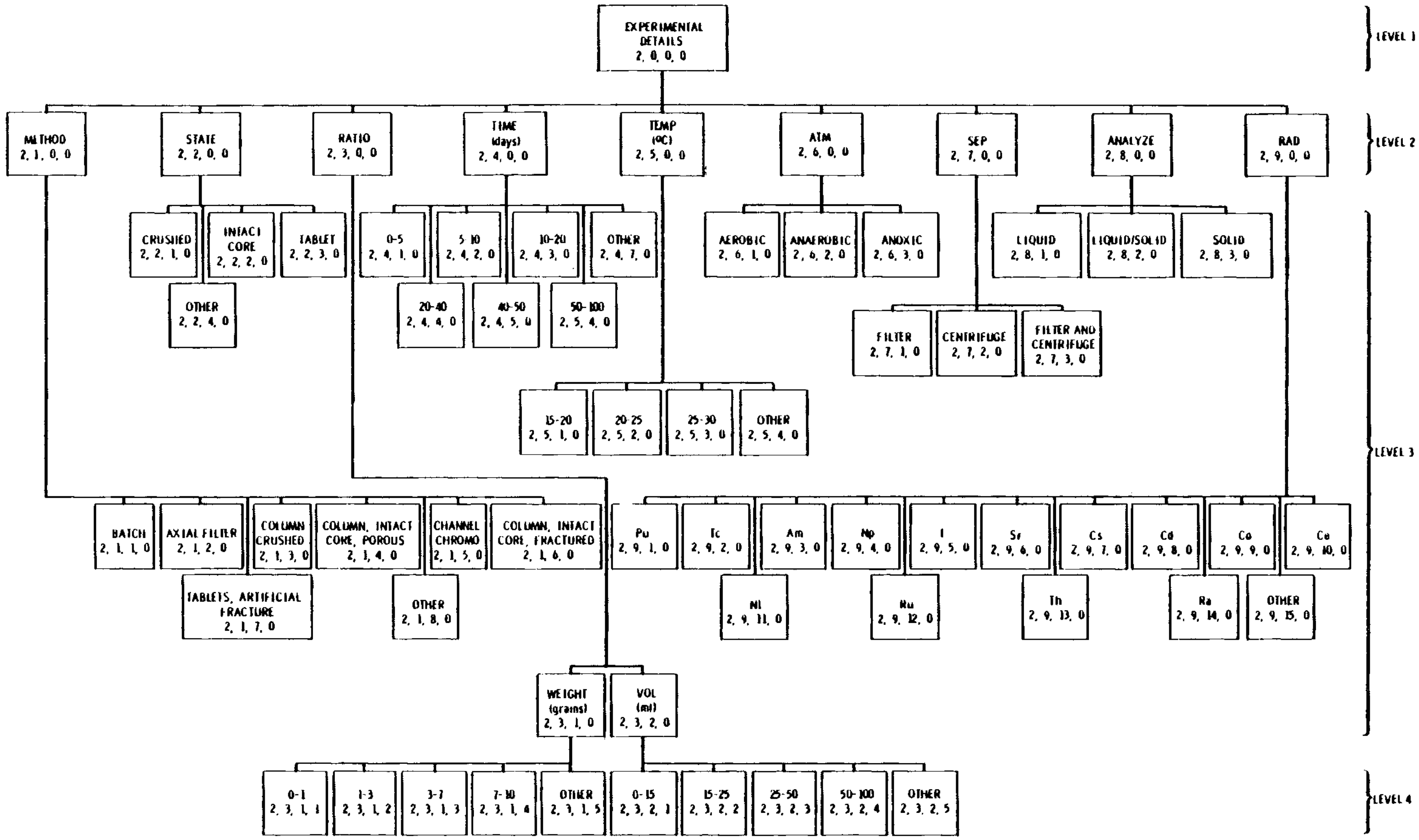
Reference	Exp. Details	Geologic Media	Aqueous Phase		Nuclide	Adsorption-Function
A. J. F. Relyea B. PNL C. WISAP Task 4 Contractor's Information Meeting Proceedings, October 2-5, 1978, to be published D. 2 E. 1978	A. Batch (3W,BC) B. Crushed 100 m C. 0.5g/15ml D. 29d E. 25 C F. Air G. Cen (70) H. L/L I. Sr, Cs	A. Microcline B. Parry Sound Ontario (Ward's Scientific) C. SiO_2 67.5 Al_2O_3 17.1 TiO_2 N. D. FeO 1.8 MnO N.D. CaO 0.1 MgO tr 0.1 K_2O 13.6 Na_2O N.D. D. Microcline - 83% $(K_{3.95})(Al_{3.95}$ $Si_{12.05}O_{32}$ Quartz - 15% (SiO_2) Calcite - 1 to 2% $(CaCO_3)$ Garnet - 1% Almandine-Pyrope Garnet, $(Fe_{2.69}$ $Mg_{4.14})(Fe_{1.00},$ $Al_{.47},Si_{5.53},$ $O_{24})$ E. 1% F. Not determined G. 1.2 ± 0.3, pH=7 H. Not determined I. E.G. (6.1 ± 1.0)	A. Beg. B. pH 8.2 Eh(mv) UNK Na 690ppm Ca 0 K 0 Mg 0 Cl 0 HCO_3 1350ppm CO_3 0 SO_4 0 Si 0 C. NO_3 UNK B UNK B UNK Tr.Mat UNK	A. End B. pH 9.25 Eh(mv) 312 Na 654ppm Ca 4ppm K 20ppm Mg 0 Cl 9.4ppm HCO_3 157.1ppm CO_3 75ppm SO_4 ND Si 30ppm C. NO_3 UNK OC UNK B 2.8ppm Tot.Fe 9.1ppm Tot.P 0.2ppm Tot.Al 4.8ppm	A. Tc B. (approx.) $1x10^{-8}$M C. TcO_4^{-1} Beg D. Wet/pH/7DF0.45 E. Not determined	A. 0.61 ± .13 B. ml/g C. Adsorption D. 3 reps

APPENDIX B

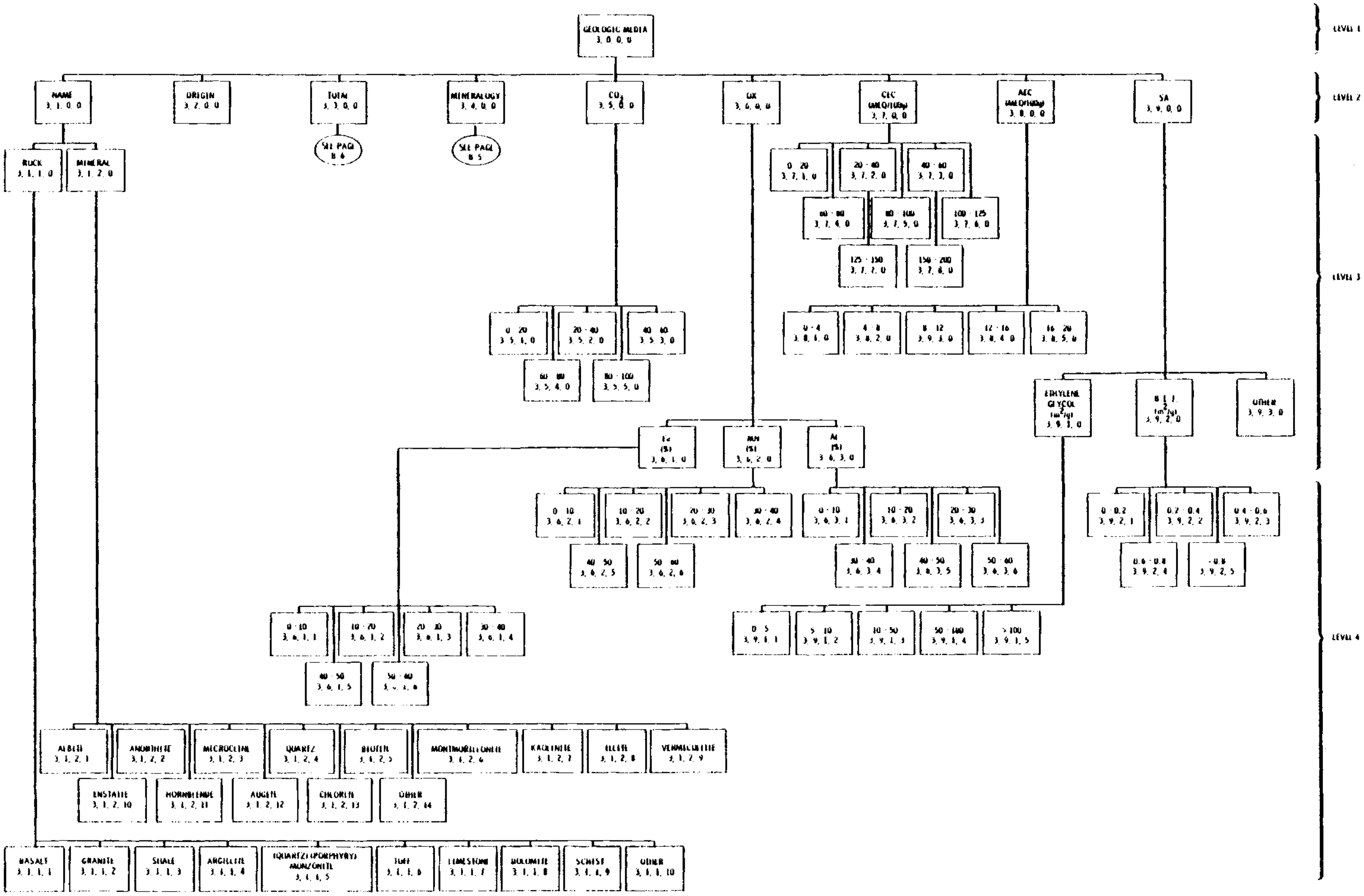
DATA INDEXING METHOD



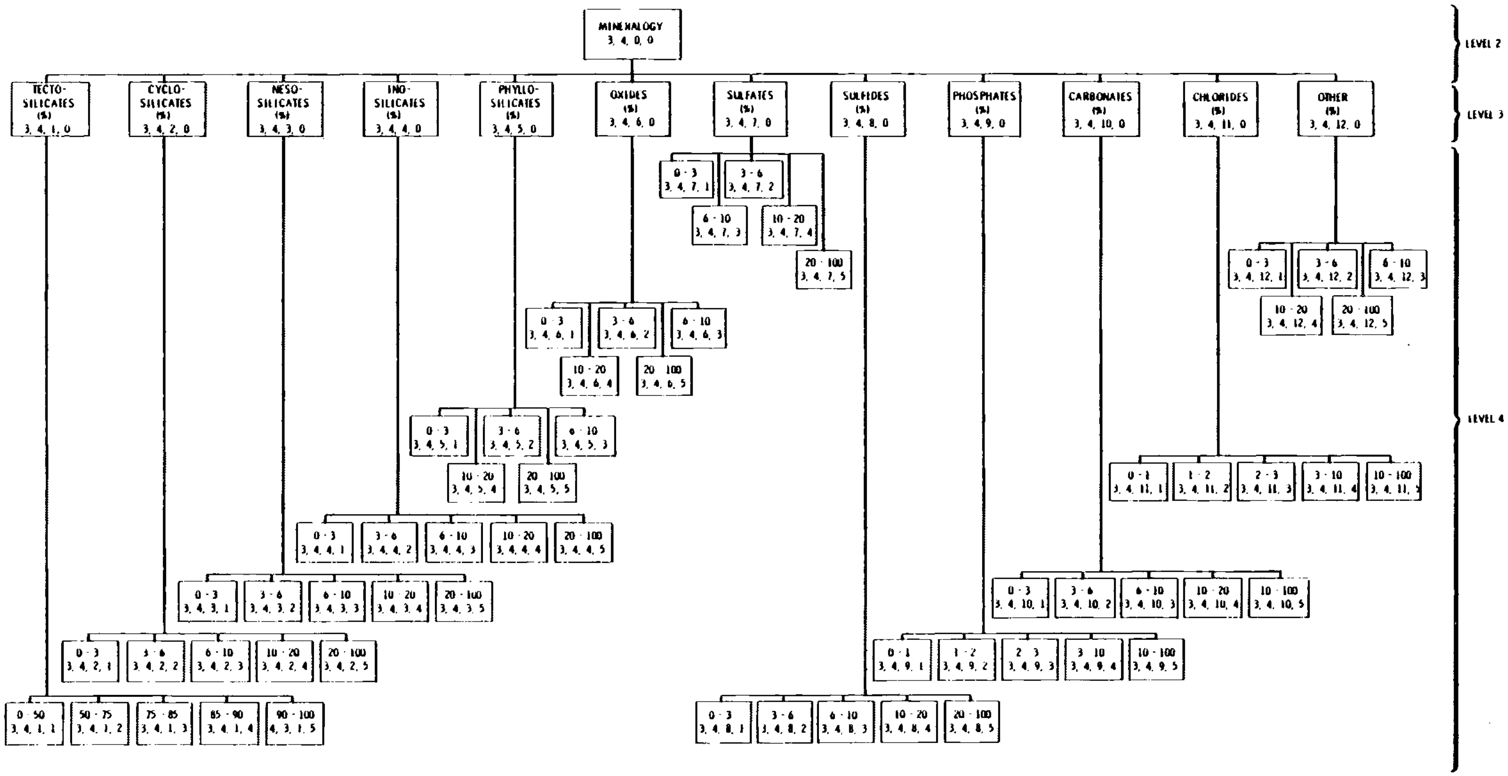
'Reference' Category Indexing Structure



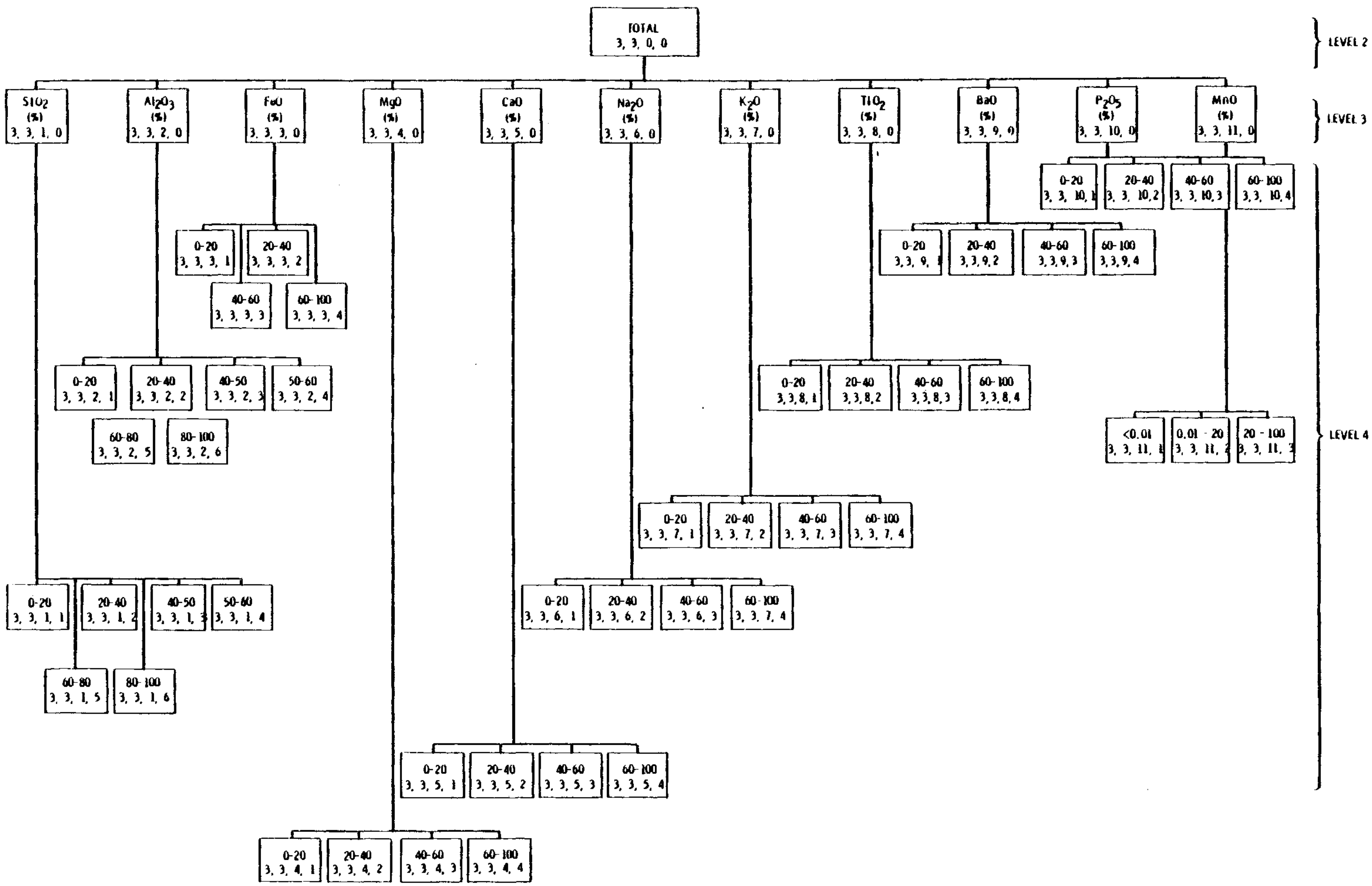
'Experimental Details' Category Indexing Structure



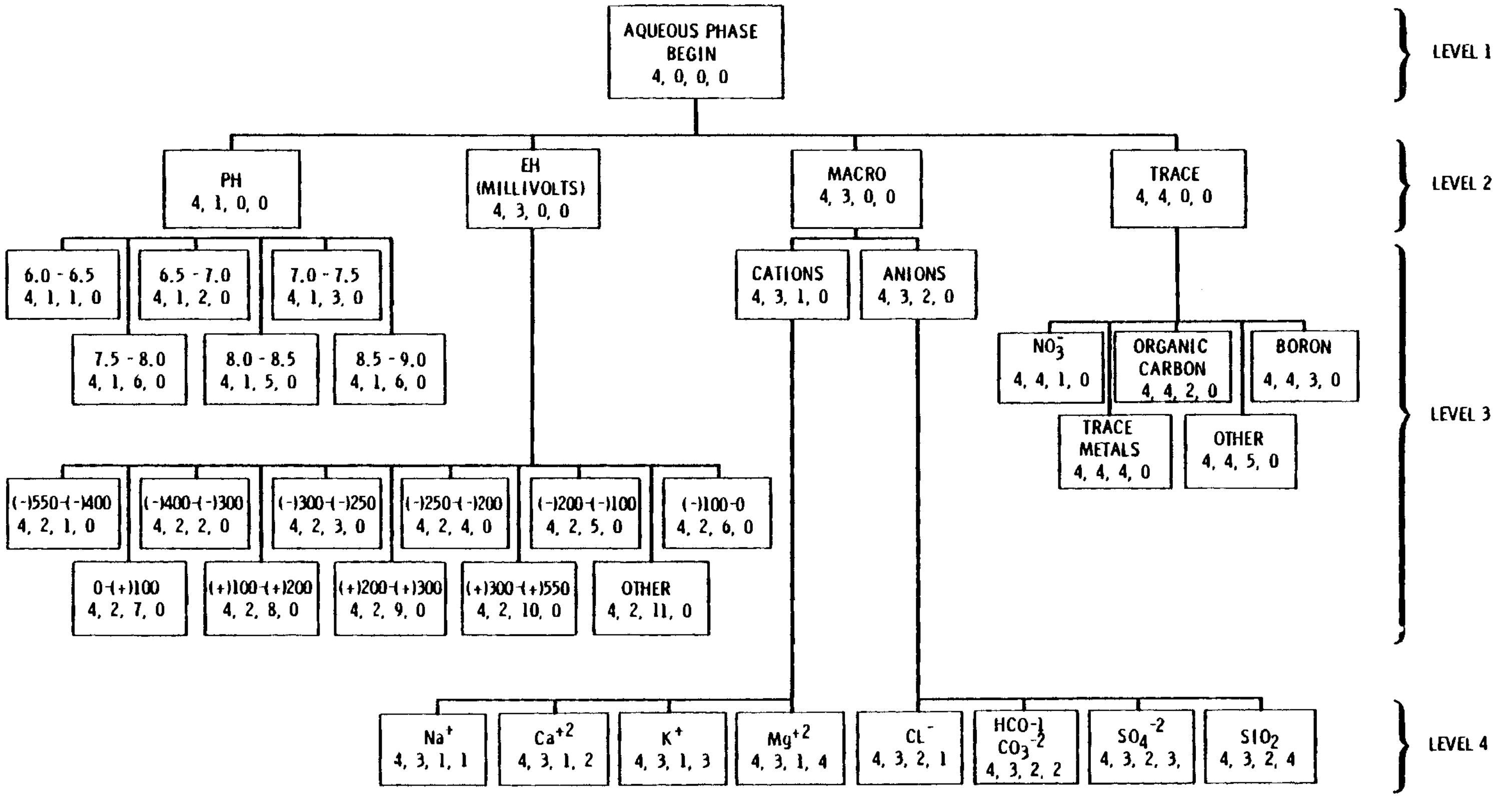
'Geologic Media' Category Indexing Structure



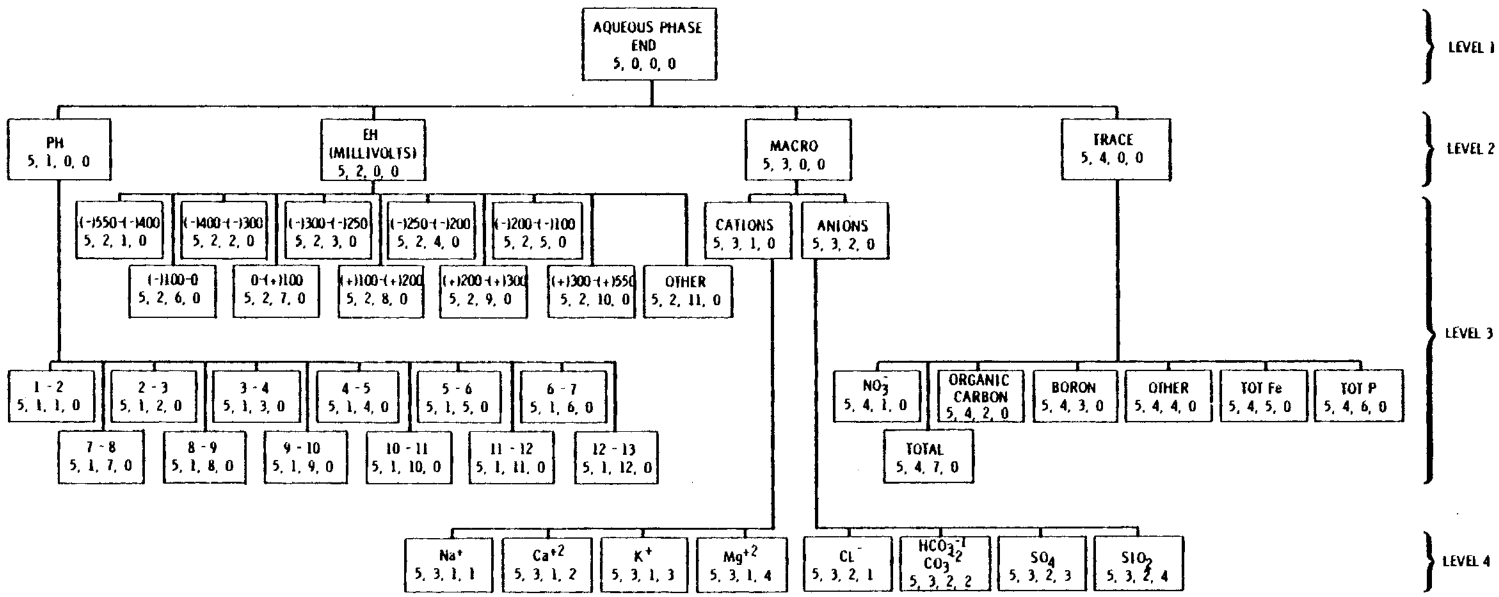
'Mineralogy' Subcategory (under 'Geologic Media' category) Indexing Structure



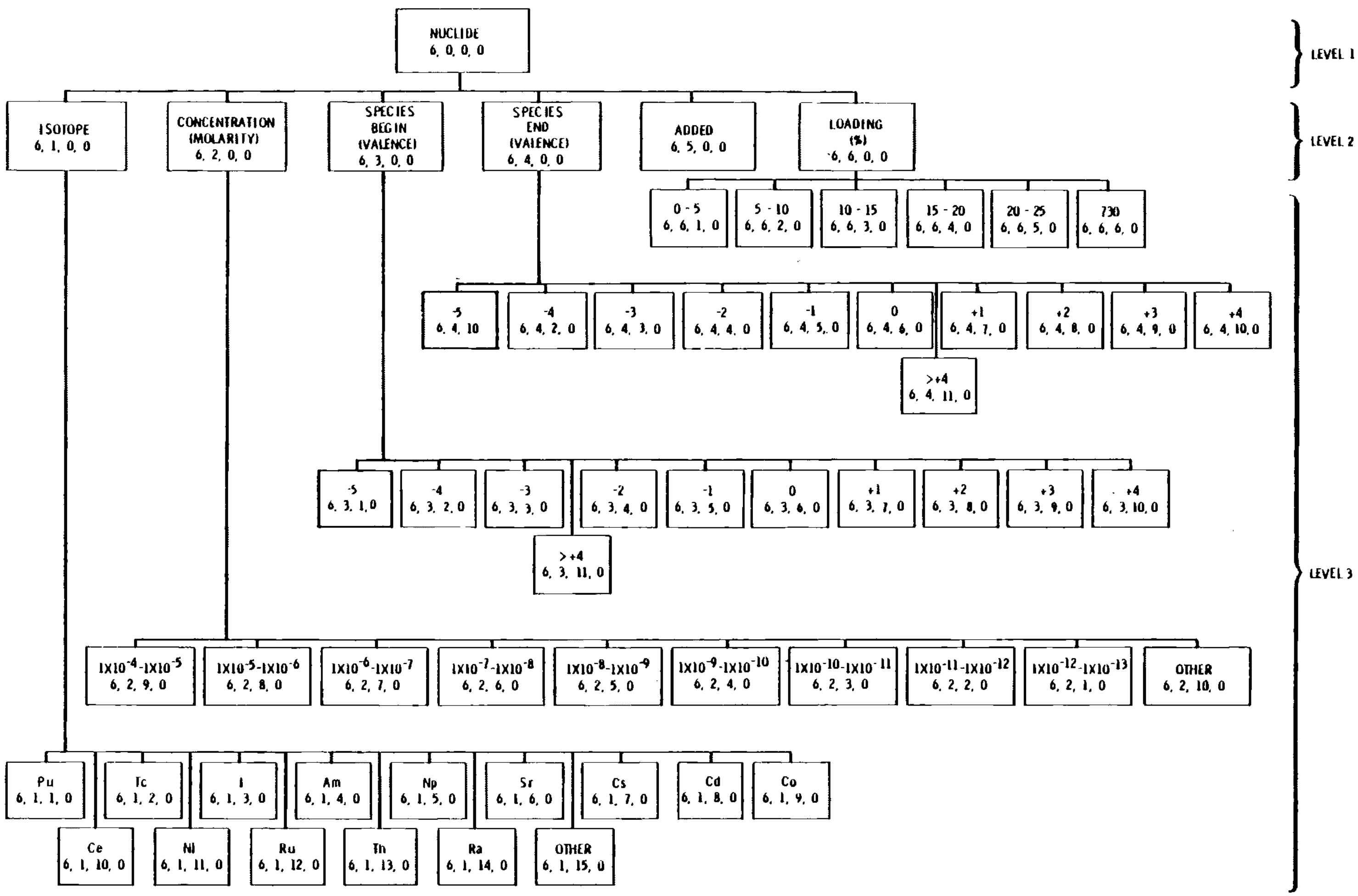
'Total' Subcategory (under 'Geologic Media' category) Indexing Structure



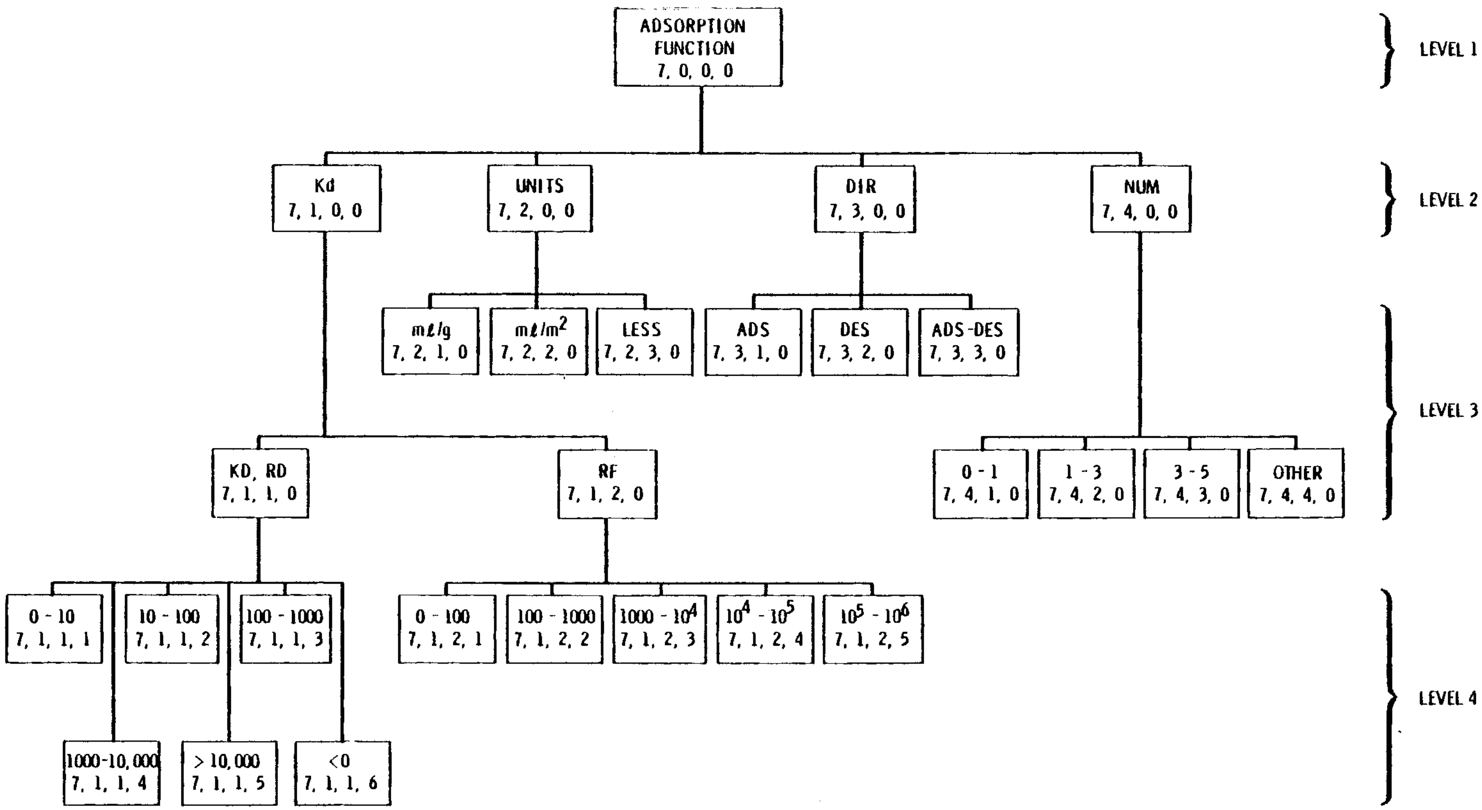
'Aqueous Phase (Begin)' Category Indexing Structure



'Aqueous Phase (End)' Category Indexing Structure



'Nuclide' Category Indexing Structure



'Adsorption Function' Category Indexing Structure

APPENDIX C

DATA INPUT METHOD

APPENDIX C

DATA INPUT METHOD

Prior to FY 1980, experimental data from WRIT contractors has been received in a format consistent with Appendix A. This data has in turn been placed in a format consistent with a coding tree found in Appendix B. Conversion of data to coding tree format is necessary prior to data input to the SIRS (Sorption Information Retrieval System) computer. All future sorption data will be submitted directly in coding tree form consistent with the following examples. The advantages from this action are:

- Minimization of data handling and number of people in contact with the data.
- Elimination of the reinterpretation of data.

For example, each contractor has his/her own shortcuts and interpretations for using the coding form (Appendix A). Interpretation of each contractor's work by PNL staff sometimes results in confusion and inaccurate transmission of data. This reinterpretation of data will not be necessary, as contractors will submit data in final coded form. The final coded form or coding tree is more quantitative than the descriptive coding form previously used. All experimental information can be recorded via the coding tree. Should an exception arise, a note to PNL regarding the discrepancy should suffice.

The coding tree of Appendix B represents the interrelationships of all data categories possible from a sorption experiment. To properly code experimental results for input to SIRS, one must identify the proper indices for each data point from Appendix B. Appendix A provides guidelines for recordable experimental data necessary to properly characterize each experiment. Appendix B supplies the indices for each experimental data point. Having located the proper indices for a data point, one must next specify the data type (1 = comment, 2 = label, 3 = numeric). Next, any numeric or comment data are recorded. Finally, a number is assigned to each individual experiment. This number is repeated in the last columns of each record or line of coded data. 80/80 sheets are to be used for recording the data. The proper columns to be used for coding are shown on page C.4. Consider the following example:

> The coding form of Appendix A has an example sorption experiment by J. F. Relyea on page A.7. This is the format in which sorption data were previously submitted to PNL. In the future, all sorption data will be submitted in the final coded format consistent with Appendix B. The batch experiment by Relyea is coded in this form on Pages C.5 to C.8. The following paragraphs give selected examples of the steps involved in coding this data. For the purposes of description, page A.7 will be used as a data source. However, formatting data in a form similar to page A.7 will not be necessary. Contractor need submit only the final coded data consistent with the following format.

The first step is associating the information under Reference on page A.7 with the proper box on page B.2, Appendix B. Relyea corresponds to the box NAME. There are no further levels of categories below NAME; therefore, the box NAME is the most unique desriptor of Relyea. The identifying indices would be 1,1,0,0. The actual name Relyea would be a comment of type 1, because a specific box with Relyea doesn't exist. This data would be coded as found on line 1, page C.5.

The second piece of information on page A.7 is PNL. A level 3 category on page B.2 exactly describes PNL and has the index of 1,2,1,0. This is a label and therefore a type 2. Line 2, page C.5 shows the proper coding.

On page A.7 under Geologic Media, there is a total chemical composition given for SiO_2. That composition is 67.5. Starting with the coding tree level 1 category GEOLOGIC MEDIA on page B.4, one proceeds to the level 2 category TOTAL (Appendix A shows SiO_2 associated with TOTAL). The tree continues to levels 3 and 4 but on a separate page. TOTAL is on B.6. Proceeding to level 3, one can find a box for SiO_2. The total chemical compositon in SiO_2 is broken down even more at level 4. The 67.5 lies within the range specified by the 60-80 box. Thus, the index indentifying SiO_2 having a value of 67.5 is 3,3,1,5. In the case of numeric data, the actual value 67.5 is also recorded on the same line, as shown on line 20 of page C.5.

These are three separate examples of how experimental data is recorded. The complete coding of all data on A.7 is shown on pages C.5 to C.8. This was accomplished by correlating each piece of data with the corresponding box or data category (Appendix B) best identifying it.

Properly coding the first few sorption experiments is time consuming. PNL staff transcribing subcontractor experimental data to the final coded form have found several ways to streamline the data recording process. Most experiments typically are quite repetitive, or at least only several experimental parameters change from one experiment to the next. A standard experiment (fully indexed) can be copied, and any changing drastically speeds up the data recording process. Also, the amount of mundane work is decreased, reducing the likelihood of errors. Each subcontractor may identify other shortcuts. All were welcome as long as experimental data is transmitted to PNL on 80/80 sheets in the format shown on the following pages.

Some special rules to keep in mind while coding:

- For overlapping numeric data, use the first index for coding. For example, take the numeric ranges 0-5 and 5-10. If the experimental data to be recorded was 5, it would be coded with the indices associated with the 0-5 range.
- In the case of label data with comments, the comments can be entered on the same line as the indices specifying the label. Refer to page A.7 in category A under <u>Experimental Details</u>. Batch (3W, BC) is properly coded on line 7, page C.5.
- For numeric data, a measurement of 'not detected' is recorded as o. A remark of 'not determined' is recorded as a comment unless a data category exists for 'other'.

80 — 80 | REQUESTED BY | DATE | PAGE OF | PROBLEM NO.

ABBCCDDEEFGGGHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHIIIIIIII

A=CONTINUATION SPACE (BLANK NORMALLY, ASTERISK IF CONTINUATION OF PREVIOUS LINE)

B=LEVEL 1 INDEX
C=LEVEL 2 INDEX } DATA CATEGORY SPECIFIER
D=LEVEL 3 INDEX
E=LEVEL 4 INDEX

F=TYPE OF DATA (1=COMMENT, 2=LABEL, 3=NUMBER)

G=LEAVE BLANK

H=ENTER ANY COMMENTS OR NUMBERS (NUMBERS MUST BE DECIMAL)

I=EXPERIMENT NUMBER (CONSECUTIVELY PER INVESTIGATOR PER FISCAL YEAR)

54-3000-463 (5-66)

80 - 80 Sheet Data Input Format

PAGE 1 OF 4

80 — 80

REQUESTED BY J. F. Relyea

DATE 03/15/80

PROBLEM NO.

	0101000001	RELYEA
	0102010002	
	0103000001	WISAP TASK 4 CONTRACTORS INFORMATION MEETING PROCEEDINGS,
*	0103000001	OCTOBER 2-5, 1978, TO BE PUBLISHED
	0104010222	
	0105030002	
	0201010002	(3W, BC)
	0202010002	< 100 µM
	0203010013	0.5
	0203020013	15.
	0205030003	29.
	0204040003	25.
	0206010002	
	0207020002	(70)
	0208010002	
	0209060002	
	0209070002	
	0301020032	
	0302000001	PARRY SOUND ONTARIO (WARDS SCIENTIFIC)
	0303010053	67.5
	0303020013	17.1
	0303080013	0.
	0303030013	1.8
	0303110013	0.K
	0303050013	0.1

54-3000-863 (9-66) AEC RL RICHLAND WASH

Sample Data Input

80 – 80

REQUESTED BY T.F. Relyea

DATE 03/15/80

PROBLEM NO

030304013	0.1
030307013	13.6
030306013	0.
030310013	0.1
030401053	98.
030401051	MICROCLINE-83%(K3.95)(AL3.95,SI12.05)O32,QUARTZ-15%(SIO2)
030410013	1.5
030410011	CALCITE-(1-2%)(CACO3)
030402013	1.
030402011	12 ALMANDINE-PYROPE GARNET(FE2.69,MG4.14)(FE1.0,AL.47,SI5.53,O24)
030501003	1.0
030600001	NOT DETERMINED
030701003	1.2
030701001	+OR-0.2,PH=7
030800001	NOT DETERMINED
030901023	6.1
030901021	+OR-1.0
040105003	8.2
040211002	UNKNOWN
040301023	690.
040302013	0.
040303013	0.
040304013	0.
040305013	0.
040306053	1550.

54-3000-863 (9-68)

Sample Data Input (contd)

80 - 80

REQUESTED BY J. F. Relyea

DATE 03/15/80

PROBLEM NO

040309013	0.
040302013	0.
040308013	0.
040401002	UNKNOWN
040402002	UNKNOWN
040405002	UNKNOWN
040404002	UNKNOWN
050109003	9.25
050210003	312.
050301023	654.
050301022	4.
050503025	20.
050304013	0.
050305023	9.4
050306053	157
050309033	75.
050307013	0.
050308033	30.
050401002	UNKNOWN
050402002	UNKNOWN
050403002	2.8
050405002	9.1
050406002	0.2
050407002	4.8

84-3000-863 (9-86)

Sample Data Input (contd)

80 – 80

REQUESTED BY J. F. [illegible]

DATE 03/15/80

PAGE 4 OF 4

PROBLEM NO.

Columns 1–10	Columns 11–80
0601 02002	
0602 06003	1.00000001
0602 06001	APPROXIMATE
0603 04002	
0605 00001	WET/PH/7DF0.45
0606 00001	NOT DETERMINED
0701 01013	0.61
0701 01011	+OR-0.12
0702 01002	
0703 01002	
0704 02003	3.

54-3000-463 (9-68) AEC-GE RICHLAND, WASH

Sample Data Input (contd)

APPENDIX D

DATA QUALITY ASSURANCE PLAN

APPENDIX D

DATA QUALITY ASSURANCE PLAN

The following is an outline of the quality assurance procedures to be implemented for the sorption data base at the end of FY-1980. The procedures listed herein are designed to address two problems: computer code documentation and input data integrity.

I. Computer Code Documentation Procedures

On a quarterly basis or less frequently if the files have been rarely updated, all the SIRS input data and computer codes will be saved on magtape/disk for permanent storage. The UIC convention used to identify the progression in time of the data base will be:

[224, 1] =version 1
[224, 2] = version 2, etc.

All programs will be saved on the PDP-11/55 computer system. Necessary input files to regenerate the data base will be present on the same tape/disk. Dates and persons involved in saving the system will be clearly labeled on the tape/disk. Entry will be made in the SIRS Log Book. A file named:

DI:HEADER.BLK

will contain any pertinent comments concerning that version of the data base (i.e., changes in this version from the previous) including: the data, version number and the name of the responsible person.

II. Input Data Integrity (steps of input)

1. Data are received from investigator and a copy made and filed (Appendix C describes data input formats).

2. One copy of the coded forms are sent to Battelle's keypunching for processing. Cards shall be verified by keypunching before their return.

3. The keypunched data is then run through program INCHEK to check for the presence of all necessary data categories and is processed to final form as needed by the main data base routines.

4. These can serve both as a simple summary and a future check on the main manipulative data base routines (interactive control programs). For example, the means and standard deviations of numeric data categories are computed.

5. Finally, all input experimental data are printed out in a readable format (grouped by investigator). Two dated copies are made. One for PNL use and another to be separated by investigator. The latter copy is then sent to the contributing investigator for his/her verification.

6. At this point, all data is stored properly for use. The data is then selectively retrieved, processed, and compared with the output from steps 3, 4, and 5.

In conclusion, this QA procedure has established necessary backup copies and provided several methods of assuring data base integrity. Summaries of experimental data are available to data base users and contributors for cross reference and checking. All data base input activity shall be summarized in the SIRS Log Book. The main entry items are:

- Number of experiments entered by each investigator
- The month and year of entry
- Person coding the data
- Person keypunching the data
- Person checking the data
- Any changes in coding procedure or method since last entry
- Date and location of any save files.

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