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ORGANIZATION AND DESIGN OF AN AUTOMATED LABORATORY INFORMATION MANAGEMENT SYSTEM FOR THE BRANCH OF GEOCHEMISTRY RESEARCH AND OPERATIONAL LABORATORY

by

ART L. SUTTON AND JOSEPH H. CHRISTIE

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U.S. Geological Survey, DFC, Box 25046, MS 973, Denver, CO 80225

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ABSTRACT

This report provides an overview for the design of a Laboratory Information Management System (LIMS) used to process data created or produced by a variety of analytical instruments in both a routine analyses and research environments in a Government laboratory. Methods of reducing and in some cases eliminating manual data entry are an important requirement of this or any other LIMS. Techniques to make expensive analytical instruments available to the user full-time for analyses are also described. This report also describes attributes of the LIMS which enable us to take advantage of current and future technology.

INTRODUCTION

A Laboratory Information Management System (LIMS) designed for a Government research lab and an operational lab doing routine analyses has many of the same requirements as a system designed for any other lab. Government labs generally have a variety of analytical instruments ranging from computer controlled state-of-the-art instruments to older instruments with little or no data handling capabilities. Typically, the labs operate only one shift per day, but have instruments and robots that are capable of 24-hour operation. Government labs generally have a higher ratio of professional chemists to technicians than private labs, thus making it important to reduce the amount of time they spend on the LIMS.

The particular labs for which this system was developed, exist in three centers across the country and in multiple buildings in two of the centers. Each center is composed of multiple projects (Neutron Activation, X-Ray, Mass Spec., etc.). Analytical requests are submitted in any of the three centers for work to be done by any project or lab. A typical job submitted in Denver might require X-Ray majors, Mass Spec. in Denver,Colorado; Neutron Activation in Reston, Virginia; and Partial Chemistry in Menlo Park, California. After a request for analyses has been submitted, it may be changed at any time. The changes must be reflected in all three systems. The LIMS processes up to 40,000 samples each year with an average of 20 to 25 elements to be determined per sample.

Analytical samples are divided into "active" and "completed" samples. The LIMS handles only the active samples. The chemical analyses results for all completed samples are transferred to a separate database for permanent storage.

Due to the many levels of management within the Government, the system must supply a wide variety of reports. These reports range from backlog and production reports for the individual analysts to monthly and yearly reports for management at various administrative levels. Accurate and timely reports of work requested, work completed, and backlogs are necessary for budgetary and other organizational decisions.

The LIMS consists of five parts: (1) a log-in system that allows new samples to be entered into a database along with the chemistry to be performed on each sample, (2) a status database that automatically keeps track of the status of the analytical work on all samples in the system after the job has been assigned to an analyst, (3) a network system that interfaces with the analytical instruments in the lab, (4) a retrieval system that provides the analytical results in printed and electronic form for the submitter, and (5) an archival system to store completed samples on magnetic tape for possible future re-entry into the LIMS. This archival system is in addition to the "completed sample" database used to store data permanently for general use.

The LIMS consists of three databases. In addition, there is an answer file (ANSWR) and a description file (DESC) for each job. A job consists of 1-40 similar samples which require the same chemistry.

The first database is a read only database that contains information concerning analytical techniques performed by each laboratory and each project within the lab. This database (AUK) allows the type of analysis (TOA) to be entered at various times throughout the analysis of a sample and the system will know what elements make up the TOA. Instead of entering 37 elements for one technique, the work can be entered by typing one value. AUK also contains the required information to display and validate requested analytical work and the analyst for each project and laboratory as it is entered into the LIMS. It also contains information relating to valid programs and offices within the Government allowed to submit samples. Government labs generally have to submit reports relating to costs or some form of "work units" to various offices. These work units can be used by the LIMS or an accounting system to predict completion dates, produce production reports and backlogs. Table 1 describes information contained in the AUK database.

The second database (SAM) is a read/write database that contains all the accounting information required to provide the necessary reports. Table 2 contains SAM information. For each job (group of similar samples) there is an answer file (ANSWR) and a description file (DESC) logically linked to SAM. The answer file (ANSWR) contains all analytical results and the necessary flags and space for Quality Assurance (QA) and Quality Control (QC) samples. DESC and ANSWR are described in tables 3 and 4.

The third database (WORKST) is a real-time status database. It monitors the analytical work as it is entered into the system and records the time and level of completion for each TOA and job. This provides a manager with the capability of knowing "what happened when" on any job or TOA in the system. Table 5 contains a description of WORKST.

SYSTEM HARDWARE AND SOFTWARE SELECTION

The selection of hardware and software was based on the requirement that we had to process requests from the instruments as quickly as possible. The system must act as a tool for chemists and technicians and get them on and off the system in as little time as possible. A real-time operating system was selected for the LIMS computer. The computer is dedicated solely to the LIMS in order to meet lab requirements. A general purpose computer would not be appropriate because it is necessary to set system priorities to meet the needs of the lab. When priorities are set to allow several computers to communicate at 9600 baud or faster, other processes slow down significantly - a reason for distributed processing. With the equipment available today, a real-time system would not be required, but a dedicated system would be.

Another requirement that is very important is that the basic design must allow for down-time of the LIMS computer without effecting the instruments. If all instruments are interfaced to the LIMS and require information and processing to operate, down-time can be very expensive. To meet this requirement, a computer was placed between each instrument to be automated and the LIMS. Some of the instruments in use had only a simple terminal and/or a printer for output. If there was a terminal, an inexpensive computer with adequate data storage and a terminal emulator was substituted. In other cases, computers with controllers, A-D converters, multi-meters and other electronic equipment had to be used. Most of the instruments today have personal computers as their interface to the LIMS. Common third party software now available makes interfacing much easier. Originally, we required that any automated instrument had to be able to store two weeks of data in case the central LIMS went down. Two weeks turned out to be excessive, because the system has never been down for more than 2 days. However, most of the personal computers commonly used today have more than sufficient storage for 2 weeks of work. There is a manual data entry option in the software to accommodate data from instruments that do not warrant automation.

The LIMS has the ability to do the calculations for individual instruments if they do not have the computing power, but this is generally done only during the early stages of setting up an instrument. It is preferable to have the computing power at the instrument. In most cases, the calculations are done on the computer controlling the instrument or on the computer in the lab linked to the LIMS.

LOG-IN SYSTEM

The log-in system allows new samples to be entered into the LIMS from three different sources. The first is a semi-automatic entry system that takes data from interactive software, and compares and expands it using data from the AUK database. Sample identifiers (lab numbers) and job (groups of samples) numbers are maintained by the system. Before development of the LIMS, sample numbers were manually typed or written many times for each sample. One survey showed a single sample number had been typed sixteen times. This did not include the number of times it was written in the labs on worksheets and various temporary reports. Now the average throughout all labs is much less than once per sample. Once the lab numbers and other description information for each sample has been generated by the computer, all instruments have access to the data. The resulting data are then stored in the SAM database and the answer files (ANSWR) linked to SAM.

The second log-in system is an automated method that accepts files created by a submittal system developed for personal computers (Christie, Jackson, and Sutton, 1990). All data are entered by the submitter except for lab numbers and the chemistry to be performed. Up to 2,000 samples can be entered in each pass by entering only the chemistry. The LIMS breaks the samples up into 40 sample jobs and supplies both the job number and lab numbers. All SAM, DESC, and ANSWR entries are made automatically in a few minutes.

The last data entry option allows previously analyzed samples to be restored from archive tapes and re-entered into the LIMS. At this point, jobs or samples can be re-analyzed, or chemistry can be added to the jobs.

After a job is logged in by any of the three methods, a printed confirmation copy of the log-in is generated for each job. This is made available to the submitter so the data can be verified. This report can also be generated at any time by an analyst in order to determine what work is being performed in addition to his/her own.

After the samples have been entered, changes can be made: (1) samples can be added, (2) samples can be deleted, (3) elements can be added to the job, (4) elements may be deleted, (5) analytical work can be moved from one laboratory to another and, (6) jobs can be deleted completely from the system.

The LIMS has system manager software that automatically schedules tasks on a regular basis with or without operator intervention. Backlogs are run at some interval, usually weekly, and a backlog database is created that can be down-loaded to the instruments or user's computers. Most users download the backlog database at night or on weekends while the LIMS and their systems are not being used.

At any time, either bar code or normal printed labels can be generated.

STATUS DATABASE (WORKST)

The status database allows any user to check the status of samples in the LIMS. Entries are automatically created and updated as samples are processed by the lab. When a job is assigned to an analyst, or an instrument requests information about the samples, an entry is created in the status database. The entry tells when the job was started, to whom it is assigned, and how many samples and elements in the job have been completed. When the data are transmitted over the network, WORKST is updated in real-time as each element is received. Because several instruments may require access to WORKST at the same time, access to the database is funneled thru a monitor program that can handle all normal interactions and eliminate "collisions." It is important that the WORKST database be properly updated, because decisions are made by the LIMS based on the status of a job. In addition to updating WORKST, there is a printed log of each transaction. This log will be discussed under "data integrity." WORKST and the log are important because realistically it is not possible to have an individual monitoring all the data that are coming into the LIMS. Several instruments may be transmitting at the same time from different labs and different buildings. Most of the time this is a computer-to-computer transaction at 9600 baud or greater without an operator at either end.

Software is available to edit the WORKST database, and to generate special reports. Instruments may send one sample and one element today, and another tomorrow until all are complete. WORKST keeps track of this work and if data entry is not complete after some selected period of time, reports are generated to make sure the analyst knows there has been a break in the flow of data.

The archive software also uses the WORKST database to determine which jobs are ready to be archived. After the archive process, the job entries are eliminated from the database.

A status program is available to allow anyone with access to the system to check the status of any job or TOA. Status is also used by submitters to check their work without having to contact the lab.

NETWORK SYSTEM (SAMNET)

The network is probably the most critical part of the system. It is a very simple RS-232 network. The protocol is ASCII with a checksum on each analytical value transmitted. Older instruments do not have the capability of using the network systems available today. When this system was designed, Local Area Networks (LANs) were not available. SAMNET requires software on each instrument to transfer data to and from the LIMS. The LIMS acts as a slave to the instruments which provides complete control to the laboratory. This is opposite the method used by most other LIMS. The communications software on the LIMS is interrupt-driven. When the instrument computer needs to make a transaction, it sends an ASCII string that tells the LIMS whether it is requesting data or sending data, and provides either a list of jobs for which it needs data or sends completed analytical data for a list of jobs it has analyzed. Data transmitted to the LIMS include a job number, TOA, element, sample number, analytical value, and the number of significant digits associated with each analytical value. The data are transmitted to an area in the system that allows the chemist to run additional software on the data if necessary. Otherwise, it is automatically moved to the LIMS. The analytical values are stored in the

ANSWR file in a format that maintains the correct number of significant digits. Data are normally transmitted from the instrument computer to the LIMS at night or early in the morning. This makes the instrument available for analyses for the full shift - a valuable asset for an instrument that may cost from $100,000 to $250,000. Before one of our new instruments was interfaced to the LIMS it took 2 hours to analyze a set of samples and over 8 hours to manually enter the data. After the system was put on line to the LIMS, data were transferred automatically at 1:00 A.M. The LIMS then prepares a printed report for the analyst which is available when he/she arrives in the morning.

An individual laboratory can operate without knowing anything about the LIMS. The labs receive a backlog once each week, or upon demand, with a list of jobs to processed. An operator runs a job from the backlog and if the job is not in his/her computer, the computer simply calls the LIMS for the data and then continues the operation. In reality, most analysts interact with the system on a regular basis, using most of the available utilities. The automated systems have access to the software to create worksheets, confirmation sheets, and partial and complete analytical reports. They can also check the status of any TOA or job.

Every job must have three approvals before it can be reported to the submitter. The jobs are approved by the analyst, the lab chief, and the sample control officer. The analyst and lab chief can transmit approvals with the analytical data over SAMNET if desired, or they can run approval software after they have received the LIMS report.

Jobs may have analytical work done in any of the three centers. There is software to send job information from center to center. A network system is generally not used to send the data. The physical sample is sent by mail and a data tape containing the LIMS information is sent with it. Analytical data can be either transmitted or returned to the requesting center on tape by mail.

Any software that runs automatically on the LIMS and on SAMNET can also be run manually if required.

In order to take advantage of LAN's in the future, software has been developed that will allow data files to be uploaded and downloaded to the LIMS for processing at a specified time. This technique is now being used over SAMNET, but will be more efficient when a formal LAN is installed.

RETRIEVAL SYSTEM

The retrieval system allows a variety of reports and electronic data sets to be created for each job. The system routinely generates a printed report for the analysts. The report begins as a preliminary report and after three levels of approval, becomes a final report. After approval, data may be retrieved in three different fixed formats. Other formats can be easily created. All formats maintain the significant digits as stored in the system. Software is available from other sources to convert these formats to spreadsheet and STATPAC formats (VanTrump, Miesch, 1977).

ARCHIVAL SYSTEM

After the analytical work has been completed on a job and the data retrieved for the submitter, the samples are allowed to "age" for a period of time. This allows changes to be made or the samples to be re-submitted for additional analytical work. After this aging process, the jobs are moved to an archival database which is not part of the LIMS and then copied to magnetic tape for permanent storage. If, in the future, the archived samples need additional analyses, they can be read back into the system and have the additional work added to the job.

TOOL KIT

As with most software systems, there is software to monitor and repair all three databases, the DESC and ANSWR files. There is software to monitor and check SAMNET. Any instrument can convert SAMNET into an interactive line that can run any LIMS software interactively and then convert the line back to the automated protocol.

DATA INTEGRITY

We use several techniques to assure data integrity. Some systems are backed up frequently, some use a "mirror" disk system and some use dual LIMS. The frequency of our backups are determined by the history of hardware and software failures and the amount of time required to restore the system. For our application, the use of mirror disk systems and/or maintaining duplicate LIMS are not worth the additional cost. The types of failures that generally destroy data are electrical and hardware failures. When these failures are experienced, they may effect both systems. In addition, if one system fails, it must later be brought up to date. This is generally a manual operation. When you have a LIMS processing a very large volume of data and no operator monitoring the processing, in addition to regular backups, you must have a method of determining what transactions have taken place since the last backup. The method used here is to do a backup of the system at the end of each week. In our buildings, problems with power seem to occur on weekends. If we are installing new software, or making some other significant changes, we will backup more often. All transactions in the LIMS are logged to disk or to a printer (SAMLOG). We generally use a printer because of the possibility of a failure of the disk containing the log. All transactions logged to the printer fall into four categories: (1) *** EVENT *** provides a list of all tasks that occurred and the time they occurred, (2) *** WARNING *** indicates a potential problem that should be investigated before it becomes an error, (3) *** ERROR *** indicates some problem with a job or with the computer operating system that must be resolved, and (4) *** TASK *** indicates a task that must be manually performed by the sample control officer. One reason a warning would occur would be if the status database (WORKST) reached 90% of capacity. At 99% an error would occur and the LIMS would shut itself down. All errors must be checked in order to make sure jobs process properly.

In case of a system failure, i.e., a crashed disk, the last backup would be restored, and then the sample control officer would execute manually all "*** EVENT ***" entries on SAMLOG. If re-transmissions from instruments were required, the instrument operator would be requested to send the data. It typically takes about four hours to restore a week's work. In the past 15 years, this process has been required only twice.

SAMLOG can also be used for debug printout during program development. This allows one to check critical elements of the software in relation to other events taking place in real-time.

SUMMARY

The current LIMS has been very effective in increasing the output from expensive analytical instruments, providing management throughout the U.S.

Geological Survey with the information they require, and reducing the manual efforts by scientists necessary to produce the required output for their customers.

The basic system requires little knowledge by the users. A lab can operate without the ability to "logon" to the LIMS. However, as time has passed, more personnel have become interested in interacting with the system and using options that originally were totally automatic or supplied information to them on printed reports. Now that most people have personal computers, word processors, and spreadsheets, we are spending more time making our output compatible with their systems.

We are in the process of converting the system to current technology hardware. By converting to a UNIX operating system with a much faster processor, we will be able to take advantage of the wide variety of third party software that we cannot currently use. Although the hierarchial database structure is faster, we hope to convert to a relational database. The faster processor should more than compensate for the difference in the speed of the databases. A relational structure will make it more efficient to generate the special reports frequently requested on very short notice.

Table 1a.--Description of data items in the AUK database

ITEMS	DESCRIPTION
NIDPKG	KEY - Code for package jobs
DESCPK	Description of package jobs
NID	KEY - Code for elements
CONVD1	Code for converting SAM element codes to RASS
DESCRT	Description for each element
WORKCT	Work units for each type of analysis (TOA)
DESCCT	Description for each TOA
UNITCT	Number of elements for each TOA
LLOA	KEY - Location of analyses (LOA)
LLOADS	Description of LLOA
PRJLDR	Lab Chief's name
WORKPJ	Work units for each package job
TOA	Key - Type of analysis (TOA)
INNID1	Elements associated with each TOA
INNID2	Elements associated with each TOA
INNID3	Elements associated with each TOA
PNORD	Order of elements within TOA
ANNO	Analyst number
ANAME	Analyst name
TECEL	Technique for elements in RASTB
DESCEL	Description of each technique (TECEL)
TECGR	Group technique number for elements in CHGTB
DESCGR	Group technique description for each element in CHGTB
DEFANO	Default analyst number for each TOA in CHGTB
WUNITS	Work Units for each TOA in CHGTB
DESC	Technique description
LOA	Valid locations for each TOA
ORDER	Element order for each TOA in data file - CHGTB
OFFNO	U.S.G.S. office number
OFDESC	Office description
BRDESC	U.S.G.S. branch description
PROG	U.S.G.S. program number
PRDESC	Program description
TECH	Technique code
DATE	Date technique added to AUK database
PRIOR	Priority for analysis of job for each office

Table 1b.--Contents of the AUK data files

SET NAME	TYPE	CONTENTS
PACKG	Manual master	List of valid package jobs
RASTB	Manual master	List of valid elements
CHGTB	Manual master	List of valid types of analyses (TOA)
LLOAA	Manual master	List of valid laboratories
PROG	Detail	List of Government programs
OFFICE	Detail	List of Government offices
PJT	Detail	List of TOA's for each package job
PNIDD	Detail	List of fixed elements for each TOA
ANNOA	Detail	List of analyst numbers and names
ELTEC	Detail	List of infromation for each element in RASTB
GRTEC	Detail	List of default information for each TOA CHGTB
WUPEL	Detail	List of elements for each misc. type TOA

Table 1c.--Data file links in the AUK database

SET NAME	SET NO	ITEM NAME	TYPE	LINKED TO DATA SET(S)
PACKG	01	NIDPKG	Integer	PJT
		DESCPK	ASCII	
RASTB	02	NID	Integer	ELTEC
		DESCRT	ASCII	
		CONVD1	Integer	
CHGTB	03	TOA	Integer	GRTEC - WUPEL - PNIDD
		WORKCT	Integer	
		DESCCT	ASCII	
		UNITCT	Integer	
		LOA	ASCII	
		ORDER	Integer	
LLOAA	04	LLOA	ASCII	ANNOA - GRTEC - ELTEC
		LLOADS	ASCII	
		PRJLDR	ASCII	
PROG	05	PROG	ASCII	
		PRDESC	ASCII	
OFFICE	06	OFFNO	ASCII	
		OFDESC	ASCII	
		BRDESC	ASCII	
		PRIOR	ASCII	
PJT	07	NIDPKG	Integer	PACKG
		TOA	Integer	
		WORKPJ	Integer	
		LLOA	ASCII	
PNIDD	08	TOA	Integer	CHGTB
		INNID1	Integer	
		INNID2	Integer	
		INNID3	Integer	
		PNORD	Integer	
ANNOA	09	LLOA	ASCII	LLOAA
		ANNO	Integer	
		ANAME	ASCII	
ELTEC	10	LLOA .	ASCII	LLOAA
		NID	Integer	RASTB
		TECEL	Integer	
		DESCEL	ASCII	
GRTEC	11	LLOA	ASCII	LLOAA
		TOA	Integer	CHGTB
		TECGR	Integer	
		DESCGR	ASCII	
		DEFANO	Integer	
		DATE	ASCII	
WUPEL	12	TOA	Integer	CHGTB
		LLOA	ASCII	
		NID	Integer	
		WUNITS	Integer	
		DESC	ASCII	
		TECH	Integer	
		DATE	ASCII	

Table 2a.--Description of data items in the SAM database

ITEMS	DESCRIPTION
JOB	KEY - Job number
LLOA	KEY - Location & lab mneumonics
PROG	KEY - U.S.G.S. Program number
DESCPG	Program name
LLOAD	Type of analyses (TOA) description
PRJLD	Project leader (Lab chief)
TOA	Type of analysis
NAME	Sample submitter's name
INDAT	Date samples were logged into SAM
OBWRK	Office - Branch requesting analyses
PJWRK	Project requesting analyses
OBREQ	Office - Branch accountable for analyses
PJREQ	Project accountable for analyses
IPRTY	Priority assigned to requested analyses
NS	Number of samples submitted for analyses in this job
LABNO	Lab number for the first sample in this job
DUE	Date analyses are due
NDT	No. of determinations for this TOA
WUNIT	Work units or dollars for this TOA
DONE	Date this TOA was completed
CONTC	Lab contact person's analyst number
CMPDA	Estimated completion date
CDATE	Date corrections were made

Table 2b.--Contents of the SAM data files

SET NAME	TYPE	CONTENTS
JOBAM	Automatic Master	Job numbers (groups of samples)
MMLOA	Manual Master	List of valid centers and labs
PROM	Automatic Master	List of valid U.S.G.S. programs
RALF	Detail	Sample submitter accounting information
TOADD	Detail	Information for laboratory analyses
RALFC	Detail	Corrected RALF information
TOADC	Detail	Corrected TOADD information

Table 2c.--Data file links in the SAM database

SET NAME	SET NO	ITEM NAME	TYPE	LINKED TO DATA SET(S)
JOBAM	01	JOB	ASCII	RALF - TOADD - RALFC - TOADC
MMLOA	02	LLOA	ASCII	TOADD -TOADC
		LLOADS	ASCII	
		PRJLDR	ACCII	
PROM	03	PROG	ASCII	RALF - TOADD - RALFC - TOADC
RALF	04	NAME	ASCII	
		INDATE	Integer	
		JOB	ASCII	JOBAM
		OBWRK	Integer	
		PJWRK	ASCII	
		OBREQ	Integer	
		PJREQ	ASCII	
		IPRTY	ASCII	
		NS	Integer	
		LABNO	ASCII	
		DUE	ASCII	
		PROG	ASCII	PROM
TOADD	05	JOB	ASCII	JOBAM
		LLOA	ASCII	MMLOA
		TOA	Integer	
		NDT	Integer	
		WUNITS	Integer	
		DONE	Integer	
		OBWRK	Integer	
		PROG	ASCII	PROM
		CONTCT	Integer	
		CMPDAT	Integer	
RALFC	06	NAME	ASCII	
		INDATE	Integer	
		JOB	ASCII	JOBAM
		OBWRK	Integer	
		PJWRK	ASCII	
		OBREQ	Integer	
		PJREQ	ASCII	
		IPRTY	ASCII	
		NS	Integer	
		LABNO	ASCII	
		DUE	ASCII	
		PROG	ASCII	PROM
		CDATE	Integer	

Table 2c.(cont.)--Data file links in the SAM database

SET NAME	SET NO	ITEM NAME	TYPE	LINKED TO DATA SET(S)
TOADC	07	JOB	ASCII	JOBAM
		LLOA	ASCII	MMLOA
		TOA	Integer	
		NDT	Integer	
		WUNITS	Integer	
		DONE	Integer	
		OBWRK	Integer	
		PROG	ASCII	PROM
		CONTCT	Integer	
		CMPDAT	Integer	
		CDATE	Integer	

Table 3.--Description of data items in the sample description file (DESC)

RECORD	WORD	TYPE	DESCRIPTION
1	1	ASCII	Location code of center where the job originated
	2-4	ASCII	Name of the original job if work has been done on these samples before 1-Blanks if no previous work was done 2-"00" if previous work was done in multiple jobs 3-Name of single previous job
	7	Integer	Number of copies of the final report
	8-64	ASCII	Names and addresses for reports and copies
	65-102	ASCII	Sub-title for report cover sheet
	103-116	ASCII	Name of the submitter
	117	Integer	U.S.G.S. Office number
	118-120	ASCII	U.S.G.S. Branch number
	121	Integer	Version No. of software creating this file
	122-124	ASCII	U.S.G.S. Program number
	125	Integer	NS - Number of samples in this job
	126-128	ASCII	Undefined - available for future use
2	1-4	ASCII	LABNO - First lab number (D-000001)
	5-11	ASCII	FLDNO - Field number
	12-32	ASCII	DESC - Description of sample(1)
	33-64	ASCII	Repeat of words 1-32 for sample(2)
	65-96	ASCII	" " " 1-32 " sample(3)
	97-128	ASCII	" " " 1-32 " sample(4)
3	1-128	.	Repeat of second record for samples 5-8
4	.	.	 9-12
.	.	.	. . . .
.	.	.	. . . .
.	.	.	. . . .
14	1-64	ASCII	Repeat of second record for samples 49-50

File characteristics:

a. The file name links DESC to data sets RALF and TOADD in the SAM database
b. Type 1(binary-random access)
c. 128 words per record
d. 4 samples per record

Table 4.--Description of data items in the ANSWR data file

RECORD	WORD	TYPE	DESCRIPTION
1	1	Integer	SREC - Starting record number for results
	2	Integer	LREC - Ending record number for results
	3	Integer	NS - Number of samples in this job
	4	Integer	NONID - Number of elements in this job
	5	Integer	Version Number for software creating this file
	6	Integer	Number of labs doing work in this job
	7-26	ASCII	List of labs doing work in this job
	27-29	ASCII	U.S.G.S. Program number
	30	Integer	U.S.G.S. Branch number
	31-33	ASCII	U.S.G.S. Project number
	34	Integer	Record number for multiple analyst codes
	35-39	Integer	QA/QC Replicate analyses
	40	Integer	Flag denoting the final location for results
	41	Integer	Flag denoting the level of completion for elements in this job
	42	Integer	Indicator of deleted elements in this job
	43		Undefined - available for future use
	44	Integer	Last date changes were made in this file
	45		Undefined - available for future use
	46	Integer	Date this job was entered from another center
	47	Integer	Date this job was transferred to another lab
	48	Integer	Date sample preperation was completed
	49	Integer	Number or comment records
	50	Integer	Flag denoting the presents of samples that are not to be analyzed
	51	Integer	Flag denoting the presence of QA/QC samples
	52-56	Integer	Sample numbers of QA/QC samples
	57	Integer	Total number of records in this file
	58-60	ASCII	Name of the last program altering this file
	61-128		Undefined - available for future use
2	1-127	ASCII	Comments and footnotes for this job
	128		Pointer to additional comment records

Table 4.(Cont.)--Description of data items in the ANSWR data file

RECORD	WORD	TYPE	DESCRIPTION
3	1	Integer	TOA - Type of analyses
	2	Integer	NID - Element code
	3	ASCII	LLOA - Location & lab mneumonics
	4	Integer	Technique code
	5-8	ASCII	Ascii descriptor for element code
	9	Integer	Analyst number for this element (may be a multiple analyst code)
	10	Integer	Aproval Date or code
	11	Integer	Flag denoting a deleted element
	12	Integer	Contact analyst number
	13	Integer	Estimated completion date
	14	Integer	NDT - Number of determinations for this TOA
	15	Integer	Cost or work units for this TOA
	16	Integer	Date this element was assigned to an analyst
	17-28		Undefined - available for future use
	29-128	Integer	Analytical results for this job 2 words/sample - See note 1
4 - n	1-128		One record for each element in the job Each record is the same as record 3.

Note 1: In order to maintain significant digits, the mantissa of the analytical result is stored in one word and the exponent and qualifier are stored in the second word.

File characteristics:

a. The file name links the file to data sets RALF and TOADD in the SAM database
b. TOA and LLOA link the file to data set TOADD in the SAM database
c. Type 2(binary-random access)
d. 128 words per record

Table 5a.--Description of data items in the WORKST database

ITEMS	DESCRIPTION
JOB	KEY - Job number (group of samples)
LLOA	KEY - Location and lab mnuemonics
ASNMIN	Minute the job was assigned
ASNHR	Hour the job was assigned
ASNDAY	Day the job was assigned
ASNMON	Month the job was assigned
ASNYR	Year the job was assigned
SCRMIN	Minute the job was finished by a lab defined by LLOA
SCRHR	Hour the job was finished by a lab defined by LLOA
SCRDAY	Day the job was finished by a lab defined by LLOA
SCRMON	Month the job was finished by a lab defined by LLOA
SCRYR	Year the job was finished by a lab defined by LLOA
ANSMIN	Minute the job was given the final approval
ANSHR	Hour the job was given the final approval
ANSDAY	Day the job was given the final approval
ANSMON	Month the job was given the final approval
ANSYR	Year the job was given the final approval
FINMIN	Minute the final report was written for the submitter
FINHR	Hour the final report was written for the submitter
FINDAY	Day the final report was written for the submitter
FINMON	Month the final report was written for the submitter
FINYR	Year the final report was written for the submitter
NOCOP	Number of copies of the final report printed
RASDAY	Day data were transferred to "completed" database
RASMON	Month data were transferred to "completed" database
RASYR	Year data were transferred to "completed" database
STATFL	Status flag used for quick determination of status of a job
DISPFL	Disposition flag
FIRMIN	Minutes data were read into a remote analytical instrument
FIRHR	Hour data were read into a remote analytical instrument
FIRDAY	Day data were read into a remote analytical instrument
FIRMON	Month data were read into a remote analytical instrument
FIRYR	Year data were read into a remote analytical instrument
LSTMIN	Minute the last data entry was made by an analytical inst.
LSTHR	Hour the last data entry was made by an analytical inst.
LSTDAY	Day the last data entry was made by an analytical inst.
LSTMON	Month the last data entry was made by an analytical inst.
LSTYR	Year the last data entry was made by an analytical inst.
NSREQ	Number of samples requested for this Job/TOA
NSDONE	Number of samples completed for the Job/TOA
INID	Type of analysis (TOA) for this Job
OVFLAG	Flag to indicate that data have been overwritten
COMPFL	Flag to indicate completion of a Job/TOA
ANNO	Analyst number for this Job/TOA

Table 5b.--Contents of the WORKST data files

SET NAME	TYPE	CONTENTS
JMAS	Automatic master	List of jobs
LMAS	Manual master	List of valid centers and laboratories
WKSTAT	Detail	SAM status for each location and laboratory
XXSTAT	Detail	Location and laboratory accumulation status

Table 5c.--Data file links in the WORKST database

SET NAME	SET NO.	ITEM NAME	TYPE	LINKED TO DATASET(S)
JMAS	01	JOB	ASCII	XXSTAT - WKSTAT
LMAS	02	LLOA	ASCII	XXSTAT - WKSTAT
WKSTAT	03	JOB	ASCII	JMAS
		LLOA	ASCII	LMAS
		ASNMIN	Integer	
		ASNHR	Integer	
		ASNDAY	Integer	
		ASNMON	Integer	
		ASNYR	Integer	
		SCRMIN	Integer	
		SCRHR	Integer	
		SCRDAY	Integer	
		SCRMON	Integer	
		SCRYR	Integer	
		ANSMIN	Integer	
		ANSHR	Integer	
		ANSDAY	Integer	
		ANSMON	Integer	
		ANSYR	Integer	
		FINMIN	Integer	
		FINHR	Integer	
		FINDAY	Integer	
		FINMON	Integer	
		FINYR	Integer	
		NOCOP	Integer	
		RASDAY	Integer	
		RASMON	Integer	
		RASYR	Integer	
		STATFL	Integer	
		DISPFL	Integer	
XXSTAT	04	JOB	ASCII	JMAS
		LLOA	ASCII	LMAS
		FIRMIN	Integer	
		FIRHR	Integer	
		FIRDAY	Integer	
		FIRMON	Integer	
		FIRYR	Integer	
		LSTMIN	Integer	
		LSTHR	Integer	
		LSTDAY	Integer	
		LSTMON	Integer	
		LSTYR	Integer	
		NSREQ	Integer	
		NSDONE	Integer	
		INID	Integer	
		OVFLAG	Integer	
		COMPFL	Integer	
		ANNO	Integer	

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