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FEASIBILITY STUDY FOR AUTOMATION OF THE CENTRAL LABORATORIES, WATER RESOURCES DIVISION, U. S. GEOLOGICAL SURVEY

William F. Morris
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MASTER

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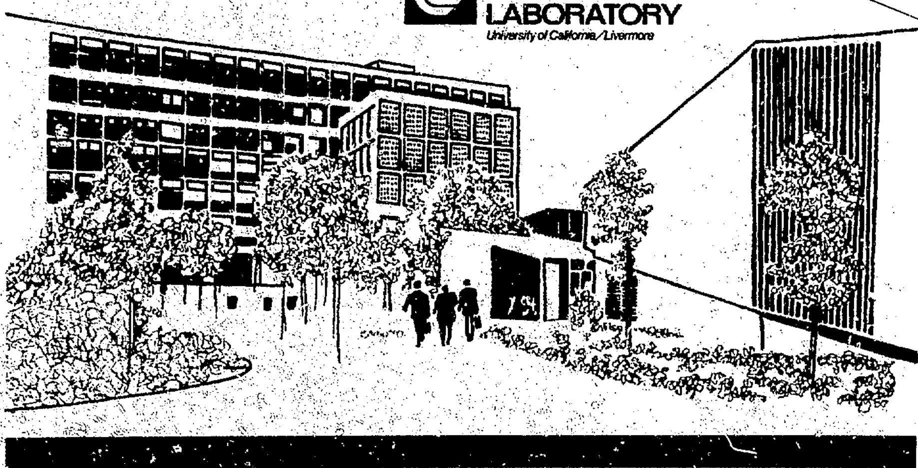

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Abstract

This study of the feasibility of further automating the Central Laboratories deals specifically with the combined laboratory operations in Salt Lake City, Utah, and Denver, Colorado, and is prepared with the understanding that such a system will also be implemented at the Central Laboratories in Atlanta, Georgia, and Albany, New York. We define the goals of automation in terms of the mission of a water analysis laboratory, propose alternative computer systems for meeting such goals, and evaluate these alternatives in terms of cost effectiveness and other specified criteria. We find that further automation will be beneficial and recommend an in-house system that incorporates dual minicomputers: one for time-shared data acquisition, processing, and control; the second for data management. High-use analytical instruments are placed on-line to the time-shared minicomputer, with a terminal at each instrument and backup data storage on magnetic tape. A third, standby computer is switched in manually should the time-shared computer go down. Field-proven, modular hardware and software are chosen. We also recommend the incorporation of the highly developed, computer-integrated instruments that are commercially available for determining petrochemicals and other organic substances, and are essential to the Laboratories' mission.

Introduction

This study uses information and data from the Central Laboratories' operations at Salt Lake City, Utah, and Denver, Colorado. In the spring of 1976, these two laboratories will be combined into a single facility, located at Denver, Colorado.

Our objective is to define the current automation requirements of the Central Laboratories and present a cost analysis of the plans that satisfy these requirements. In brief, the study shows that the Central Laboratories have already benefitted appreciably from the use of remote computer facilities in Reston, Virginia. We find, however, that there are drawbacks to the use of a remote system that hinder the laboratories from realizing their full potential. We propose alternatives to overcome these drawbacks and hence to approach more closely the ideal concept of laboratories that can perform many parameter determinations simultaneously and quickly.

Although not addressed in this feasibility study, a functional specification of a system for Denver must consider the needs of the U.S.G.S. Water Resources Laboratories in Atlanta, Georgia, and Albany, New York, so that any system implemented at Denver can be easily replicated at Atlanta and/or Albany.

The mission of the Central Laboratories is to provide basic data on the quality of water resources through comprehensive and rapid analytical services to the districts and field projects in the 50 states. These comprehensive services have included a wide variety of physical tests and chemical and instrumental determinations of inorganic substances, pesticides, herbicides, and radionuclides in water samples. The services are now being extended to include the determination of petrochemicals in water to provide data for assessing the impact on water resources of the exploration and use of fossil fuels. This latter effort is in keeping with the Laboratories' responsibility to develop new and more effective analytical procedures and produce reliable data.

The Central Laboratories endeavor to provide these services at the lowest expenditure of manpower, time, and money commensurate with good quality control. Although the workload is high, the staff strives to attain a short turnaround between the time samples arrive in the laboratory and the time results are reported, so as to supply analytical and physical data promptly to the sample submitter and to the U.S.G.S. Hydrological Data Bank (WATSTOR).

How the Laboratories Fulfill Their Mission

The Central Laboratories fulfill their mission by employing procedures that maximize throughput without sacrificing analytical accuracy and precision. The Salt Lake City and Denver laboratories are organized into interdependent specialized sections, each being responsible for specific operations and analytical procedures.

At each facility, parallel determinations are made of a number of parameters on a single sample. Manual, semi-automated, and automated methods are used, and each laboratory has been moving toward completely automated facilities. With the combining of Salt Lake City and Denver laboratories, the opportunity for more efficient automation is obvious.

The Central Laboratories make use of remote computer facilities of the U.S.G.S. in Reston, Virginia. The computer generates job schedules that list the determinations to be made on each sample. The computer calculates calibration curves and sample results from data entered off-line via a terminal located in Salt Lake City. The computer also makes quality control checks on the sample analyses, generates analytical reports, and enters appropriate data into U.S.G.S. files and national data bases.

ANALYSES PERFORMED

There are nearly 300 different chemical and physical determinations that the combined Salt Lake City and Denver laboratories are prepared to make on any water sample. An updated list of the parameters that can be determined is released each year by the Central Laboratories.[1] About 50 additional parameters can be calculated from these direct determinations. Details of many of the analytical procedures are found in Ref. 2. Some of the atomic absorption procedures are based on provisional methods.

The determinations that are most frequently made in the Salt Lake City laboratory are specific conductance, pH, and concentrations of chloride, sulfate, calcium, magnesium, bicarbonate, sodium, potassium, silica, fluoride, and (nitrate + nitrite) as nitrogen. These constitute about 60% of all determinations carried out. The future promises a change in emphasis relative to the kinds of determinations that will be made and the matrices in which the determinations will be made. For example, there will be many more determinations of cyanide, chromium, lead, phenols, oils and grease, and trace metals, and there will be more water sediment and other hydrogeological samples. Currently the Salt Lake City laboratory performs about 500,000 tests per year and reports about 1 million water-quality parameters on about 40,000 samples. The samples arrive at an average rate of about 160 per day; the number for any one day varies from 25 to nearly 400.

Quality control samples and standards constitute about 10% of the laboratory sample load and include standard reference water samples, in-house calibration standards, blind samples, and interagency quality-control (round robin) samples. Statistical studies of precision show that relative standard deviation ranges between 5 and 20% for major (mg/liter) through minor (μg/liter) parameters. For most determinations of major parameters, the accuracy, expressed as positive or negative percent bias, is 2%. For determinations of minor and trace parameters there is considerable variation, ranging from less than 1% to as much as 50%, depending on the parameter and the level being determined.

DIVISION OF RESPONSIBILITY

The laboratory chief has administrative assistants in Salt Lake City and Denver. The staff includes management personnel for quality control and production, professional chemists, data processing personnel, laboratory technicians, and clerical assistants. Laboratory operations are divided into sections, according to primary responsibility or service, and each section is directed by a supervisor. The sections are: sample receiving, AutoAnalyzer,* atomic absorption analysis, special and manual methods, emission spectroscopy, chromatography, radiochemistry, and automated data processing. When the Salt Lake City and Denver laboratories are combined, the sections will be divided differently to maintain efficient operation.

INSTRUMENTATION

Instrumentation in the Salt Lake City and Denver laboratories includes four AutoAnalyzers ranging from one to five channels each, eight atomic absorption spectrophotometers, an automated analytical balance, a direct-reading emission spectrometer, gas and liquid chromatographs, a gas chromatograph - mass spectrometer, two spectrophotometers, a titrimeter, various carbon analyzers, radiochemical counting equipment, a fluorimeter, conductivity and pH meters, and other common laboratory instruments and equipment.

DATA PROCESSING

Data processing is now handled through a DATA-100, Model 70 terminal

*Reference to a company or product name does not imply approval or recommendation of the product by the University of California or the U.S. Energy Research & Development Administration to the exclusion of others that may be suitable.

that communicates with two IBM 370/155 computers of the U.S.G.S. in Reston, Virginia. The terminal is card oriented and has a line printer. The Reston computer program receives all sample identification information, generates laboratory-work-request job sheets and job data cards (upon which analytical data are to be entered), applies received input data to the calibration data in storage to compute the analytical results, performs quality-control checks, outputs final analysis sheets, stores the data in the national files, and makes appropriate cost accounting entries.

INFORMATION AND DATA FLOW: RECORDS AND REPORTS

The Salt Lake City laboratory produces and uses a number of records and reports, most of which are retained in the sections for only a short time after the analytical data have been reported and filed. The flow of information and data starts with the requester. The job requester submits Log-Inventory information sheets along with the samples. They supply details to the sample-receiving section relative to sample identification, field measurements, and the parameters to be determined. The information is logged into a receiving-section record book, and the Log-Inventory sheet is passed on to the data processing section.

Using a keypunch, the data processing section prepares Log-Inventory cards in order to transmit the sample information via the Central Laboratory DATA-100 terminal to the U.S.G.S. Reston computer.

The Central Laboratories' program residing in the Reston computer sets up a file of parameters to be determined and initiates cost accounting. It also formulates job sheets and job data cards, which are transmitted back to the Salt Lake City laboratory. The job sheets are generated for each section and list the sample numbers along with the parameters to be determined by that section. The analyst uses the job sheet to set up his work schedule, record information in his records, and keep track of the samples. The job data cards, upon which the analysis data are punched, are kept in the ADP section.

When a sample is run, the analysis data are produced in the laboratory in several different forms (printed tapes, data record sheets, etc., depending on the method or instrument) and given to the data processing section. The information is keypunched on the job data cards and transmitted to the Reston computer, where data reduction and quality control calculations are performed and the analysis report is formulated. The report is transmitted back to the laboratory and outputted on a line printer. Cost-accounting cards accompany the report and are used to maintain an accounting of work and funds for each requester of the laboratory's services.

The analysis report is reviewed by the laboratory's quality control officer who, if he approves the report, sends it to the requester. If he rejects one or more constituent results, a rerun is requested and eventually a revised report is obtained. The cost-accounting card is processed back through Reston to confirm the adequacy of header information in the WRD (for Water Resources Division) station header file so that the approved sample data can be passed into the WATSTOR file.

Important Features of the Existing System, Drawbacks of a Remote System, and Benefits of Further Automation

The existing laboratory system has several important features that demonstrate the effectiveness of automation and reveal advantages to be gained by further automation. For example, the use of remote computer facilities to perform the complex tasks of scheduling, data reduction, collation, and reporting has improved laboratory operations, management, and cost-accounting procedures. Although benefits have been realized at the Central Laboratories through the use of remote computer facilities, further benefits can be achieved by incorporating in-house computer facilities that will overcome certain of the drawbacks of a remote computer system. For example, an in-house system will greatly reduce the numerous transcriptions of information that are required in the present system. These transcriptions occur throughout the flow of information from one medium to another (e.g., from log sheets, data records, and recordings, to computer cards). These occur before the information is transmitted to the computer. They are a likely source of error and consume a large amount of time. Keypunching of cards and verification of punched data is also a time-consuming process and a source of error. In addition, for economic reasons the return of output from the computer is usually on an overnight basis. In the course of processing a group of samples, at least two overnight transmission-reception turnarounds with the Reston computer take place. These involve: (1) the transmission of the sample

Log-Inventory information to Reston and the reception of the work schedules and job data cards at the laboratory and, (2) transmission of analysis data to Reston and reception of the analysis report at the laboratory. Several transmissions of data are made to Reston before the analysis report is received at the laboratory, because many different parameters are determined in one sample over the course of several days. On-line quality control data are not available as the analysis proceeds in the laboratory. They become available only when the calculation in Reston is completed and the analysis report is returned to the laboratory. This delays the rerunning of samples should quality control criteria not have been met.

The laboratory is set up to perform multiple analytical tests virtually simultaneously on each sample. Thus a data base of multiple test results for each sample is established simultaneously. This system was devised in order to produce a complete analysis report of multiple tests on any one sample in as short a time as possible. It is an important concept, but it cannot be realized fully until the analytical tests being performed simultaneously are placed "online" to a computer for data reduction, quality control, and reporting.

The laboratory administration has pointed out other areas where improvements can be made.[3] These include the logistics of distributing many samples from the receiving section to the various laboratory sections, and the problems of performing frequent sample dilutions and of introducing large numbers of samples into the analysis instruments. (For example, during the test year 1971-1972, more than 10,000 dilutions were performed.) In these areas, direct automation would benefit efficient laboratory operation.

The Approach to Further Automation

GOALS TO BE ATTAINED

The goals of automating the Central Laboratories have been stated in other reports.[3,4] The goals we state below are the result of our review of the laboratories in Salt Lake City and Denver with a view to how they can best be further automated to satisfy demands for increased production and analytical research capabilities, and to provide a prototype for the automation of all the Central Laboratories.

Virtually all of goals detailed below will lead to increased laboratory efficiency:

- To speed up the logging in of samples and the setting up of files of parameters to be determined.
- To establish the files in the Central Laboratories and in Reston.
- To make available probable values for the parameters to be determined.
- To incorporate on-line automated analysis methods capable of on-line data acquisition, data processing, and quality control screening.
- To provide, at the same time, efficient techniques for the off-line entry of data from low-use and non-automated methods and instruments, and to eliminate punched cards as a method of computer communication.
- To provide a method for introducing and processing rerun samples quickly.
- To incorporate automated sample-changer and dilution systems that can be applied to a variety of instrumental methods.
- To establish an effective automated method for distributing samples.
- To maintain data backup so that laboratory operations will not be interrupted, and accumulated data will not be lost, in the event of a component malfunction within the system.
- To provide methods for promptly assessing laboratory performance, examining the status of an analysis, and reporting routine analytical data.

TECHNOLOGICAL AND ECONOMIC CONSTRAINTS

The Central Laboratories have adopted a stepwise approach to automation in order to maintain effective operation. The approach is prudent and was taken after weighing the constraints of manpower, time, costs, and available technology. Considering the goals stated in the previous paragraph and the automation required, it is wise to continue the stepwise approach.

The laboratories should continue their use of highly developed, commercially available instrument systems for determining petrochemicals and other organic substances. Such systems (e.g., chromatographs) can be obtained with integrated computer hardware and software that have been proven over years of development.

Frequently used instrumental methods for the determination of inorganics should be placed on-line in the automated system. Data from low-use instruments and methods not linked directly to the on-line automation system can be entered from off-line terminals.

The entire automation system should be integrated in-house to effectively manage the data from all the sources: on-line instruments, commercially available instrument systems, and non-automated methods.

With regard to automated sample distribution, there is little doubt that improved methods for distributing samples can be realized by incorporating an automated materials-handling system. However, it is consistent with the stepwise approach to defer such development and to consider including it separately after an effective laboratory automation has been implemented and evaluated. Sample diluters pose a different kind of problem. Proven technology has not yet been developed to provide on-line automatic dilution of samples. However, such a development could proceed in parallel with the automation of laboratory methods and instruments.

CANDIDATE INSTRUMENTS FOR AUTOMATION

At least 18 instruments are candidates for on-line automation in the new Denver laboratory. A brief description of each instrument and the measurements performed are given below.

Chromatography

A variety of chromatographic instruments are used in the laboratory for determining organic substances. As noted above, the acquisition of already developed, automated chromatographs is the preferred approach. The data from these systems may be fed to a central, shared computer and collated with data from other analytical instruments and methods.

Beckman Conductance Meter

This instrument is essentially a Wheatstone bridge. Specific conductance is measured when a variable resistance is adjusted to equal the resistance between two platinized electrodes immersed in the water sample. Conductance is measured on most samples that arrive in the laboratory. The value is used to calculate an approximate dilution factor for subsequent analyses performed in the various sections.

Radiometer-Copenhagen Titration System

This system performs repetitive titrations and can pipet the sample, clear the pipet, pipet a reagent, perform the titration, record the volume of titrant for the end-point, and print out the concentration of the sample. This system is used frequently to determine the alkalinity of water, which is a function of carbonate and bicarbonate content.

Technicon AutoAnalyzer

The AutoAnalyzer performs continuous-flow, simultaneous chemical analyses. The system aspirates multiple samples in sequence, brings the samples and reagents together for reaction, and continuously moves the sequence of samples through predetermined analysis steps. A reaction that produces a colored solution is included in the analysis procedure. The analyzer pumps the colored solution through a colorimeter, where absorption of the analyte of interest in measured. The concentration, which is proportional to absorption, can be displayed on a recorder or a digital printer. Four Technicon AutoAnalyzer systems carry a large workload in the laboratory. The following combinations of analytes are determined on the four separate AutoAnalyzers: (1) sulfate and chloride, (2) iron and phosphorus (HPO_3), (3) silica, phosphorus, nitrate, nitrite, and fluoride, and (4) nitrogen (Kjeldahl).

A new system for measuring pH and specific conductance is a candidate for automation. It is made up of components from the Technicon AutoAnalyzer and Radiometer-Copenhagen instruments. Water samples are introduced by means of a Technicon sampler and proportional pump, and the measurements are made with a Radiometer-Copenhagen potentiometer. It is expected that this instrument will determine pH and specific conductance on all samples received by the Denver laboratory.

Atomic Absorption Spectrometer

The atomic absorption spectrometer is used to determine metals in water samples. The instrument consists of a characteristic atomic-line source (hollow-cathode lamp) of the metal to be determined, a flame source for exciting the metals in the sample, a monochromator to select light of the appropriate wavelength, and a photomultiplier tube to detect the light. Water samples are aspirated into the flame, which stands between the hollow cathode lamp and the monochromator-detector. Neutral atoms of the metal of interest absorb the characteristic light from the hollow-cathode source, and the decrease in light energy (absorption) is detected and measured. The value can be read on a digital display in absorbance units, or directly in concentration, which is proportional to absorbance.

Atomic absorption spectrometers are used to determine many metals in a large number of samples. Five spectrometers (Perkin-Elmer Model 306) are used to determine individually Ca, Mg, Na, K, and Hg. Three spectrometers (Perkin-Elmer Model 503) are used for the determination of approximately 18 other metals.

Ultraviolet and Visible Spectrophotometer

The spectrophotometer consists of interchangeable tungsten-filament (visible) and hydrogen (ultraviolet) lamps, sample-solution cells, a monochromator, and a detector. The solution cell containing the sample is placed in the light path between the source lamp and the monochromator-detector. Light passing through the solution is absorbed by the analyte of interest over a wavelength band characteristic of the analyte. Measurements are made in absorbance units; absorbance is proportional to concentration. Oil, grease, phenol, boron, bromine, and vanadium are the most frequent spectrophotometric determinations. Two Coleman Model 55 spectrophotometers are used.

Total Organic Carbon Analyzer

Total organic carbon is determined using an Oceanographic International carbon analyzer. The glass-ampule technique is used, and the instrument consists of a sample-preparation unit and an analyzer unit. Up to 10 ml of sample are placed in a borosilicate ampule, and potassium persulfate is added. The mixture is acidified and purged with oxygen to remove pre-existing carbonate. The ampule is sealed, and the organic matter is oxidized to CO_2. It is then transferred to the analyzer unit where the seal is broken, and the quantity of carbon as CO_2 is measured with a nondispersive infrared analyzer. Over 4,000 total-organic-carbon analyses were performed on the instrument last year.

Mettler Electronic Balance

The Mettler Electronic Balance is composed of the balance itself (Model HE20), a balance control (Model BE20), and an electronic digital readout (Model BA28). The system is linked to a programmable calculator that accepts the weight value from the electronic balance and calculates the appropriate result depending upon the analyses being performed. The system is used most often for the determination of dissolved and suspended solids in water.

Optical Emission Spectrometer

The emission spectrometer is used for multielement analysis of water samples and residues. The sample is excited to emit light, which is dispersed in a grating spectrometer to form a spectrum of the elements in the sample. The spectrum is focused along the focal plane of the spectrometer, where carefully arranged slit-aperture photomultiplier tubes (channels) detect the spectrum lines of the elements of interest. The detected signal from each channel is processed, and the system outputs absolute intensities, intensity ratios, or concentrations. A Jarrell-Ash Plasma AtomComp spectrometer will be installed in the new facilities in Denver. Although the system will contain its own computer for control and computations, it should be linked to a laboratory automation system to attain enhanced capability for storage, data reduction, and quality assurance.

JOB SCHEDULING, COORDINATION, AND SAMPLE MANAGEMENT ACTIVITIES TO BE AUTOMATED

A number of activities related to scheduling, coordination, and data management are tied to the remote computer in Reston, Virginia. The usual response time of the remote system to an input is overnight. Thus the laboratory must gear its activity to the turnaround time of the remote system, and therefore does not realize full, efficient operation. On some occasions, when the Reston system is down, the Central Laboratories' job scheduling ceases, and a backlog of samples is created.

In view of this problem, it would be of great benefit to develop a local management system in the Central Laboratories. The local system would perform only those management functions that would provide efficient operation of each laboratory. The following is a brief listing of the minimal functions:

- Provide local job-parameter files for logging information and data.
- Provide job schedules.
- Provide methods for determining the status of a sample.
- Provide a means for reviewing the locally completed analysis, including quality control.
- Provide a means for approving the locally completed analysis before transmitting the result to Reston, Virginia.

FUNCTIONAL REQUIREMENTS OF THE CENTRAL LABORATORIES

The requirements for a system that will fulfill the Central Laboratories' goals within the stated constraints can be discussed in terms of three categories: inputs, outputs, and the interconnecting functions. These are summarized in Appendix A. The primary intent of the schematic in Appendix A is to summarize the important required functions and their relationship and to remind the reader of hardware and software requirements.

Proposed Alternative Systems for Fulfilling the Central Laboratories' Requirements

In devising concepts of systems to fulfill the Central Laboratories' requirements, we have judged that the following two factors weigh heavily:

• The decision of the Central Laboratories to automate in steps.

• The requirement that the automation system be reliable to the extent that laboratory operations, once automated, are not interrupted, and no data are lost in the event of a component failure.

In view of the above factors, small multiple-processor automation systems appear to be superior to a large-computer automation system. They allow for automation of the most critical and most frequently run analyses as a first step, with the option to expand the system to a network of computers to include other analyses and data management procedures, and to provide standby facilities in the event of failure within the on-line operating system.

We propose three alternative system concepts and variations. We describe them in the next section and in Appendix B in terms of schematic diagrams, relative advantages and disadvantages, and costs of hardware, software, and interface design and fabrication. In some cases, specific vendor equipment costs are shown. These are not intended to reflect a recommendation as to the vendor, but rather to show a typical cost for the item.

Each system can be built up (over a period of time) from a simpler version.

Bear in mind that this feasibility study presents available possibilities — that is, possible systems that can be compared on the basis of advantages, disadvantages, and costs. In following sections we will list guidelines for evaluating the alternative systems and a cost/benefit analysis that evaluates the worth of each of these systems on the basis of performance and (time and dollar) effectiveness.

SYSTEM NO. 1

Figure 1 shows a schematic of system 1. The fundamental building block is the programmable calculator with a mass-memory device and CRT display. The system is composed of multiple units of the fundamental building block for on-line acquisition and processing of data from individual analytical instruments. The system also includes a minicomputer system for in-house data management. The minicomputer is equipped with disk, magnetic tape, and essential input/output devices. Additional input/output terminals are provided for the receiving section and other laboratory sections, for the entry of off-line information and data into the management system.

A number of features should be incorporated into the system. The programmable calculator should include a versatile keyboard, a multi-line CRT display, a mass-memory device (e.g., cassette tape), and a capability for programming in a high-level language. These features provide convenient operation and interaction, the capability to write and modify programs with relative ease, and facilities for backup storage of data.

The input/output terminals for off-line use by the receiving section and non-automated instruments and methods should include local memory (cassette tape) for backup storage and, if equipped with CRT display, the ability to view selected lines of a large data set.

The in-house data management system, in addition to providing job matrices, work schedules, collations, and reports, should also contain programs for the reduction of data entered from the off-line instruments and methods.

Variations of System 1

The variations of system 1 are in keeping with the stepwise automation approach. The variations are:

1A) Exclude in-house data management, while continuing data management in Reston, Virginia. This variation would employ a simpler concentrator computer (relative to a data management computer) to prepare information and data for transmission to the Reston system.

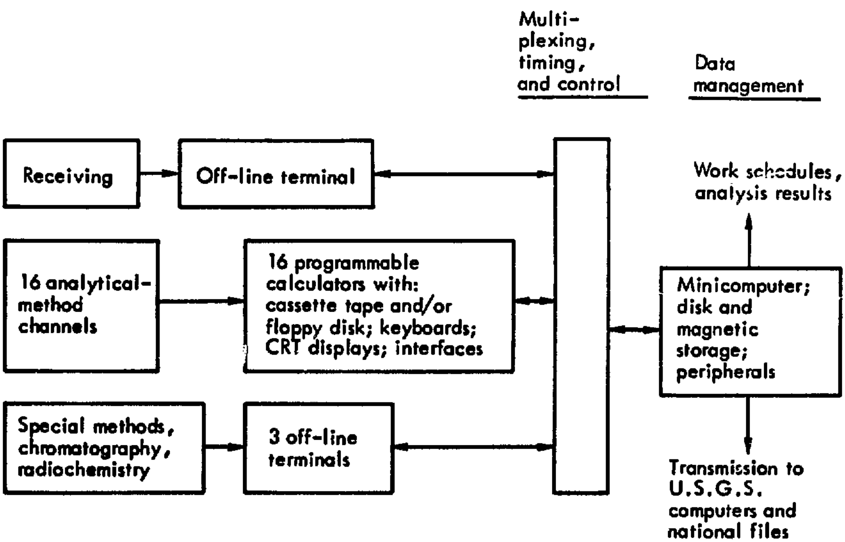

Fig. 1. Schematic of system 1. See Fig. B1 in Appendix B for details.

1B) Provide a few on-line, programmable calculator systems for the essential high-use analytical instruments, and a number of "roll around" systems to be used where needed "for current requested analyses." Such a system could be adopted in lieu of a full complement of calculators as shown in the system No. 1 schematic.

1C) Adopt a hybrid system, that is, programmable calculators for the simpler analyses (for example, conductivity and spectrophotometry) and a time-shared minicomputer for the more complex, high-throughput instrumental methods such as the multichannel Technicon AutoAnalyzers and the atomic absorption spectrometers.

Costs for System 1

Table 1 gives the overall costs for system 1 and each of the variations. See Appendix B for detailed listings of the costs for computer hardware, software, and interface design and fabrication.

Table 1. Costs for system 1 and variations.[a]

System	Cost (thousands)	
1	$717	
1A	585	
1B	597	$497[b]
1C	769	669[b]

[a]See Appendix B for details of the configurations and typical costs.

[b]Without data management.

Advantages of System 1

The programmable-calculator system has the following advantages:

1) The building-block units allow for stepwise automation.

2) Each unit provides data storage backup for each analytical instrument by means of cassette tape.

3) Each unit is relatively inexpensive. Thus, the laboratory is able to retain a standby unit in the event of failure of an on-line unit.

4) The small dimensions and weight of each building-block unit permit "roll around" automation systems that may be linked to an analytical instrument currently in high use.

Disadvantages of System 1

1) The complete system as shown in Fig. 1 is expensive.

2) There is limited core memory in each calculator unit for storing programs. Certain instrumental methods require large applications programs which, if placed in a calculator system, would have to be segmented and chained into the core from a disk.

3) Although a single calculator unit is relatively small compared to a minicomputer, 16 calculator units with peripherals may occupy an excessively large amount of space in the laboratory.

4) A calculator system in the laboratory will be exposed to acid fumes,

etc. Thus, each system may require an enclosure to protect it from the laboratory environment.

5) The relatively large number of building blocks in the system increases the likelihood of maintenance problems.

SYSTEM NO. 2

Figure 2 shows system 2. This system incorporates dual minicomputers, one for time-shared data acquisition, processing, and control, and the second for data management functions. The system includes a third minicomputer to serve as a standby in the event of failure of the time-share processor.

High-use analytical instruments are placed on-line to the time-share processor. Input/output terminals are available to each instrument, and data storage backup is provided by a magnetic tape unit at the processor.

If the on-line time-share processor fails, the standby unit would be manually switched into the system. With this manual switching approach, rather than automatic switching, some data may be lost. However, it would be cost effective to make the limited number of reruns required after a system failure rather than to bear

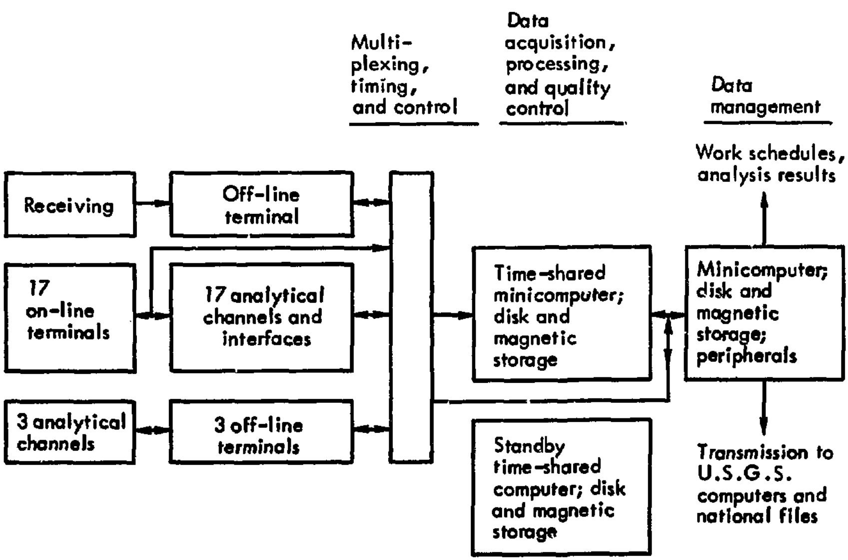

Fig. 2. Schematic of system 2. See Fig. B2 in Appendix B for details.

the high cost of an automatic switching system.

As in system 1, the system should incorporate features including appropriate input/output terminals at the on-line and off-line instruments and the ability to program in high-level language.

Variations of System 2

The variations of system 2 sacrifice redundancy. However, backup is retained by reducing certain tasks to a lower priority. The variations are:

2A) The standby time-share processor is excluded from the system. If the on-line time-share processor fails, the functions of data acquisition, processing, and control would be taken over by the data management processor. The data management functions would be temporarily suspended or continued at a lower priority until the time-share processor was returned to on-line service.

2B) In-house data management is excluded from the system in favor of data management in Reston, Virginia. Two time-share processors would be used: one for data acquisition, processing, and control for the high-use instruments, and the second for similar functions for the low-use instruments. The second processor would also be used as a concentrator to prepare information and data for transmission to Reston. If either of these two processors fails, its functions would be taken over by the other. Concentrator tasks would be set at a lower priority.

Costs for System 2

Table 2 gives the costs of system 2 and its variations. For each system, the cost is compiled from the detailed listing of costs for computer hardware, software, and interface design and fabrication shown in Appendix B.

Table 2. Costs for system 2 and variations.[a]

System	Maximum (thousands)	Minimum (thousands)
2	$687	$606
2A	602	521
2B	497	446

[a]For a breakdown of the costs in this table, see Appendix B. Estimated minimum costs reflect the availability of software and hardware designs from systems designed for the U.S. Environmental Protection Agency.

Advantages of System 2

1) The system can be built in steps.
2) A minimum version of the system can service all of the high-use instrumental methods on a time-share basis.
3) The system is compatible with other systems developed for the water analysis laboratories of the

U. S. Environmental Protection Agency (EPA). Therefore, certain hardware and software developments are transferable, with a significant savings in cost.

Disadvantages of System 2

1) Neither the minimum system nor the manually switched dual-processor system provides complete, continuous operational backup.

SYSTEM NO. 3

System 3, shown in Fig. 3, incorporates an interconnected grid of minicomputers. Esser ally ea section of the laborato. 'as its own time-share processor for data acquisition, processing, and control for a number of instruments, e.g., for the six spectrometers in the atomic absorption laboratory. In the grid arrangement shown in Fig. 3, the four laboratory computers are tied to one another, and if one fails, one or more of the other computers share its functions. Thus, laboratory operations can continue. Magnetic tape provides the backup data storage for each laboratory processor.

Variation of System 3

In a variation of system 3, the number of time-share processors is cut from 4 to 2. The system then resembles system 2.

Costs for System 3

The cost of system 3 (including computer hardware and software, and interface design and fabrication, as compiled in Appendix B) is estimated at $864,000. This cost does not include the cost of hardware and software to automatically switch among the computers within the grid should one of them go down.

Advantages of System 3

1) The network can be built up in steps.

2) The system provides backup for continuous operation and storage of data.

3) It is capable of accepting many inputs and of operating complex programs, and is therefore amenable to expansion of laboratory tasks and automation of methods and instruments not included in the initial automation.

4) The time-share minicomputer building-block of this system is compatible with EPA systems. Therefore, certain hardware and software developments are transferable, with a significant savings in cost.

Disadvantages of System 3

1) The complete system as shown in Fig. 3 is expensive.

2) If automatic switching within the grid of computers is adopted, the cost will be greater.

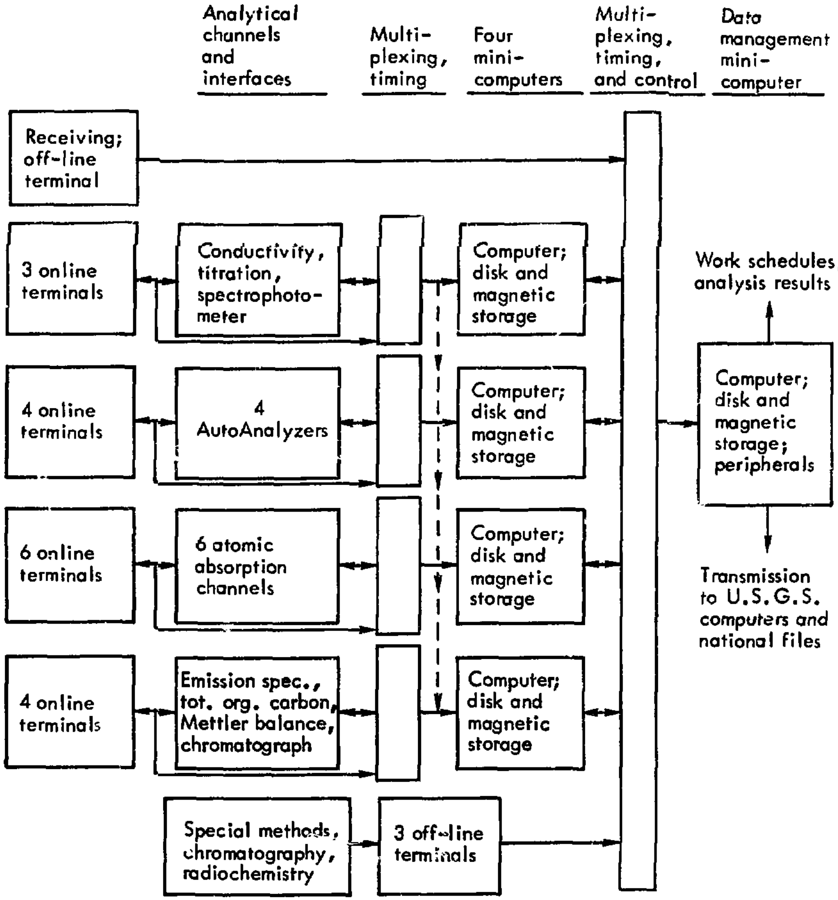

Fig. 3. Schematic of system 3. See Fig. B3 in Appendix B for details.

Evaluation of the Proposed Systems

We have pointed out the goals to be attained by further automation, summarized the requirements of the laboratories in a schematic diagram, and proposed three alternative automation systems and their variations.

We will now formulate a set of criteria for evaluating the proposed systems. The aim of this evaluation is to identify the automation system that best meets the Central Laboratories' requirements as we see them.

TIME RESPONSE

The system should generate job parameter files and work schedules immediately after the samples have been received by the laboratory. Hence, the data management system must accept information or data in fractional seconds to seconds. Such a time response will also be needed when data are entered from the high-throughput, on-line analytical instruments.

Information and data must be retrieved from the management data base in no more than a few minutes, and preferably just a few seconds. This requirement is especially important in scheduling laboratory work, determining the status of an analysis, and preparing reports.

HARDWARE AND SOFTWARE CAPABILITIES

The computer system should be easily programmable by the analyst in the laboratory; it should have a versatile, vendor-supported operating system and provide a data management language; it should have a wide variety of characteristics, facilities, and peripherals that qualify it to handle the complex tasks of the laboratory and to take on new tasks in the future. Appendix C gives more details of the desirable hardware and software capabilities.

HARDWARE BACKUP CAPABILITY

It is advisable to maintain computer backup facilities (an extra computer) in the event the primary computer fails, so that laboratory operations may continue uninterrupted. A redundant system should have a second processor in standby mode ready to be brought into operation manually or automatically. In the case of the Central Laboratories, uninterrupted operation is not critical enough to warrant the expense of the extra hardware and software that would be needed to automatically switch to a standby computer. Thus, manual switching to standby is recommended.

DATA STORAGE AND BACKUP CAPABILITIES

Mass storage should be available for the backup storage of information and data that are being accumulated during laboratory operations. It must retain the information and data until the final results have been stored in the U.S.G.S. and national files and the analysis report has been written. Furthermore, the user should be able to retrieve data relatively easily from the backup mass-storage, and extensive software for sorting and collating should not be required.

GROWTH POTENTIAL

The system should be modular, to allow for expansion. The computer operating system should make efficient use of its resources and should be sufficiently versatile to allow for growth in time-sharing, data management, data communications, and task coordination.

In Table B6 of Appendix B we have evaluated the proposed alternative systems in terms of system costs and the criteria described above. This method of evaluation allows us to judge the merits of each system relative to both "quantifiable" benefits and "unquantifiable" criteria. The quantifiable benefits are treated in detail in the following section.

Recommended System

The capabilities and moderate cost of system 2 qualify it as the most suitable system to meet the needs of the Central Laboratories. The achievement of good time reponse by means of on-line instrumental analysis and in-house data management is the most important need of the Central Laboratories. System 2, incorporating state-of-the-art minicomputers, will fulfill that need. The hardware and software requirements and hardware backup can be met by field-proven modular systems that can be acquired for system 2. These can be expanded to accommodate growth. Although data storage backup by means of magnetic tape will not be exclusive for each instrument, shared backup will be available at the time-shared processor or on magnetic tape at the management processor. Thus, a number of alternative schemes for data backup can be pursued and implemented.

COMPARISON OF COSTS AND BENEFITS

The income and operating costs of the Central Laboratories are directly related to the number of tests performed. Since the operation of a laboratory involves a coordinated effort among management and all of the individual sections, it is reasonable to average costs and income over the entire staff. For this cost/benefit analysis, figures from the Salt Lake City laboratory will be used as an example. The income of the laboratory for FY 1975 was

$1,285,799, and the effort during that period was 43.3 employee years. Thus, the average income (related to tests) was $30,000 per staff member.

Table 3 summarizes the results of our cost/benefit study. We have analyzed the effort currently being expended in all sections of the Salt Lake City laboratory relative to the effort that would be required with the recommended automation. The automation will bring about increased efficiency, which has been expressed in employee-years of effort made available to perform additional tests. The dollar value of this increased efficiency has been calculated by multiplying the average income per staff member times the employee-years made available by automation. See Appendix D for a detailed table of this cost/benefit study.

The efforts of only 22 members of the staff are included in the calculations shown in Table 3. The analysis did not include employees

Table 3. Benefits of automation.

Laboratory effort category	Efficiency increase due to automation[a] (employee-years per year)	Dollar value of increased efficiency[b]
Section supervisors	0.55	$16,500
Production supervisor	0.50	15,000
Quality control section	1.00	30,000
Section 1		
Sample receiving	0.38	11,500
Alkalinity and conductivity	0.34	10,000
Section 2		
Technicon AutoAnalyzers	0.83	25,000
Section 3		
Atomic absorption	0.77	23,000
Section 4		
Carbon determinations	0.53	16,000
Spectrophotometer and balance	0.08	2,500
ADP section	2.00	60,000
Total benefits	6.98	$209,500

[a]"Effort increment," i.e., effort by present techniques minus effort after automation.

[b]Effort increment multiplied by the average income per staff member.

Table 4. Annual operating costs.

Item	Present system	Proposed system
Data-100 terminal (rent and maintenance)	$15,000	—
IBM keypunch (rent and maintenance)	4,000	—
IBM sorter (rent and maintenance)	1,800	—
Line printer (rent and maintenance)	1,000	1,000
System maintenance by computer manufacturer	—	9,000
CPU and disk accesses (in Reston)	42,500	20,000
Transmission costs	10,000	4,000
On-line disk (Reston)	7,500	7,500
Paper for line printer and terminals	1,200	1,500
IBM cards	1,000	—
Magnetic tape	—	500
Electronics engineer (salary, benefits, and overhead)	—	45,000
Total costs	$84,000	$88,500

whose tasks we judged were not affected by the recommended automation. This includes, for example, secretaries, analysts performing chemical preparations and non-automatable tasks, and certain managerial functions. The approach is conservative and is intended to make the analysis as credible as possible.

The cost/benefit analysis relative to effort shows that the incorporation of additional automation will make available nearly 7 employee-years per year of effort to perform additional tests. Translated into dollars by the formula shown previously, this will increase the laboratory income by $209,500.

In addition to effort it is important to compare operating and maintenance costs of the present Salt Lake City automated data processing system relative to the recommended automation. Table 4 summarizes that comparison and indicates higher costs of $4,500 yearly for the recommended automation. Again we have made a conservative analysis, especially with regard to reduced Reston system costs for CPU time, disk accesses, and transmissions that would result with the new automation. An optimistic analysis would reduce the Reston costs still further.

The operating and maintenance costs for the recommended automation include the addition of an electronics engineer to the Central Laboratories staff. It would be beneficial to include an engineer on the staff not only to maintain the system but also to be responsible for system upgrading and future growth. If a staff engineer is not added, the annual cost for maintaining the system would then be estimated at 10% of the cost of the system hardware, or approximately $30,000 per year.

COSTS AND BENEFITS RELATIVE TO PAYOUT TIME AND LIFE OF THE SYSTEM

As shown above, the recommended automation will yield the equivalent of $209,500 in available effort each year at an operating and maintenance annual cost of $4,500 over that of the present ADP system. Thus, the net benefit is equivalent to $205,000 per year in available effort.

If one assumes the expected service life of the system to be 5 years, the net benefit after 5 years, taking into account the one-time investment cost of $602,000, will be $202,000. This value was calculated using the following formula:[5]

$$B_{(5\ \text{years})} = \frac{b}{n}\left[\frac{(1 + (i/n))^{5n} - 1}{(i/n)(1 + (i/n))^{5n}}\right] - c$$

where,

b = net benefit per year, $205,000

i = interest rate, 10% per annum

n = period (12, if compounded monthly)

c = one-time investment cost of the system, $602,000.

The break-even point or payout time for the recommended system is 3.5 years and was calculated as follows:

$$T = -\left[\ln\left(1 - (ic/t)\right)\right]/i$$

The payout time of 3.5 years is less than the 5-year service life of the system and thus characterizes the system as economically desirable.

SUMMARY OF BENEFITS

From a cost/benefit point of view the recommended automation system is economically justifiable. It will accrue the net equivalent of $202,000 in available effort for the Salt Lake City laboratory alone over an expected service life of 5 years. Also, the original investment cost of the system will have been paid up in 3.5 years.

The Central Laboratories will benefit in other ways as well. They will be able to incorporate more quality assurance checks and will be able to virtually eliminate calculation, transcription, and keypunching errors. They will be able to accomplish good turnaround on the reporting of analyses and will improve production control techniques through the use of in-house sample management. More timely scheduling of work and determination of the status of jobs will result.

Soon, the Central Laboratories will experience increased demands for their services. The automation recommended in this study will put the laboratories in a better position to meet those demands and to expand still further as future needs unfold.

Acknowledgment

This study was prepared under
U.S.G.S. Order No. 15013.

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Appendix A

Functional Schematic of the Central Laboratories, U.S.G.S.

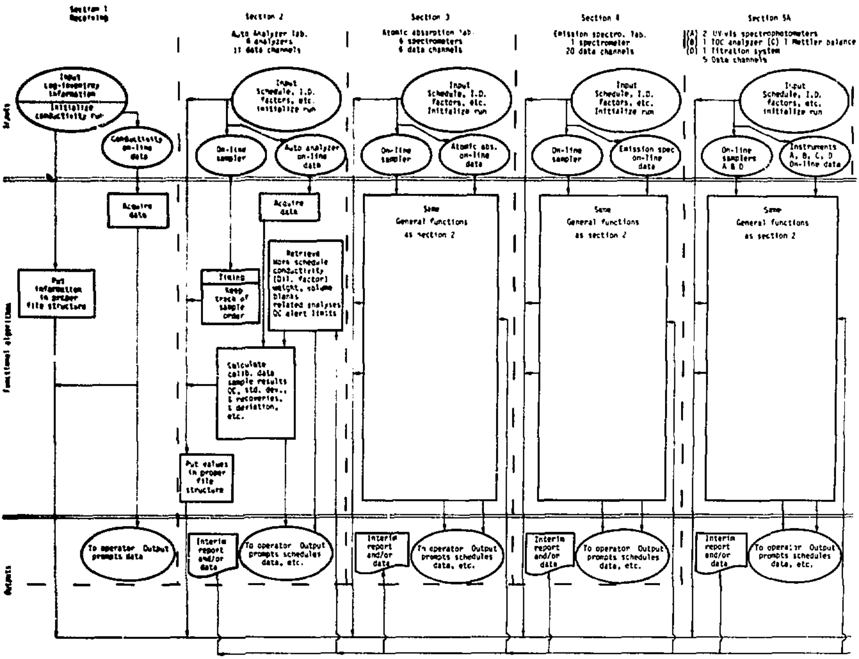

Fig. A1. Functional schematic of the Central Laboratory, U.S.G.S.

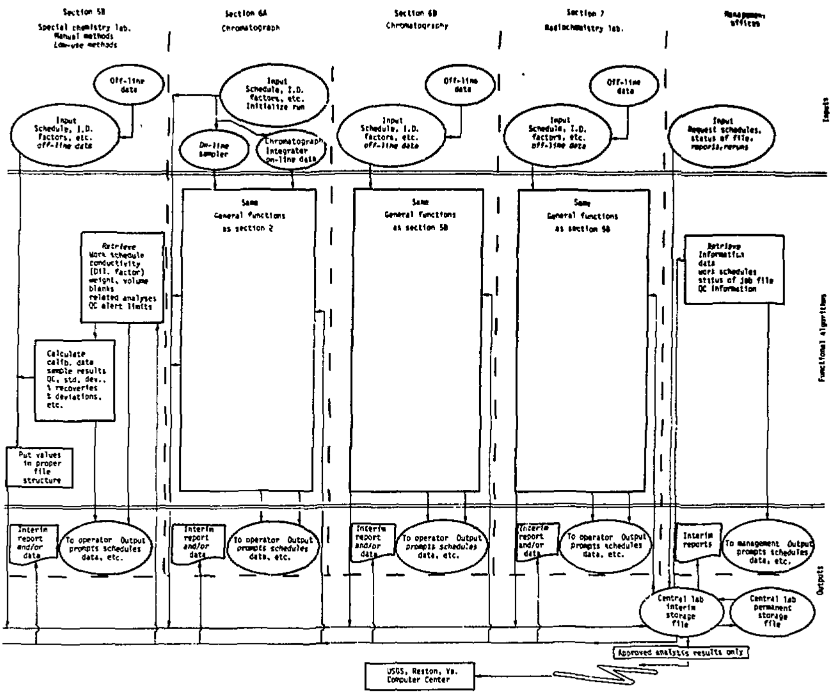

Fig. A1. (Continued from facing page.)

Appendix B

Costs for Computer Hardware and Software, and Interface Design and Fabrication

SYSTEM NO. 1

Table B1. Cost of computer hardware for system 1.

Description	Unit cost, (thousands)	No. of units	Total cost, (thousands)
Programmable calculator with CRT, 32K memory, single tape cassette (78K bytes), disk (252K bytes), Wang Laboratories, Inc.	$17.1	14	$239.4
Minicomputer main frame (for data mgmt.), Data General, Eclipse	40.0	1	40.0
Fixed-head disk, 262M	14.0	1	14.0
Moving-head disk, 12M	18.5	1	18.5
Magnetic tape, 9 track	8.5	1	8.5
Paper-tape reader	1.3	1	1.3
Rack	2.0	1	2.0
Memory map and protection unit	3.5	1	3.5
Minicomputer operating system software	1.0	1	1.0
Line printer, Centronics, 102A	6.8	1	6.8
Terminal, for off-line uses, Hewlett-Packard 2640A	3.0	3	9.0
Communications device, Bell Telephone 201	0.2	1	0.2
Total cost			$344.2

Table B2. Cost of computer software for system 1.[a]

Description	Cost (thousands)
Beckman conductance meter	$14.0
London titrimeter	22.0
Coleman 55 spectrophotometer[b]	18.0
Jarrell-Ash emission spectrometer[c]	
Technicon AutoAnalyzer[b]	15.0
Perkin-Elmer atomic absorption spectrometers	20.0
Total-organic-carbon analyzer[b]	10.0
Mettler balance[b]	10.0
Reverse-phase chromatograph	15.0
Concentrator program[d]	(20.0)
In-house data management[b]	100.0
Total cost	$224.0

[a]BASIC-language applications programs, including assembly-language codes for specific tasks, e.g., data acquisition.

[b]Applications programs for these instruments have been (or will have been) developed for the Environmental Protection Agency for use with Data General computer systems. Modification of these programs to U.S.G.S. needs and assuming a Data General system would reduce software costs by approximately 30%.

[c]An applications program for Jarrell-Ash emission spectrometer is available from Jarrell-Ash Company with purchase of the instrument.

[d]Required to prepare data for transmission to Reston if in-house sample data management is not provided.

Table B3. Cost of interface design and fabrication for system 1.

Description	Design cost[a] (thousands)	Fabrication cost per unit (thousands)	Number of units	Total cost (thousands)
General interface	($6.0)	$14.0	2	$34.0
Beckman conductance meter	3.0	3.0	1	5.0
London titrimeter	6.0	8.0	1	14.0
Coleman 55 spectrophotomer	(4.0)	3.0	1	7.0
Jarrell-Ash emission spectrometer	7.0	7.5	1	14.5
Technicon AutoAnalyzer, II	(6.0)	4.5	4	24.0
Perkin-Elmer Model 306 atomic absorption spectrometers	(2.5)	3.0	4	14.5
Perkin-Elmer Model 503 atomic absorption spectrometers	(2.5)	4.0	2	10.5
Total-organic-carbon analyzer	(3.0)	3.0	1	6.0
Mettler balance	(5.0)	5.0	1	10.0
Chromatograph	4.0	4.5	1	8.5
Total cost				$149.0

[a]Numbers in parentheses indicate that the interface design has been developed for the Environmental Protection Agency for use with Data General computer systems. Therefore, design costs would not be incurred for a Data General system.

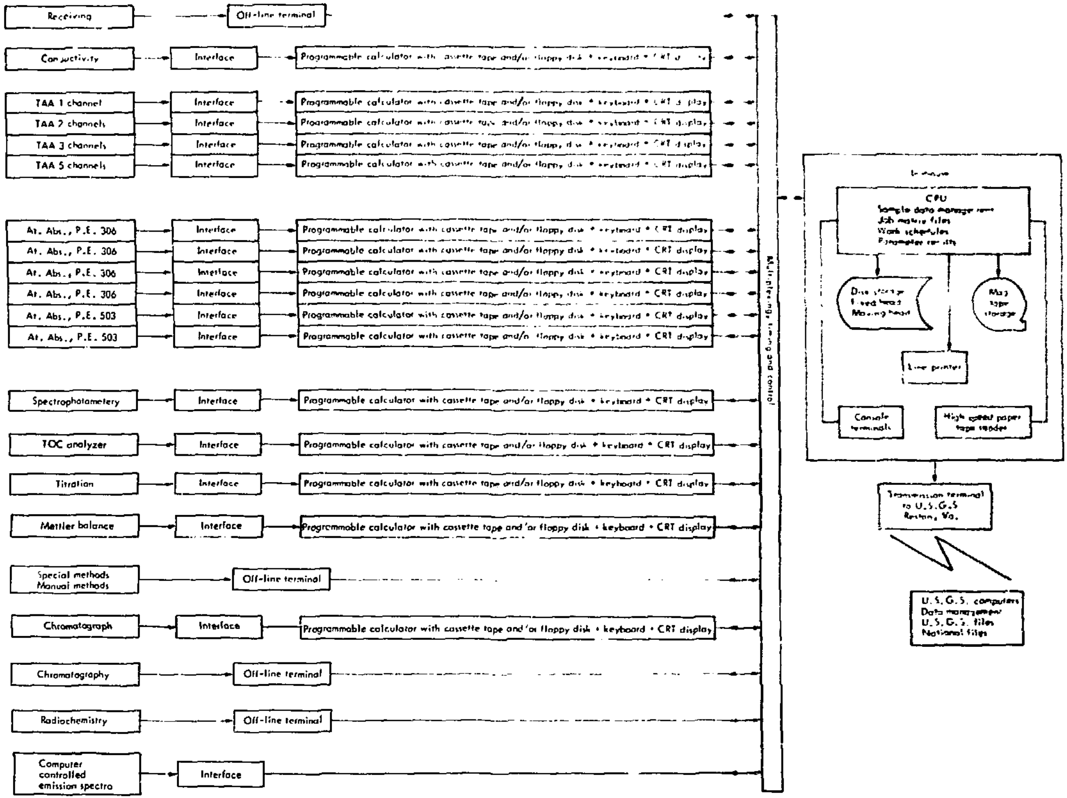

Fig. B1. Schematic of system 1.

SYSTEM 1, VARIATION 1A

Computer Hardware

Costs for computer hardware and peripherals are lower by about $32,000 relative to system 1. This provides a concentrator computer rather than a data management computer.

Total cost: $312,000

Computer Software

Total cost: $124,000

(Costs would be reduced by eliminating data management programming.)

Interface Design and Fabrication

No change in costs relative to system 1.

Total cost: $149,000

SYSTEM 1, VARIATION 1B

Computer Hardware

The lowest limit in the number of programmable calculators for the system would be 7.

The costs would be reduced by $120,000 relative to system 1.

Total cost: $224,000

Computer Software

Same as system 1.

Total cost: $224,000

Interface Design and Fabrication

Same as system 1.

Total cost: $149,000

SYSTEM 1, VARIATION 1C

Computer Hardware

4 Programmable calculators

1 Minicomputer (time-share)

1 Minicomputer (time-share backup)

1 Minicomputer (in-house sample management)

Total cost: $396,000

Computer Software

Same as system 1.

Total cost: $224,000

Interface Design and Fabrication

Same as system 1.

Total cost: $149,000

SYSTEM NO. 2

Table B4. Cost of computer hardware for system 2.

Description	Unit cost (thousands)	No. of units	Total cost (thousands)
Minicomputer, main frame, Data General, Eclipse	$40.0	3	$120.0
Fixed-head disk, 262K	14.0	3	42.0
Moving-head disk, 12M	18.5	3	55.5
Magnetic tape, 9 track	8.5	3	25.5
Paper-tape reader	1.3	3	4.0
Rack	2.0	3	6.0
Memory map and protection unit	3.5	3	10.5
Minicomputer operating system software	1.0	1	1.0
A/D converter, 14 bit	2.5	2	5.0
Line printer, Centronics, 102A	6.8	2	13.6
On-line data terminal, Lear-Siegler, ADM-1	1.0	14	14.0
Off-line data terminal, Hewlett-Packard	3.0	4	12.0
Console terminal, Texas Instruments, Silent 700	1.5	3	4.5
Communications device, Bell Telephone 201	0.2	1	0.2
Total cost			$313.8

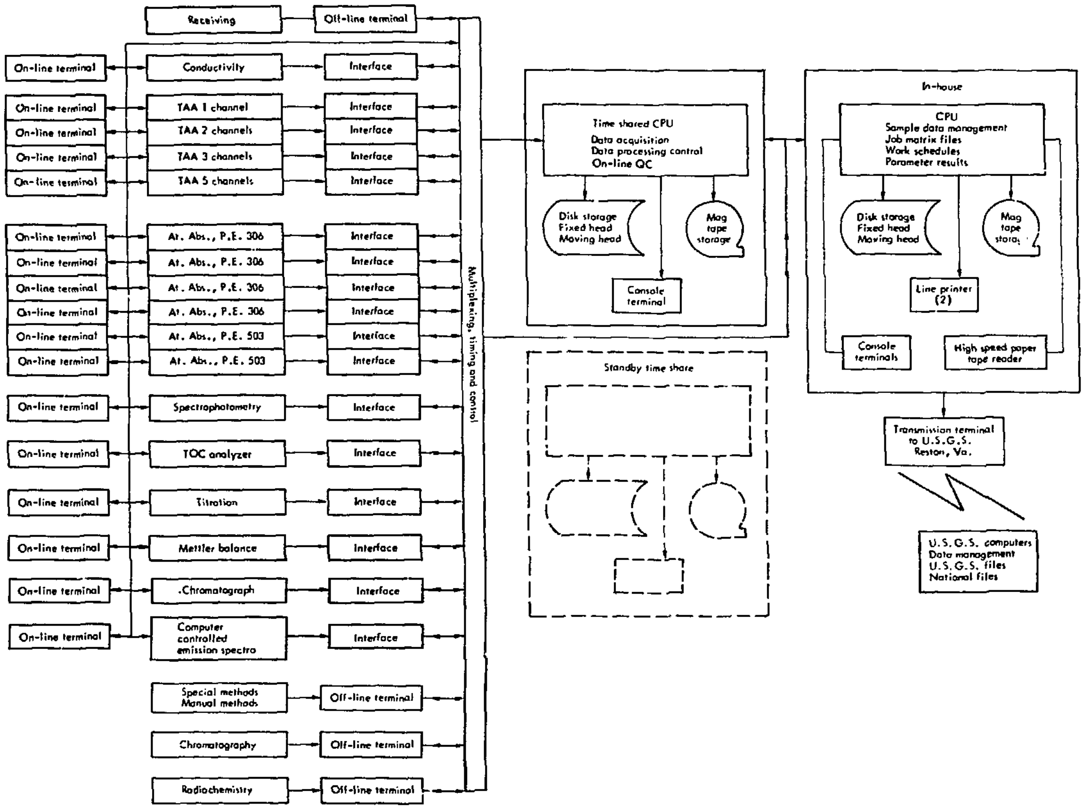

Fig. B2. Schematic of system 2.

Computer Software

Software specifications for system 2 are assumed to be about equivalent to system 1. Therefore, refer to system 1 for details.

Total cost: $224,000

Interface Design and Fabrication

Interface design and fabrication costs are assumed to be approximately equivalent to system 1. Therefore, refer to system 1 for details.

Total cost: $149,000

SYSTEM 2, VARIATION 2A

Computer Hardware

Exclusion of the standby processor would reduce costs by $90,000 relative to system 2.

Total cost: $224,000

Computer Software

Software costs would be increased by $5,000 to transfer applications programs to the data management computer.

Total cost: $229,000

Interface Desig and Fabrication

Same as system 2.

Total cost: $149,000

SYSTEM 2, VARIATION 2B

Computer Hardware

Costs for computer hardware and peripherals are lower by $90,000 relative to system 2. This provides a concentrator computer rather than a data management computer.

Total cost: $224,000

Computer Software

Costs are reduced by $100,000 relative to system 2 by elimination of data management programming.

Total cost: $124,000

Interface Design and Fabrication

No change in costs relative to system 2.

Total cost: $149,000

SYSTEM NO. 3

Table B5. Cost of computer hardware for system 3.

Description	Unit cost (thousands)	No. of units	Total cost (thousands)
Minicomputer, main frame, Data General, Eclipse	$40.0	5	$200.0
Fixed-head disk, 262K	14	5	70.0
Moving-head disk, 12M	18.5	5	92.5
Magnetic tape, 9 track	8.5	5	42.5
Paper-tape reader	1.3	5	6.5
Rack	2.0	5	10.0
Memory map and protection unit	3.5	5	16.5
Minicomputer operating system software	1.0	1	1.0
A/D converter, 14 bit	2.5	2	5.0
Line printer, Centronics, 102A	6.8	2	13.6
On-line data terminal, Lear-Siegler, ADM-1	1.0	14	14.0
Off-line data terminal, Hewlett-Packard	3.0	4	12.0
Console terminal, Texas Instruments, Silent 700	1.5	5	7.5
Communication device, Bell Telephone, 201	0.2	1	0.2
Total cost			$491.3

Computer Software

Software specifications for system 3 are assumed to be approximately equivalent to system 1. Therefore, refer to system 1 for details.

Total cost: $224,000

Interface Design and Fabrication

Same as system 1.

Total cost: $149,000

SYSTEM 3, VARIATION 3A

Costs for computer hardware, software, interface design, and fabrication are approximately the same as system 2.

Total cost: $687,000

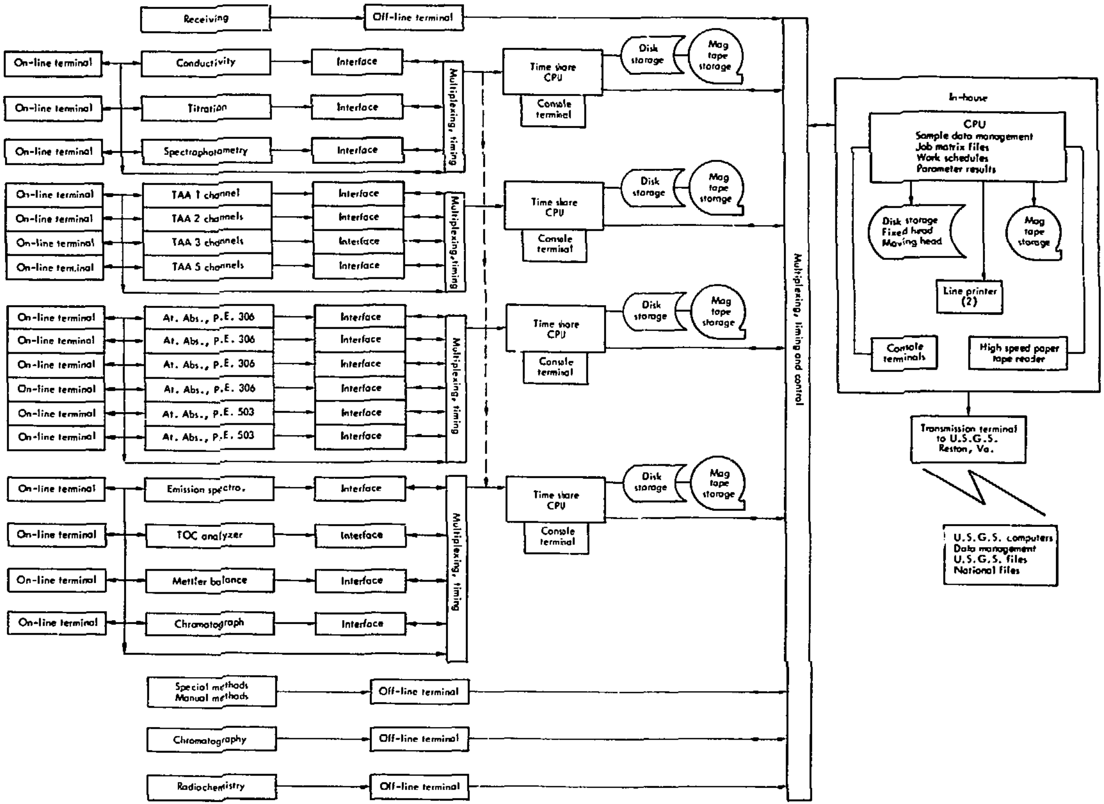

Fig. B3. Schematic of system 3.

Table B6. Evaluation of the alternative systems.

System	Cost	Time Response Capability	Hardware and Software Capabilities
No. 1 Multiple Programmable Calculators + In-house Sample Data Mgmt. Minicomputer	$710K	Meets Requirements. 1) In-house Sample Data Mgmt. 2) On-line analyses.	Some limitations. 1) Operating system less versatile than that of a minicomputer 2) Limitations in size of core memory (32K) in calculators
No. 1A Multiple Programmable Calculators Remote Data Mgmt.	$608K	Does not meet requirements. A poor time response with remote data management.	Same limitations as No. 1 (above)
No. 1B Limited Number of Programmable Calculators + "Roll-Around" Calculators + In-house Sample Data Mgmt. Minicomputer	$590K	Meets requirements. 1) In-house Sample Data Mgmt. 2) On-line analyses	Same limitations as No. 1 (above)
No. 1C Hybrid System Programmable Calculators + Time-share Minicomputer + In-house Sample Data Mgmt. Minicomputer	$762K	Meets requirements. 1) In-house Sample Data Mgmt. 2) On-line analyses	Limitations are not present if minicomputer with good operating system is incorporated in hybrid system.
No. 2 Time-share Minicomputer + Backup minicomputer + In-house Sample Data Mgmt. Minicomputer	$588K	Meets requirements. 1) In-house Sample Data Mgmt. 2) On-line analyses	Meets requirements if minicomputers with capabilities shown in Appendix B are incorporated in system.
No. 2A Time-share Minicomputer In-house Sample Data Mgmt. Minicomputer (no separate time-share computer for backup)	$496K	Some limitation. If Sample Data Mgmt. CPU has to take over on-line instrument tasks (functioning as backup), data mgmt. tasks will be slowed (lower priority).	Meets requirements same as No. 2 (above).
No. 2B Time-share Minicomputer +Backup Minicomputer Remote Data Mgmt.	$429K	Does not meet requirements. Poor time response with remote data management.	Meets requirements same as No. 2 (above).
No. 3 Network System 4 Time-share Minicomputers + In-house Sample Data Mgmt. Minicomputer.	$851K	Meets requirements. 1) In-house Sample Data Mgmt. 2) On-line analyses	Meets requirements if minicomputers with capabilities shown in Appendix B are incorporated in system.

Table B6. (Continued from facing page.)

Hardware Backup Capability	Data Storage Backup Capability	Growth Potential
Meets requirements. Redundant hardware can be made available with standby programmable calculator	Meets requirements. Cassette tape data storage backup exclusive to each automated instrument. No sorting required.	Limitations. Growth requires addition of programmable calculator and peripherals for each new laboratory instrument to be automated. Proliferation of calculator units creates space and location problems.
Meets requirements same as No. 1 (above)	Meets requirements same as No. 1 (above)	Limitations same as No. 1 (above)
Limitations. Hardware backup may be impaired if a limited number of calculator units are available.	Meets requirements same as No. 1 (above)	Limitations same as No. 1 (above)
Meets requirements. Redundant hardware is a relatively high investment cost with incorporation of minicomputer.	Limitations. Incorporation of a minicomputer (time-sharing) in the hybrid systems leads to limitations shown in No. 2 (below)	Limitations are not present if minicomputer with good operating system is incorporated in the hydrid system.
Meets requirements with backup minicomputer.	Limitations. Magnetic tape for data storage backup is shared by multiple instruments. Availability on demand for updating is limited. Sorting of data required when data has to be retrieved.	Meets requirements if minicomputers with capabilities shown in Appendix B are incorporated in system.
Meets requirements. However, since the hardware backup is the Data Mgmt. computer, additional software will be required to allow the Data Mgmt. CPU to take over time-share processing. This cost is shown. Also note that switching will be manual, therefore, some data loss may occur.	Limitations same as No. 2 (above)	Meets requirements same as No. 2 (above)
Meets requirements same as No. 2 (above)	Limitations same as No. 2 (above)	Meets requirements same as No. 2 (above)
Meets requirements. Note: If automatic switching among the network of CPU's is required for backup, then additional hardware and extensive software will be needed	Limitations same as No. 2 (above)	Meets requirements same as No. 2 (above)

Appendix C
Capabilities of System Hardware and Software

There are three major parts to a computer system: the central processing unit (CPU), the peripheral input/output devices, and the operating system. The first two parts compose the hardware of the system, while the latter contains the software that ties the CPU and peripherals together and enables the users' applications programs to run smoothly. While many systems can meet the minimum hardware capabilities for the Central Laboratories, only a few can satisfy the important criteria set for operating-system software.

A typical minimum-capability system can be acquired from a number of manufacturers. This would include, for example, a 16-bit-word-length CPU with 64K bytes of core memory expandable to 256K bytes or greater. Peripheral devices would include high-speed paper tape, magnetic tape, fixed-head and moving-head disks, a medium-speed line printer, and teletypewriter or display terminals for the computer console and for each of the on-line automated instruments.

Although the above hardware configuration can be supplied by a number of computer manufacturers, each manufacturer supplies a different operating-system software package, and these must be studied carefully to be certain that the most appropriate system is chosen. Two important points about the operating system are: (1) it must be supported by the supplier, and (2) it should be a field-proven system. It is not unusual for a reliable manufacturer to guarantee his support of the operating system software for as long as five years. This has been found necessary because often times system bugs are not discovered until long after delivery of the computer system. One should also be cautious about the acquisition of computers with new or prototype operating systems. We have observed that such systems are beset with problems initially and may not be delivered on schedule because the supplier has encountered unforeseen difficulties. The disadvantage of this cautionary stance is that new, possibly more powerful, systems may be rejected. However, the advantages of a proven system are worthwhile, especially when one considers that users other than U.S.G.S. will have tested the system and their experiences can be drawn upon.

A number of features characterize a versatile computer operating system. The following paragraphs deal with some of the important characteristics and the benefits derived from each.

MODULAR DESIGN

The system should be modular in design, possess a variety of machine configurations, and permit the user to easily select desired system features. Thus, the user will be able to build executive programs from vendor and user routines and tailor them to meet the specific needs of the laboratory. The modular operating system is an important feature, which provides versatility in building the initial installation and permits future changes and growth.

FLEXIBLE SCHEDULE

The operating system must be capable of scheduling and allocating program control to many analytical instruments (users) performing many tasks. The scheduling should be such that each user appears to have exclusive access to system resources such as disk files, the instrument I/O terminal, or the system line printer. The flexible scheduling system provides the capability for on-line multi-instrument time-sharing of a single computer.

MULTIPLE AND HIGH-LEVEL LANGUAGE SUPPORT

The system should be capable of supporting many language processors, such as BASIC and FORTRAN as well as assembly language. For the occasional programmer-analyst, the high-level BASIC language provides a convenient and relatively simple means for program development. It is the most widely used interactive language available and can be supplied in multi-user versions for time-sharing applications. A strong point in favor of BASIC is that it can be modified on-line and tested virtually immediately after modification. A potential disadvantage lies in the fact that BASIC is an interpreted code and thus runs more slowly than a compiled code such as FORTRAN.

DATA MANAGEMENT CAPABILITIES

The system software for file management should permit the user to create, access, and manipulate large data bases. Such a software package would provide a basis for building an in-house data management system.

OTHER FEATURES

A number of other features are required if an effective time-sharing system is to be realized. A versatile disk-file management capability should be available wherein data can be accessed randomly, sequentially, or contiguously. File protection must be included to ensure against inadvertent or unauthorized access.

To make the most efficient use of core storage, the user should have available effective program-swapping, chaining, and overlaying techniques.

Foreground-background program operation is another desired feature. It permits apparent simultaneous functioning of unrelated programs that share basic system resources. This feature would be especially useful in emergency backup situations where tasks normally performed by two computers could be taken over by a single processor.

Appendix D
Benefits of Automation

Table D1. Comparison of the effort expended with present techniques to that expended when automated techniques are used. The increase in efficiency is presented at the end of each subsection as "Effort available for additional activities."

Tasks	Effort expended (employee-years per year) At present	With automation
Section supervisors		
Respond to sample status inquiries	0.15	0.15
Handle requests for special analyses	0.25	0.10
Monitor special quality-control samples	0.25	0.10
Perform special studies	0.30	0.30
Generate special reports	0.25	0.25
Schedule work for section	0.45	0.20
Routine analytical tasks in section	0.75	0.75
Management tasks	0.60	0.60
Total effort	3.00	2.45
Effort available for additional activities	—	0.55 ←
Sample receiving (Section 1)		
Unpack shipments	0.50	0.50
Read and transcribe information from bottles	0.13	0.07
Number the bottles	0.25	0.25
Read and transcribe information from log-inventory sheet	0.50	0.25
Enter information in logbook	0.13	0.06
Arrange bottles in trays	0.06	0.06
Distribute samples	0.06	0.06
Special and rush sets efforts	0.12	0.12
Respond to inquiries and problems	0.25	0.25
Total effort	2.00	1.62
Effort available for additional activities	—	0.38 ←

Table D1. (Continued)

Tasks	Effort expended (employee-years per year) At present	With automation
Alkalinity and conductivity (Section 1)		
Set up instrumentation	0.05	0.05
Prepare samples and standards	0.25	0.25
Perform clerical operations	0.19	0.02
Operate instrumentation	0.29	0.29
Perform calculations; transcribe data	0.19	0.02
Shut down instrumentation	0.03	0.03
Total effort	1.00	0.66
Effort available for additional activities	—	0.34 ←
Technicon AutoAnalyzers (Section 2)		
Set up instrumentation	0.59	0.59
Prepare samples and standards; make dilutions	1.19	1.19
Perform clerical operations	0.60	0.10
Operate instrumentation	2.34	2.34
Perform calculations; transcribe data	0.43	0.10
Shut down instrumentation	0.25	0.25
Total effort	5.40	4.57
Effort available for additional activities	—	0.83 ←

Table D1. (Continued)

Tasks	Effort expended (employee-years per year) At present	With automation
Atomic absorption (Section 3)		
Set up instrumentation	0.29	0.29
Prepare samples and standards; make dilutions	1.34	1.34
Perform clerical operations	0.43	0.08
Operate instrumentation	1.34	1.34
Perform calculations, transcribe data	0.50	0.08
Shut down instrumentation	0.10	0.10
Total effort	4.00	3.23
Effort available for additional activities	—	0.77 ←
Carbon determinations (Section 4)		
Set up instrumentation	0.20	0.20
Prepare samples and standards	1.30	1.30
Perform clerical operations	0.40	0.06
Operate instrumentation	0.75	0.75
Perform calculations, transcribe data	0.25	0.06
Shut down instrumentation	0.10	0.10
Total effort	3.00	2.47
Effort available for additional activities	—	0.53 ←

Table D1. (Continued)

Tasks	Effort expended (employee-years per year) At present	With automation
Spectrophotometer and electronic balance (Section 4)		
Set up instrumentation	0.05	0.05
Prepare samples and standards	0.33	0.33
Perform clerical operations	0.05	0.02
Operate instrumentation	0.16	0.16
Perform calculations, transcribe data	0.07	0.02
Shut down instrumentation	0.05	0.05
Total effort	0.71	0.63
Effort available for additional activities	—	0.08 ←
ADP section		
Transcribe sample identification and analytical data to cards	2.06	0.00
Maintain card files	0.88	0.00
Computer programming	0.06	1.00
Total effort	3.00	1.00
Effort available for additional activities	—	2.00 ←

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