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# A FEASIBILITY STUDY FOR THE COMPUTERIZED AUTOMATION OF THE LABORATORY SERVICES BRANCH OF EPA REGION IV

W.G. Boyle, Jr.
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LAWRENCE
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*University of California/Livermore*

LAWRENCE LIVERMORE LABORATORY
*University of California/Livermore, California/94550*

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# Contents

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## ABSTRACT

This report is a study of the feasibility of computerized automation of the Laboratory Services Branch of the Environmental Protection Agency's Region IV. The LSB provides analytical support for a number of EPA divisions; its primary function at present is compliance monitoring, field surveys, and oil identification. Automation of the LSB is not only feasible but also highly desirable. Automation systems are proposed that will make major improvements in analytical capacity, quality control, sample management, and reporting capabilities. Most of these automation systems are similar to those already developed and installed at other EPA laboratories. These systems have options that include limited modifications suggested as a result of the study of the LSB Laboratory, and also include communications hardware and software for a Sample File Control host computer. It is estimated that the initial cost of three of the four options considered would be recouped in approximately three years through increased capacity and efficiency of operation.


## 1. INTRODUCTION

The EPA has recognized for some time that its laboratories would benefit from computerized automation, and since 1973 the EPA's Environmental Monitoring and Support Laboratory (EMSL) and Lawrence Livermore Laboratory have been working together on automation plans. The approach has been to make individual studies of a few typical laboratories and develop automation systems that could be used with only minor modifications — in other similar laboratories. This effort, conducted under Interagency Agreement No. EPA-IAG-D6-0321, has become known as the Pilot Laboratory Automation Project. Members of the LLL Chemistry and Materials Science Department with broad experience in computer automation of laboratory operations have been assigned to the project. Automation systems have already been designed and put into operation at three EPA laboratories: two operated by the Environmental Research Center at Cincinnati, and the Central Regional Laboratory, Region V, at Chicago.

Five laboratories are being studied for automation: Region III Annapolis Field Office; Kansas City Region VII Surveillance and Analysis Division; Edison, New Jersey, Region II Surveillance and Analysis Division; NEIC, Denver; and the Laboratory Services Branch of Region IV, Athens, Georgia. This report concerns the proposed automation of the Analytical Services Section of the Laboratory Services Branch at Athens, hereafter referred to as the LSB.

Five major objectives will be accomplished by automating the EPA's sample analysis laboratories:

- Increased instrument capacity.
- Improved accuracy and precision of analytical results.
- Reduced time and tedium for the analyst.
- Reduced clerical time and errors.
- Improved access to the analytical data.

Section 2 of this report presents the features we consider important in meeting the objectives of a laboratory automation system. Section 3 describes Region IV's LSB. Section 4 describes the four alternative systems considered for automation of the LSB, with a summary of advantages and disadvantages. Section 5 describes system components and summarizes costs. Section 6 summarizes operating benefits and calculates the years required to recover expenses, and the balance after five years. Details of the cost-benefit analysis and other supplementary information are given in the appendixes.

# 2. FEATURES REQUIRED TO MEET THE AUTOMATION OBJECTIVES

This section describes the features required to achieve the automation objectives listed in Sec. 1. Related material is in Appendix E in the form of guidelines followed in evaluating various proposed automation systems for the LSB. Some of these features require or are enhanced by Sample File Control (SFC), which will be designed and implemented on existing PDP 11/70 computers by the EPA; SFC will require a data link from the proposed automation system.

A. To maximize instrument capacity, the computer must be able to take readings from the instrument output at the time a sample signal is present, and to sense and control the introduction of new samples. Concentrations are calculated immediately and quality control checks are made on stream. On fully automatic instruments, the operator is notified immediately if something goes wrong with a run so that it can be corrected. On semimanual operations, the computer saves time between samples by relieving the operator of the need to read and calculate concentrations.

B. Digital reading of the instruments by a computer is inherently more precise than visual reading, and covers a broader dynamic range. In addition, accuracy is improved by using some of the increased sample capacity that the computer provides to run more standards, spikes, and duplicates.

Computer automation provides two important kinds of quality control (QC). The first kind of QC is passive; it results from the fact that the flow of information is always under computer supervision, with no hand transcription of data once it is entered into the system. If the system makes a mistake, it is almost invariably the kind of mistake that humans find preposterous. Such errors are easy to spot.

The second kind of QC provided by computer automation is active. The arithmetic power of the computer permits easy implementation of analysis algorithms and statistical tests which are very laborious to do by hand or even with a modern calculator. Additional operator effort is required, but minimal. The analyst must pipet additional duplicate samples and standards, and spike a certain fraction of samples.

Passive and active QC alert the operator to trends in system behavior and permit corrective action before, or as soon as, obvious false results are produced.

C. The computer easily handles the tedious, repetitive work that operators have done in the past, and frees them for tasks that better utilize their talents. There are several major ways the computer helps the analyst. It reads all the data and calculates the concentration of samples and the curves for standards, displaying this information immediately so that the analyst can plan his work more effectively. With more extensive data storage, such as SFC, the analyst will be able to select a set of samples for a particular test from the system storage, and to arrange the samples in a pattern including check standards and rerun samples in an order that minimizes interference. The analyst will be able to obtain a summary of work that needs to be done and work that has been done, and to create tables of output data. It will also be possible to retrieve stored data, interparameter quality control values, and compliance limits to help with dilutions and alert users to samples that need special attention.

D. The computer saves clerical time and reduces clerical errors because it eliminates all hand transcription of information and data after the initial sample-identifying information has been entered. It will print reports suitable for filing or distribution and will maintain an inventory logbook.

E. At least one month's accumulation of analysis data can be stored in computer system files. These data can be associated with everything that is known about the sample. With the proper software, information can be made available in a variety of formats for report preparation. It can also be used to look at trends of instrumental behavior (for example, calibration drift), check quality control parameters, and prepare work accountability reports. Records of custody and records of assurance that proper procedures were followed are of use in some legal proceedings.

F. An automation system should have certain other features to be effective. The computer system should easily be able to accommodate additional instruments and perform additional automatic functions. Help from personnel outside the automated laboratory should be minimized. The operator should be able to use the computer as an extremely powerful calculator off-line. The laboratory scientist must be able to make necessary changes when new information, procedures, and operations are instituted.

Some of these features are discussed in more detail in Appendix E.

# 3. DESCRIPTION OF THE LSB

## Laboratory Operations

The Analytical Services Section of the LSB provides analytical support for a number of the Region IV Surveillance and Analysis Division's functions, including compliance monitoring, enforcement, air and water quality, and hazardous material control. Currently, the LSB's primary function is in water quality chemistry, with heavy emphasis on trace organic identification and identification of oils in oil spills.

The automation systems proposed for other EPA installations have been concerned mostly with inorganic measurements. Although the Analytical Services Section is heavily involved in organic work, this study will be primarily concerned with inorganic analysis. We hope that a system similar in concept to previous systems can be provided, and that it will use much of the hardware and software developed for them. The system will be flexible enough, however, to allow some changes. For instance, the Hewlett-Packard integration system is included in the study. Before the current heavy emphasis on organic analyses, a considerable number of inorganic measurements have been made by Region IV. This information is used in this study. It is possible that the emphasis will again swing toward inorganic measurements. In the meantime, it is conceivable that the system can be used for some organic data processing while still handling most of the inorganic work.

### Sample Handling

Samples received at the field laboratory with accompanying identification are logged into a Field Sample Log Book. Information recorded in the field log includes: sample log number, station identification , date and time collected, date and time received, who delivered the sample, and who received the sample in the laboratory. Sample log numbers are coded to identify the year the samples were collected, the laboratory receiving the sample, and also include a specific serial sample number.

Samples received at the central laboratory with accompanying identification are assigned consecutive numbers and are logged into the Master Sample Log Book as with the field log. The Master Sample Log Book also contains a description of the disposition of every log number used, and whether obtained from the field operations or the central laboratory.

Most data now generated in the field and central laboratory are entered into bound data books. Final results of all analyses are transferred to a report form and forwarded either to the requestor or to the data processing unit for key punching. A copy of the final data report form is filed in a chronological file maintained by the sample custodian. A project file is also prepared.

There are variations on the details of these procedures for some samples (for example, air surveillance filters or samples for organic analysis by gas chromatography and/or mass spectroscopy), but in general it is necessary to keep detailed records of both sample locations and data which are generated by and related to the samples.

### *Quality Control*

The following quality control checks on inorganic analyses are performed and the data is recorded in the analyst's notebook:

- Calibration standards are read at the beginning of a run and again at the end, if required. Usually 6 to 8 standards are used for preparation of a calibration curve.
- A check standard in the concentration range of the sample is run approximately every tenth sample.
- A reference sample, when available, is analyzed with each run.
- About 10% of the samples are run as duplicates.
- From 2 to 5% of the samples analyzed are spiked with an amount of the constituent approximately equal to the original amount in the sample.

## Analytical Systems to be Automated

Up to 40 different parameters are often measured from a sample. These parameters include about 20 trace metals; several nutrients, such as various forms of nitrogen and phosphorus; anions such as chloride, sulfate, cyanide, and fluoride; and tests for such characteristics as total organic carbon and chemical oxygen demand.

### Atomic Absorption Spectrophotometry

Trace metals are determined by measuring the amount of light absorbed by atoms at a discrete wavelength. A hollow-cathode lamp is used to generate the discrete wavelength of light characteristic of the metal of interest. Part of the sample is transferred to a flame or furnace in a reproducible manner. The flame converts part of the sample to atoms in the unexcited state, which can absorb the light from the hollow cathode and change the amount of light striking a detector. The detector generates an electrical signal which is converted to a voltage proportional to the amount of light absorbed by the metal atoms in the flame. The voltage is recorded and the amount of that particular metal in the test solution is calculated by comparison with a standard solution containing a known amount of the metal.

Two atomic absorption instruments, a PE 460 and a PE 403, together with one automatic sampler would be automated. The detector output signal would be conditioned and interfaced for computer reading. The sampler would be interfaced so that the computer would control the rotation of the turntable, and the raising and lowering of the aspirator used in flame analysis. A computer analysis algorithm would automatically time sampler positioning, reading of the signal, and correlation of the signal with the sample identification number. The PE 460 is also used in the graphite furnace mode. One modification of the standard system would allow automation of the PE 403 when it is used to analyze for mercury vapor separated from samples.

### Technicon AutoAnalyzers (TAA)

Many chemical species are measured by Technicon AutoAnalyzers. In this instrument the species of interest is converted to a colored solution by a series of precisely controlled chemical reactions that take place in a continuously flowing stream in which a known proportion of sample and reagent solutions are drawn into the system and moved through it by a peristaltic pump. Processes for different constituents require different steps in the chemical procedure, such as filtration, digestion in hot concentrated acids, reduction, and time delays to allow each step to reach equilibrium. Finally, the colored solution flows through a colorimeter cell and absorbs light in the wavelength band of the colorimeter. The amount of light absorbed is detected by a photodetector and recorded as an output voltage on a strip-chart recorder; the amount of the chemical species of interest is calculated by comparing the recorded voltage with that for a standard solution containing a known amount of the determined species.

A maximum of eight channels of Technicon AutoAnalyzers with their automatic samplers would be automated. These would consist of six channels of the Technicon AutoAnalyzer I and two channels of AutoAnalyzer II. The detector output signal of each colorimeter would be conditioned and interfaced for computer reading. Separate computer-analysis algorithms would be provided for each colorimeter, and they would automatically time the signal reading and correlate signals with sample identification numbers.

One of the present type I instruments being used in a sampling mode with a PE 403 atomic absorption unit as the detection unit for mercury determinations so that the data should really be considered AA data. The extra TAA channel is added for possible future use.

### Total Organic Carbon Analyzers

Total organic carbon is determined by combustion of organic matter to convert the carbon to carbon dioxide, which is detected as it passes through an infrared analyzer. A measured volume of the test solution is injected into a combustion furnace and swept through by a continuously flowing stream of oxygen, converting the sample liquid to water vapor and carbon dioxide. The water vapor is condensed and trapped out as the gases are carried out of the furnace, and the carbon dioxide is carried through the infrared detector and released to the exhaust. The infrared detector generates an electrical signal which is converted to a voltage proportional to the amount of carbon dioxide passing through the detector. The voltage is recorded on a strip-chart recorder, and the amount of organic carbon present in the injected solution is calculated by comparing the recorded voltage with that for a standard solution containing a known amount of organic carbon.

A Beckman 915 Total Organic Carbon Analyzer would be automated. The detector output signal would be conditioned and interfaced for computer reading. A computer-analysis algorithm would automatically time the signal reading and correlate the signal with the sample identification numbers.

### HP-3385A Integrator

A modification of the standard system would allow data to be transmitted to the computer system from an HP-3385A integrator used in conjunction with a gas chromatograph. These data could then be used for further calculations and report writing.

### Data Processing Automation

A major portion of the analyst's time is required to correlate strip-chart recordings with sample identification numbers, to calculate values for each constituent determined, and to prepare quality control reports. In addition, the analyst must usually fill out reports for the various offices involved and for his own files. The calculations will be done by the proposed system at frequent intervals during the course of the analysis. Warning signals and messages can be generated on the basis of QC sample values. Many of the final reports will be generated by the system.

Finally, a data link to a Sample File Control program may be part of the automation system. This would enable the SFC running on another computer (a PDP 11/70 used for other data processing also), to log samples, and control and document the progress of each from the time it reaches the sample acceptance station until the final report is written.

# 4. ALTERNATIVE SYSTEMS FOR AUTOMATION OF THE LSB

The intention of the LSB project is to make software and hardware development for any particular EPA laboratory transferable to others in the Agency. Many operations are similar, thus automated procedures developed for one laboratory can often be used in another with little or no change. The benefits of automation will differ from one laboratory to another, depending upon the emphasis given to a particular operation. In this section we compare four different approaches to automating the LSB to the alternative of leaving the laboratory as it is. The approaches are as follows:

A. Install a Data General-based automation system with hardware and software selected from the system package developed for the EPA laboratories.

B. Install the selected system with modified software for new instruments not previously automated.

C. Install the selected system with a communications package to transfer data to a PDP-11/70 computer.

D. Conduct all operations on a PDP-11/70 to be procured for the Region IV Surveillance and Analysis Laboratory with a data link to a Region IV PDP-11/70 in Atlanta to be used as a back-up.

Option B adds an HP-3385A integrator and the PE 403 in the mercury analysis mode to the standard system.

Options C and D include SFC functions to be performed on a PDP-11/70 according to specifications being developed under another contract. These specifications are being circulated for approval throughout the Agency's laboratories.

The consideration of systems from other suppliers presents formidable obstacles because of the existing investment in engineering and software design applicable to Data General systems and EPA's commitment to the DEC PDP-11/70.

A summary of advantages and disadvantages for the four just discussed alternative systems follows the basis for comparison.

## No Further Automation—Basis for Comparison

This means leaving the LSB as it stands and including any existing automation that may have been applied previously.

Advantages

- The large amount of capital funds that would have been spent for computer hardware with automation could instead be used for other purposes such as additional laboratory equipment.
- No time would need to be spent to train personnel in automation procedures.

Disadvantages

- Continued man-hours spent in routine, uninteresting tasks.
- Continued calculational, transfer, and typographical errors.
- No immediate indication of faulty conditions.
- No easy way to produce consolidated reports, workload listings, and status reports.

## Existing Automation System—Alternative 1

This is the system presently operating in two laboratories at the Environmental Research Center, Cincinnati, and in the Region V Central Regional Laboratory, Chicago. There may be some differences in hardware to take advantage of the latest models, but most of the software would be the same as that presently running.

Advantages

- Reduction in man-hours spent in routine, uninteresting tasks.
- Reduction in calculational, transfer, and typographical errors.
- Immediate indication of faulty conditions.
- Software debugged and tested by others.

Disadvantages

- Cost of the computer system and extra hardware.
- Time required to train personnel.
- Space required by computer system.
- Software not idealized for all functions of the LSB.

### Modified Automation System—Alternative 2

This system uses most of the hardware and software of Alternative 1. However, some changes would be made to fit the operation of the LSB such as addition of the HP-3385A integrator and the AA mercury analyzer.

Advantages

- All advantages of the first alternative except that some software would not be debugged and tested by other laboratories.
- Programs would be adapted to the particular needs of the LSB.

Disadvantages

- All disadvantages of the first alternative except that the software would be optimized to the LSB's needs.
- Additional software cost.
- Debugging would be slower because others would not be using the identical software.

### Modified Automation System with SFC Handled by Another Computer (PDP-11/70)—Alternative 3

This is the same system as described for Alternative 2 except that the SFC is handled by a separate PDP-11/70 computer.

Advantages

- All the advantages of the first and second alternatives except for debugged software.
- Programs would still be adapted to the particular needs of the LSB.
- SFC software support from the Regional/ADP Branch.
- Easy creation of consolidated reports, status reports, and workload listing.
- Simplified operation of the instruments because of automated work plans produced by the SFC.
- Automated updating of statistical quality control criteria.

Disadvantages

- All the disadvantages of the first alternative except that the software is tailored to Region IV's needs.
- Considerable extra software cost.
- Extra hardware costs for the data link between computers.

### Using Another Computer for the Entire Automation System—Alternative 4

This is the same as the preceding system except that the automation and SFC are handled by a PDP-11/70 computer.

Advantages

- All the advantages of the third alternative.

Disadvantages

- Much greater software costs.
- Extra peripheral hardware costs to redesign system interfaces.

## 5. SYSTEM COMPONENTS AND COSTS

This section describes system components, including cost estimates when applicable.

Table 1 compares the costs of four alternative systems for the LSB. The alternative of leaving the LSB without further automation is not shown in Table 1 because it represents no cost change. Figure 1 is a schematic of the hardware system required for the four alternatives.

### Hardware

The system hardware is listed here. The specific costs can be found in Appendix A, Tables A-1 and A-2.

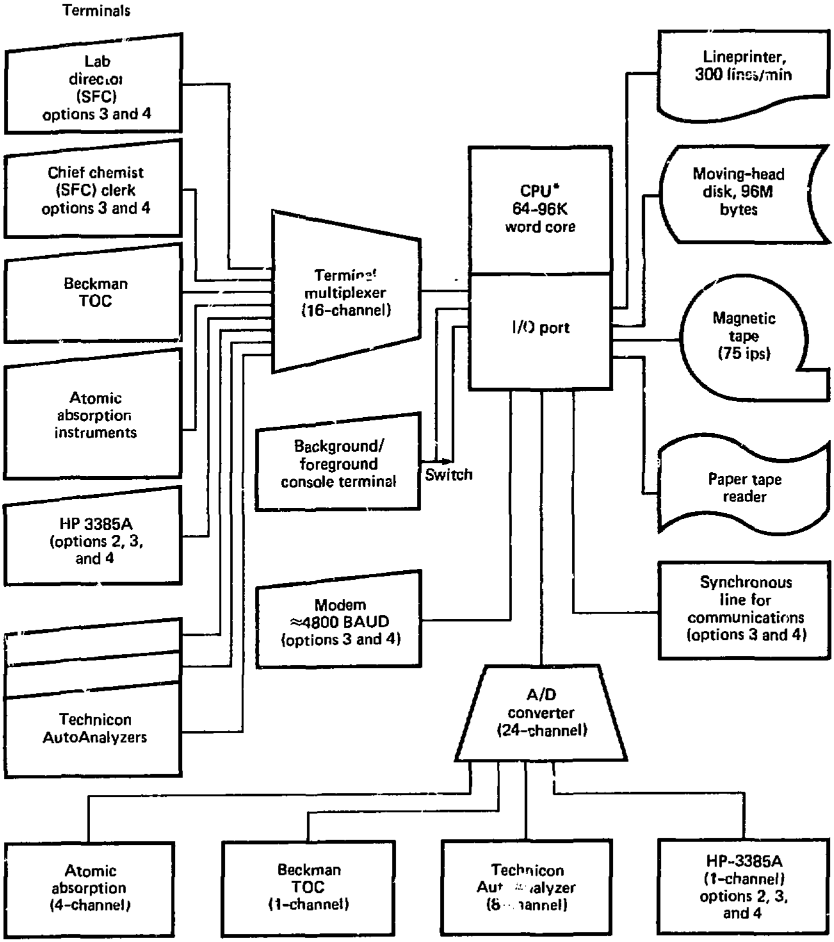


Fig. 1. Schematic of proposed hardware system for Region IV LSB.

**Table 1. Comparative costs for the four alternatives proposed for the LSB.**

| One-time costs | Alternatives 1 | 2 | 3 | 4 |
|---|---|---|---|---|
| Computer and peripherals | $ 77,962 | $ 77,962 | $121,062 | $195,610 |
| Terminals | 12,000 | 14,000 | 23,800 | 23,800 |
| Site preparation | 20,000 | 20,000 | 20,000 | 20,000 |
| Installation | 33,500 | 33,500 | 33,500 | 33,500 |
| Instrument interface | 32,200 | 38,825 | 38,825 | 43,325 |
| Spare parts and test equipment | 10,000 | 10,000 | 10,000 | 10,000 |
| Software | -- | 23,500 | 43,500 | 173,000 |
| Total one-time costs | $185,662 | $217,787 | $290,687 | $499,235 |
| **Operating expense (annual)** | | | | |
| Vendor's hardware maintenance | $10,200 | $10,200 | $15,400 | $24,400 |
| In-house hardware and software maintenance | 17,500 | 17,500 | 52,500 | 52,500 |
| Telephone communications Modem Bell Series (4800 baud) | -- | -- | 5,000 | 5,000 |
| Total annual costs | $27,700 | $27,700 | $72,900 | $81,900 |

## Computer

The computer for the first three alternatives is an ECLIPSE S/230. It is similar to the NOVA 840 computers used in the other EPA facilities, but it is almost twice as fast. It uses the same operating system as the NOVA, MRDOS, so that most software is transportable. Alternatives 1 and 2 will require 64K words of core. Alternative 3 will require 96K words. Alternative 4 would also require 96K words of core, but the PDP-11/70 core — an EPA standard system — is added in 64K words.

Costs are those of May 1977. Costs for most of the Data General components can be found in the GSA Authorized ADP Scheduled Price List. [1] Costs for most of the Digital Equipment Corporation components can be found in the PDP-11 end-user product summary and the price list supplement.[2]

## Disk Storage

A rapid-access storage of programs and data is provided by the disk system. A moving-head disk is recommended because of its fast data transfer properties. The proposed version of the standard EPA system incorporates the Data General model 6060 moving-head disk with a storage capacity of 96 megabytes.

## Magnetic Tape

Magnetic tape is used as the primary backup medium for the system. It is also important for long-term bulk storage and for the transfer of data from one location to another. The proposed system includes a magnetic tape drive running at 75 inches per second (ips).

## *Line Printer*

The line printer is needed to produce workload listings, sample wheel patterns, notebook results, final results and progress reports, as well as listing of programs. The recommended line printer prints 300 lines per minute.

## Paper Tape Reader

The paper tape reader is used for system start-up and to load diagnostic programs when the disk or tape is not available. As an interim measure, it has been used to transfer data from instruments with their own computer into the Data General system.

## Analog-to-Digital Converter System

The analog-to-digital converter reads signals coming from all the different automated instruments. The proposed converter is the same as in the present systems, and has a resolution of one part in 16,384 ($2^{14}$) of a full-scale signal. Although 16 channels would be sufficient for the currently defined automation systems, we feel another 8 channels should be present for system expansion and alternate use in case of malfunction. (The extra channels are added in eight channel sections.)

### Terminals

The terminals are the major means of entering information into the computer system other than the analog-to-digital converter. They are also used to report interim data and issue warnings during automated runs.

Two different terminal types are proposed. One is a quiet hard-copy device. This is used with the computer console to control system operation. A switch is provided for background/foreground operation. At least one other would be available for use wherever hard copy is needed.

The terminal used with most instruments is a cathode ray tube (CRT) type. This type has the advantage of more rapid display and not creating large amounts of unneeded paper. Some have the ability to roll back, that is, redisplay information already scrolled off the screen. The estimated cost of either terminal is $2000. Six terminals are proposed for Option 1, and seven terminals for Option 2. For Options 3 and 4 with SFC, two more special terminals are recommended. They have CRT display, hardcopy unit, and telecommunication accessories. Each terminal costs $4900.

### Instrument Interfaces

These units convert the output of each instrument to a signal usable by the computer. Also, a digital interface drives the computer-controlled sample wheel. Where possible, units designed for previous systems will be used. The interfaces for the Perkin-Elmer 460 atomic absorption instrument and the HP-3385A integrator will have to be designed, since these instruments have not been interfaced previously. Purchase of a newer model HP-3385A will be much more economical than designing an interface for the present one. This newer instrument has a virtual built-in interface.

### Sample Wheel

A sample wheel fully controlled by the computer is proposed for use with an atomic absorption instrument. Similar wheels have been delivered to the other installations. The wheel can hold up to 40 samples, and has a solenoid valve for automatic blank injection.

## Software

Software requirements are discussed below. Detailed costs can be found in Appendix A, Tables A-3 and A-4.

### Existing BASIC Language Software

The following programs are available:

- Single-channel Technicon II AutoAnalyzer.
- Up to three channels Technicon II AutoAnalyzer.
- Up to three channels Technicon I AutoAnalyzer.
- Beckman total organic carbon analyzer (inorganic carbon removed with acid).
- Flame mode, manual atomic absorption.
- Flame mode, automatic (sample wheel) atomic absorption.
- Graphite furnace mode, manual atomic absorption, single and double beam.
- Same as preceding with AS-1 autosampler program.
- Multielement emission spectrometer.
- Mettler electronic balance.
- UV/Vis spectrophotometer.

Describing each program in detail is beyond the scope of this study. Detailed specifications are available for most programs as separate documents.[3-6] These programs include the following general and similar functions:

- A method of creating standard curves using first-, second-, or third-degree polynomials.
- Calculating unknowns by interpolating between the two nearest standards.
- Immediate display of concentration as soon as unknowns are run.
- Correction for instrument and reagent blank.
- Calculation of spike recovery.
- Calculation of error in check standards.
- Calculation of difference between duplicates.
- Calculation of statistical error bands, using the Shewhart or Cusum method.
- An operator's notebook report, including all raw and final data.
- A final report for distribution.

For alternative 1 there would be minimal software development costs.

### Modified Software

Since no two laboratory's functions are exactly alike, there are bound to be differences in software needs. Unfortunately, software is the largest part of the cost of any system; the fewer changes made in it, the less costly the system. Also, it becomes impossible for the central facility at the Environmental Research Center (ERC), Cincinnati, to maintain the programs as different versions proliferate. Modifications would be limited to features that have a wide demand.

It is beyond the scope of this report to detail all modifications the LSB would like to see. These differences are spelled out in the functional descriptions. Examples of desired modifications follow.

A. A program is needed to handle the determination of mercury using a Technicon AutoAnalyzer sampler and atomic absorption detection.

B. Software is desired to handle the output from a Hewlett-Packard Integrator used with gas chromatography columns.

C. An SFC data link is essential to reduce the analyst's burden and the number of transcription errors between sample log-in and final consolidated reports.

Alternative 2 would include the costs for A and B. Alternative 3 would also include the cost for the SFC data link. Alternative 4 requires more software modification because these programs do not exist in a form compatible with the PDP-11/70.

### *Documentation*

The following is a list of documents supplied with the automation system:

- User instruction manuals.
- BASIC program descriptions including listings, flow charts and narrative description of relevant modules, files and file structure, chaining, variable lists and narrative description of assembly language calls relevant to the BASIC programs.
- Description of assembly language calls with listings.
- Prints, descriptions, and spare parts lists for custom hardware, interfaces, and samplers.

The cost of these items is included in the estimate of software and hardware costs.

### Miscellaneous Expenses

These expenses include costs for site preparation, installation, spare parts and test equipment, operating costs, and modems or communication links. The cost breakdown is as follows:

- Site preparation

  This is the cost of preparing a room of 300 to 400 $ft^2$ to house the computer, with adequate electrical service and air conditioning. It also includes pulling cables from instrument sites to the computer room. A nominal figure is $20,000.

- Installation

  This cost is estimated to be $33,500, based on previous installations. It includes shipment of the system, installation at the Athens laboratory, hardware and software check-out, operational testing, and training personnel.

- Spare parts and test equipment

  To maintain the system, a minimum complement of spare parts and test equipment must be acquired. Spare parts should include items such as control logic cards, power supplies, operational amplifiers, relays, and connectors. The cost for a recommended quantity of these items is approximately $3000. The major test equipment item, an oscilloscope, will cost approximately $7000. Thus, approximately $10,000 ahould be set aside for both spare parts and test equipment.

- Operating costs

  Hardware operating costs are estimated at 12% of the cost of the computer, plus peripherals per year. Software operating costs will depend on the options. For software maintenance of options 1 and 2, about 0.5 of a full-time employee (FTE) is needed. For options 3 and 4, another FTE is needed for SFC maintenance.

It should be made clear that new skills and capabilities will be required by Region IV LSB to implement and maintain an efficient automation system. ERC, through its experience with laboratory automation, has summarized these requirements.[7]

# 6. OPERATING BENEFITS AND PAYOUT

Table 2 shows the benefits and payout time estimated for the four alternatives. For convenience a condensed version of Table 1 (costs) is incorporated in this table.

### Instrument Time Savings

Each instrument to be automated has its own internal procedure and requirements for tending. Appendix B shows identifiable actions that occupy a chemist's time and the best estimates of how his time is distributed. The estimates are based on EPA analytical chemistry laboratory experience; we confirm that they fall within the range of reasonable times for such procedures. These are summarized in Table 3.

**Table 2. Comparative costs and benefits for the four alternatives systems proposed for the LSB.**

| | Alternatives | | | |
|---|---|---|---|---|
| Total one-time costs | 1 | 2 | 3 | 4 |
| Operating benefit (annual) | $185,662 | $217,787 | $290,687 | $499,235 |
| Savings in personnel (FTE) | 2.87 | 3.43 | 5.42 | 5.42 |
| Equivalent cost saving | 100,160 | 119,710 | 189,160 | 189,160 |
| Operating expense (annual) | 27,700 | 27,700 | 72,900 | 81,900 |
| Net annual benefit (cost saving - operating expense) | 72,460 | 92,010 | 116,260 | 107,260 |
| *Payout time for system (years)* | 3.11 | 2.83 | 3.02 | 6.57 |
| Accumulated balance at five years | $ 89,000 | $131,000 | $150,000 | -$93,600 |

**Table 3. Summary of estimated savings in *manpower* requirements at the LSB with the proposed automation system.**

| Manpower saved by replicate instrument automation | Full-time employee |
|---|---|
| Atomic absorption | 0.77 |
| AutoAnalyzers | 1.93 |
| Total organic carbon | 0.17 |
| Subtotal | 2.87 |
| For full automation add | |
| HP-3385A | 0.56 |
| Subtotal | 3.43 |
| Manpower saved by automated management functions | |
| *Managers' reports and projections* | 1.18 |
| Workload lists | 0.31 |
| Work accountability reports | 0.11 |
| *Update records* | 0.19 |
| Quality control | 0.20 |
| Subtotal | 1.99 |
| Total manpower saved by full automation | 5.42 |

## Managerial Time Savings

The savings resulting from management functions performed by the computer, as defined in the LSB *functional specifications for the SFC*, are derived from a model. This model is discussed in Appendix C; the benefits are summarized in Table 3.

Although the LSB *effort might be expected* to grow, this growth is not explicitly included in the benefit from automating the instruments. The impact of growth will be felt on both automated and nonautomated analyses. For simplicity, and to estimate conservatively, we assume the effort level of 30,000 *determinations per year represents a mean* over the five-year payoff period. This number is applied to the management model. More detailed growth estimates do not significantly change the payout period shown in Table 2.

## Comparison of Benefits

Manpower savings are shown in Table 3. They are divided into sections for the different alternatives. The proposed alternatives to the standard system owe their increased manpower savings and increased one-time costs mainly to the following factors:

### Inclusion of Sample File Control

The manpower saving of 1.99 is gained at the expense of $20,000 as part of the shared software cost.

### Automation of the HP-3385A

The manpower saving of 0.56 attributed to automating this instrument is gained at a cost of $18,500 *in* software and $6,600 in hardware.

## Estimating the Value of Benefits

While no benefit is assigned to other, less significant changes to the existing system, their importance to user acceptance should not be minimized. Most of them may also be useful to other EPA laboratories.

The annual operating benefit for the alternative systems are the 2.87, 3.43, and 5.42 FTE as shown in Table 3. These benefits are carried to Table 2.

The operating benefits are converted to a dollar value on the basis of the mean manpower costs for the payout period (Appendix D) so that a direct comparison to costs can be made. A value of $34,900 for one man-year was used. The net annual benefit is the operating benefit less the annually incurred cost.

The payout time is calculated on the basis of 10% per annum, discounting annual compounding. Given the ratio of initial cost to annual benefit, C/B, the payout time, T, is estimated as

$$T = -\log(1 - I \cdot C/B)/\log(1 + I)$$
$$= -\log(1 - 0.1C/B)/0.04139,$$

where i is the discount rate, 0.1/y.

The net benefit realized in five years is estimated as

$$B_5 = B \cdot [1 - (1 + I)^{-5}]/I - C = 3.791B - C$$

(See Ref. 8.)

System service life is defined to be five years within the EPA.

It should be noted that some benefits and advantages of computer automation do not lend themselves to a cost-factor equivalent. Such benefits include fewer transcription errors, staff access to an easily programmable, problem-solving computer, shorter turnaround time between sample in and report out, and more attention devoted to analytical methodology. The availability of EPA automatic data processing personnel will be another advantage, because these people will be able to interact effectively between the user and the operating system.

# REFERENCES


1. GSA Authorized ADP Schedule Price List for Data General Corporation, Contract Number GS-00C-0085, October 1, 1976 through September 30, 1977.
2. PDP-11 End-User Product Summary, January 1977 and Insert for Prices and Order, January 1977.
3. R. W. Crawford and L. P. Rigdon, *Total Organic Analyzer: Functional Description*, Lawrence Livermore Laboratory, Rept. UCRL-52045 (1976).
4. R. W. Crawford and G. W. Barton, Jr., *Technicon AutoAnalyzers: Functional Description*, Lawrence Livermore Laboratory, Rept. UCRL-52046 (1976).
5. R. W. Crawford and H. S. Ames, *Sample File Controller: Functional Description*, Lawrence Livermore Laboratory, Rept. UCRL-52047 (1976).
6. R. I. Bystroff, W. G. Boyle, Jr., and G. W. Barton, Jr., project leader, *Atomic Absorption Instrument Functional Description*, Lawrence Livermore Laboratory, Rept. UCRL-52065 (1976).
7. H. S. Ames, G. W. Barton, Jr., R. I. Bystroff, R. W. Crawford, A. M. Kray, M. D. Maples, *A Feasibility Study for the Computerized Automation of the Annapolis Office of EPA Region III.*, Lawrence Livermore Laboratory, Rept. UCRL-52052 (1976), Appendix 6 (prepared by B. P. Almich, ERC, Cincinnati (1976)).
8. F. J. Stermole, *Economic Evaluation and Investment Decision Methods*, Investment Evaluation Corporation, Golden, Colorado (1974).


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# APPENDIX A

# COSTS OF HARDWARE AND SOFTWARE

In this appendix we give a detailed breakdown of the costs of hardware and software for the LSB system. Table A-1 compares the costs of the central computer and peripherals for the four proposed alternative systems. Table A-2 estimates the cost for interfaces for the four alternatives. Table A-3 estimates the cost of rewriting software to operate on a PDP-11/70 system, and Table A-4 uses this estimate in arriving at the software costs for the last three alternatives. Alternative 1 would not require software expense. Table A-5 summarizes the annual operating costs and the basis used for the figures. Finally, Table A-6 is a rough estimate of the minimum data storage requirement for a representative system.

**Table A-1. One-time costs for the central computer and peripherals for the four alternative systems.**

| Item[a] | Alternatives 1 and 2 | Alternative 3 | Alternative 4 |
|---|---|---|---|
| Computer with 64 to 96K words core memory, floating point processor, memory map, and real-time clock | $29,520 (64K) | $36,080 (96K) | $71,500 (128K)[b] |
| Moving-head disk, 96MB | 22,542 | 22,542 | 36,750 (88MB) |
| *Magnetic tape* | 8,118 | 8,118 | 26,500 |
| Line printer | 8,528 | 8,528 | 11,800 |
| Paper tape reader | 1,804 | 1,804 | 5,060 |
| Analog/digital converter, 24-channel | 7,350 | 7,350 | 7,350 |
| System cabinet | 2,850 | 2,850 | -- |
| Multiplexer asychronous line | 3,600 | 3,600 | 3,600 |
| Computer system software | 1,000 | 1,000 | 3,660 |
| Communications hardware synchronous line adaptor (laboratory end) | -- | 1,100 | 1,300 |
| Communications hardware full/half duplex synchronous interface at PDP-11 | -- | 3,100 | 3,100 |
| Additional disk, 88 MB at PDP-11 | -- | 32,340 | 32,340 |
| Totals | $85,312 | $128,412 | $202,960 |

[a]Most items are discounted 18%.
[b]Only sold in 64K-word increments.

Table A-2. Estimated interface costs for the four alternative systems.

| Type of interface | Alternatives | | |
|---|---|---|---|
| | 1 | 2 and 3 | 4 |
| General interface | | | |
| Design | $ 0 | $ 0 | $ 4,500 |
| Fabricate | 7,300 | 7,300 | 7,300 |
| AutoAnalyzers I, II (8) | | | |
| Fabricate | 18,000 | 18,000 | 18,000 |
| AA PE 403 | | | |
| Fabricate | 1,300 | 1,300 | 1,300 |
| AA PE 460 | | | |
| Design | 3,000 | 3,000 | 3,000 |
| Fabricate | 1,300 | 1,300 | 1,300 |
| TOC | | | |
| Fabricate | 1,300 | 1,300 | 1,300 |
| HP Integrator | | | |
| Design | N.A. | 600 | 600 |
| Fabricate | N.A. | 6,025[a] | 6,025 |
| Totals | $32,400 | $38,825 | $43,325 |

[a]This fabrication cost is the cost of a new instrument, the HP-3385A, with an ASCII output service plug.

Table A-3. Cost of rewriting EPA software to operate on a digital equipment PDP-11 system.

| Programs to be rewritten | Assembly language code | Basic language code |
|---|---|---|
| Computer system | $41,000 | – |
| Technicon AutoAnalyzer | 12,000 | $30,000 |
| Atomic absorption | 7,000 | 21,000 |
| TOC | 3,500 | 15,000 |
| Subtotals | $63,500 | $66,000 |
| Total | $129,500 | |

Table A-4. Summary of new software costs.

| Software | Alternatives 2 | 3 | 4 |
|---|---|---|---|
| Instrument applications | N.A. | N.A. | $129,500 (rewrite cost) |
| HP integrator | $18,500 | $18,500 | $ 18,500 |
| PE 403 Hg analyzer | 5,000 | 5,000 | 5,000 |
| Communication with SFC | N.A. | 20,000 | 20,000 |
| Total | $23,500 | $43,500 | $173,000 |

Table A-5. Annual operating costs for the four alternative systems.

| Operating cost category | Alternatives 1 and 2 | 3 | 4 |
|---|---|---|---|
| Maintenance of the computer hardware and peripherals (vendor supplied) | $10,200[a] | $15,400[a] | $24,400[a] |
| In-house maintenance of interface hardware and software | $17,500[b] | $52,500[c] | $52,500 |
| Estimated annual costs for telephone communications | -- | $ 5,000[d] | $ 5,000 |

[a]Estimated to be equivalent to 12% of the cost of the computer and peripherals.

[b]Approximately one-half of the time of a full time employee (FTE) is needed for options 1 and 2.

[c]Approximately one FTE is needed for SFC, plus the additional 0.5 FTE is still estimated at $35,000 (see Appendix 4).

[d]Annual telephone communication costs include the following: Modem, Bell series (4800 baud), $2,400/y; telephone line, $300/y; FTS charge, $2,300/y.

**Table A-6. Estimated minimum data-storage requirements (in 8-bit bytes) for the proposed LSB system, based on 100 samples and standards.**

| Instrument | BASIC program | Data files | Number of files | Total | Assembly language patch |
|---|---|---|---|---|---|
| Atomic Absorption | 70,000[a] | 25,000 | 6 | 220,000 | 6,000 |
| Technicon AutoAnalyzer I | 40,000 | 115,000 | 4 | 500,000 | 5,000 |
| Technicon AutoAnalyzer II | 40,000 | 115,000 | 5 | 615,000 | 5,000 |
| HP 3385A | 30,000 | 30,000 | 3 | 120,000 | 5,000 |
| Beckman TOC | 25,000 | 25,000 | 2 | 75,000 | 3,000 |
| Sample File Control | 200,000 | 100,000[b] | 1 | 2,400,000[c] | 5,000 |
| Total | | | | 3,930,000 | 29,000 |

If software for two AA's and five TAA's is stored we need: 6,150,000 bytes.

[a]Several Programs.

[b]One day's worth of data. Provisions will be made to store at least one month's worth of data.

[c]One month's data plus application programs.

# APPENDIX B

## MANPOWER SAVINGS AS A RESULT OF INSTRUMENT AUTOMATION

We have adopted a model in which the total time needed for any one instrumental sample analysis, t, is broken into a number of increments which are then summed and modified by the following equations:

$$t = p + (1. + f)(w + i + c) + fd,$$

where

- t = total chemist time needed for each sample,
- p = time for preparation of sample and log book,
- w = time needed to write introduction in the logbook and introduce sample into the instrument,
- i = chemist time needed tending instrument,
- c = time needed to calculate and transcribe results,
- d = time taken for dilution,
- f = fraction of samples diluted;

and

$$e = tqr \frac{H}{H-S},$$

where

- e = the effective chemist time taken per sample,
- t = total time calculated by the previous formula,
- q = quality control factor (total determinations/unknown),
- r = fraction of samples retested,
- H = time of a work session,
- S = time to set up instrument at the beginning of each work session, shut it down at the end, and run standards.

Table B-1 summarizes the savings (man-years per year), and Tables B-2 through B-8 give the results for the instruments to be automated. In Tables B-2 through B-8, times given in the columns headed "present techniques" are consistent with values received from LSB. Times given in the columns headed "automated techniques" are our estimates of the times needed after automation.

**Table B-1. Summary of savings (man-years per year).**

| Instrument | Present | Automated | Savings |
|---|---|---|---|
| AutoAnalyzer I | 1.85 | 0.57 | 1.28 |
| AutoAnalyzer II | 0.94 | 0.29 | 0.65 |
| Atomic absorption spectrophotometers | 1.65 | 0.88 | 0.77 |
| Total organic carbon analyzer | 1.21 | 1.04 | 0.17 |
| HP-3385A integrator | 1.33 | 0.77 | 0.56 |

Table B-2. Estimated savings with automation for Technicon AutoAnalyzer I (total Kjeldahl nitrogen).

| Item | Symbol[a] | Present techniques | Automated techniques | Difference |
|---|---|---|---|---|
| Preparation of sample, min | p | 3.33 | 3.33 | 0.0 |
| Write log, introduce sample, min | w | 0.89 | 0.24 | 0.65 |
| Instrument time for chemist, min | i | 8.89 | 0.89 | 8.0 |
| Calculate and transcribe results, min | c | 3.33 | 0.0 | 3.33 |
| Dilution of off-scale samples, min | d | 5 | 5 | 0.0 |
| Fraction of samples diluted | f | 0.1 | 0.1 | 0.0 |
| Total chemist time per determination, min | t | 18.25 | 5.07 | 13.18 |
| Retest factor | r | 1.01 | 1.01 | 0.0 |
| Quality control factor | q | 1.27 | 1.27 | 0.0 |
| Setup and shutdown time per session, min | S | 96 | 96 | 0.0 |
| Hours per work session, h | H | 6 | 6 | 0.0 |
| Effective chemist time per determination, min | e | 31.93 | 8.87 | 23.06 |
| No. of determinations per chemist-day | | 15.04 | 54.1 | 39.06 |
| No. of determinations assumed/y | | 2430 | 2430 | 0 |
| Chemist-days needed/y | | 162 | 45 | 117 |
| Chemist-years needed/y | | 0.72 | 0.20 | 0.52 |

$$t = p + (1. + f)(w + i + c) + fd,$$

$$e = trq\frac{H}{H - S}$$

[a]Symbols apply to equations at bottom of table.

*Table B-3.* **Estimated savings for Technicon AutoAnalyzer I ($SO_2$ and $NO_2$ air filters run singly).**

| Item | Symbol[a] | Present techniques | Automated techniques | Difference |
|---|---|---|---|---|
| Preparation of sample, min | p | 1.5 | 1.5 | 0.0 |
| Write log, introduce sample, min | w | 0.90 | 0.24 | 0.66 |
| Instrument time for chemist, min | i | 2 | 0.5 | 1.5 |
| Calculate and transcribe results, min | c | 1.5 | 0.0 | 1.5 |
| Dilution of off-scale samples, min | d | 5 | 5 | 0 |
| Fraction of samples diluted | f | 0.1 | 0.1 | 0 |
| Total chemist time per determination, min | t | 6.84 | 2.82 | 4.02 |
| Retest factor | r | 1.01 | 1.01 | 0 |
| Quality control factor | q | 1.27 | 1.27 | 0 |
| Setup and shutdown time per session, min | S | 60 | 60 | 0 |
| Hours per work session, h | H | 8 | 8 | 0 |
| Effective chemist time per determination, min | e | 10.03 | 4.13 | 5.90 |
| *No. of determinations* per chemist-day | | 47.87 | 116.22 | 68.35 |
| No. of determinations assumed/y | | 2000 | 2000 | 0 |
| Chemist-days needed/y | | 41.78 | 17.21 | 24.57 |
| Chemist-years needed/y | | 0.19 | 0.08 | 0.11 |

$$t = p + (1. + f)(w + i + c) + fd,$$

$$e = trq \frac{H}{H - S}$$

[a]Symbols apply to equations at bottom of table.

Table B-4. Estimated savings for remaining methods with Technicon AutoAnalyzer I ($PO_4^{\equiv}$, $SO_4^{=}$, $F^-$, etc.).

| Item | Symbol[a] | Present techniques | Automated techniques | Difference |
|---|---|---|---|---|
| Preparation of sample, min | p | 2.93 | 2.93 | 0 |
| Write log, introduce sample, min | w | 1.76 | 0.47 | 1.29 |
| Instrument time for chemist, min | i | 5.86 | 0.59 | 5.27 |
| Calculate and transcribe results, min | c | 2.93 | 0 | 2.93 |
| Dilution of off-scale samples, min | d | 5 | 5 | 0 |
| Fraction of samples diluted | f | 0.1 | 0.1 | 0 |
| Total chemist time per determination, min | t | 15.04 | 4.60 | 10.44 |
| Retest factor | r | 1.01 | 1.01 | 0 |
| Quality control factor | q | 1.27 | 1.27 | 0 |
| Setup and shutdown time per session, min | S | 60 | 60 | 0 |
| Hours per work session, h | H | 8 | 8 | 0 |
| Effective chemist time per determination, min | e | 22.04 | 6.74 | 15.30 |
| No. of determinations per chemist-day | | 21.78 | 71.26 | 49.48 |
| No. of determinations assumed/y | | 4610 | 4610 | 0 |
| Chemist-days needed/y | | 212 | 65 | 147 |
| Chemist-years needed/y | | 0.94 | 0.29 | 0.65 |

$$t = p + (1. + f)(w + i + c) + fd,$$

$$e = trq\frac{H}{H - S}$$

[a]Symbols apply to equations at bottom of table.

Table B-5. Estimated savings with automation for Technicon AutoAnalyzer II ($NH_3$ and $NO_2^- + NO_3^-$).

| Item | Symbol[a] | Present techniques | Automated techniques | Difference |
|---|---|---|---|---|
| Preparation of sample, min | p | 3.16 | 3.16 | 0 |
| Write log, introduce sample, min | w | 1.89 | 0.51 | 1.38 |
| Instrument time for chemist, min | i | 6.31 | 0.63 | 5.68 |
| Calculate and transcribe results, min | c | 3.16 | 0 | 3.16 |
| Dilution of off-scale samples, min | d | 5 | 5 | 0 |
| Fraction of samples diluted | f | 0.1 | 0.1 | 0 |
| Total chemist time per determination, min | t | 16.15 | 4.91 | 11.24 |
| Retest factor | r | 1.01 | 1.01 | 0 |
| Quality control factor | q | 1.27 | 1.27 | 0 |
| Setup and shutdown time per session, min | S | 60 | 60 | 0 |
| Hours per work session, h | H | 8 | 8 | 0 |
| Effective chemist time per determination, min | e | 23.67 | 7.20 | 16.47 |
| No. of determinations per chemist-day | | 20.28 | 66.70 | 46.42 |
| No. of determinations assumed/y | | 4280 | 4280 | 0 |
| Chemist-days needed/y | | 211 | 64 | 147 |
| Chemist-years needed/y | | 0.94 | 0.29 | 0.65 |

$$t = p + (1. + f)(w + i + c) + fd,$$

$$e = trq\frac{H}{H - S}$$

[a]Symbols apply to equations at bottom of table.

## Table B-6. Estimated savings with automation for atomic absorption analysis.

| Item | Symbol[a] | Present techniques | Automated techniques | Difference |
|---|---|---|---|---|
| Preparation of sample, min | p | 7.82 | 7.82 | 0 |
| Write log, introduce sample, min | w | 0.98 | 0.17 | 0.81 |
| Instrument time for chemist, min | i | 2.0 | 0.42 | 1.58 |
| Calculate and transcribe results, min | c | 4.89 | 0 | 4.89 |
| Dilution of off-scale samples, min | d | 5 | 4.8 | 0.2 |
| *Fraction of samples diluted* | *f* | 0.06 | 0.06 | 0 |
| Total chemist time per determination, min | t | 16.45 | 8.73 | 7.72 |
| Retest factor | r | 1.01 | 1.01 | 0 |
| Quality control factor | q | 1.36 | 1.36 | 0 |
| Setup and shutdown time per session, min | S | 60 | 60 | 0 |
| Hours per work session, h | H | 8 | 8 | 0 |
| Effective chemist time per determination, min | e | 25.83 | 13.71 | 12.12 |
| No. of determinations per chemist-day | | 18.58 | 35.02 | 16.44 |
| No. of determinations assumed/y | | 6908 | 6908 | 0 |
| Chemist-days needed/y | | 372 | 197 | 175 |
| Chemist-years needed/y | | 1.65 | 0.88 | 0.77 |

$$t = p + (1. + f)(w + i + c) + fd,$$

$$e = trq \frac{H}{H - S}$$

[a]Symbols apply to equations at bottom of table.

**Table B-7. Estimated savings with automation for Beckm~n total organic carbon analyzer.**

| Item | Symbol[a] | Present techniques | Automated techniques | Difference |
|---|---|---|---|---|
| Preparation of sample, min | p | 10.14 | 10.14 | 0 |
| Write log, introduce sample, min | w | 3.38 | 3.38 | |
| Instrument time for chemist, min | i | 27.03 | 27.03 | [illegible] |
| Calculate and transcribe results, min | c | 6.76 | 0 | 6.76 |
| Dilution of off-scale samples, min | d | 5.0 | 4.8 | 0.2 |
| *Fraction of samples diluted* | *f* | *0.05* | *0.05* | *0* |
| Total chemist time per determination, min | t | 49.42 | 42.31 | 7.11 |
| *Retest factor* | *r* | *1.01* | *1.01* | *0* |
| Quality control factor | q | 1.15 | 1.15 | 0 |
| Setup and shutdown time per session, min | S | 60 | 60 | 0 |
| Hours per work session, h | H | 8 | 8 | 0 |
| Effective chemist time per determination, min | e | 65.59 | 56.16 | 9.43 |
| No. of determinations per chemist-day | | 7.32 | 8.55 | 1.23 |
| *No. of determinations assumed/y* | | 2000 | 2000 | 0 |
| Chemist-days needed/y | | 283 | 233 | 40 |
| Chemist-years needed/y | | 1.21 | 1.04 | 0.17 |

$$t = p + (1. + f)(w + i + c) + fd,$$

$$e = trq \frac{H}{H - S}$$

[a]Symbols apply to equations at bottom of table.

Table B-8. Estimated savings with automation of data from HP-3385A.

| Item | Symbol[a] | Present techniques | Automated techniques | Difference |
|---|---|---|---|---|
| Preparation of sample, min | p | 82 | 82 | 0 |
| Write log, introduce sample, min | w | 15.36 | 15.36 | 13.82 |
| Instrument time for chemist, min | i | 9.6 | 9.6 | 0 |
| Calculate and transcribe results, min | c | 77 | 0 | 77 |
| Dilution of off-scale samples, min | d | 5 | 5 | 0 |
| Fraction of samples diluted | f | 0 | 0 | 0 |
| Total chemist time per determination, min | t | 183.96 | 106.96 | 77 |
| Retest factor | r | 1 | 1 | 0 |
| Quality control factor | q | 1.3 | 1.3 | 0 |
| Setup and shutdown time per session, min | S | 20 | 20 | 0 |
| Hours per work session, h | H | 8 | 8 | 0 |
| Effective chemist time per determination, min | e | 249.55 | 145.09 | 104.46 |
| No. of determinations per chemist-day | | 1.92 | 3.31 | 1.39 |
| No. of determinations assumed/y | | 575 | 575 | 0 |
| Chemist-days needed/y | | 299 | 174 | 125 |
| Chemist-years needed/y | | 1.33 | 0.77 | 0.56 |

$$t = p + (1. + f)(w + i + c) + fd,$$

$$e = trq \frac{H}{H - S}$$

[a]Symbols apply to equations at bottom of table.

# APPENDIX C

# MANPOWER SAVINGS AS A RESULT OF SAMPLE MANAGEMENT AUTOMATION

We have chosen to develop a linear model for sample management operations. The results for the model are validated against the sample management estimates for the LSB.

We first identify the sample management functions as follows:

- Work plans and sample log-in.
- Sample load projections.
- Workload selection.
- Interim reports.
- Sample summary reports.
- Query reports.
- Form letters.
- Work accountability reports.
- Updating files for status and results.
- Quality control reports and updating files for quality control.

These items correspond to the functional description of the SFC system.

Each function is considered in terms of how much effort is expended with and without sample file control. Each function is modeled as some number of transcriptions, filing and retrieving of files, and data checking or tallying. Times for the various processes are estimated for example as follows:

- Transcriptions $t = 6$ s.
- File and retrieve $f = 4$ min.
- Checking $c = 3$ s.

These numbers include the time for correcting transcription errors.

In ultimately converting the time in minutes to man-years, a 7-h day is assumed to allow for human overhead (efficiency), and a 250-d work-year is used. The factor is

$$k = \frac{1}{60 \times 7 \times 250} = 9.52 \times 10^{-6} \text{ man-year/min.}$$

To count the number of transcriptions or checking, only a portion of the information in the SFC is used for a given report. The following average maximum numbers of each data type are obtained from the functional description of the sample file:

- Data that describe the study 8
- Data that describe the sample 15
- Data that describe the analysis 9

To count the number of reports per year, we obtained the following estimates from the LSB:

| Report type | Frequency | Annual frequency used in the model, N |
|---|---|---|
| Workload list | Daily | 250 |
| Interim, short | Daily | 250 |
| Interim, long | Weekly | 50 |
| Study status | Weekly | 50 |
| Query | Twice daily | 500 |
| Sample load | Tri-weekly | 15 |
| Work accountability reports | Twice monthly | 24 |

We take rounded figures for the key parameters describing the level of effort at the LSB.

| | |
|---|---|
| Number of determinations per year, D | 30,000* |
| Number of samples logged per year, S | 6,500 |
| Number of studies (projects) per year, P | 260 |
| Number of samples per study, $S_p$ | 25 |
| Number of determinations per sample, $D_s$ | 5† |
| Mean time to complete study, $T_p$ | 25 |

On the following pages the assumptions made in developing the benefit models for each managerial function are discussed. In general, the most efficient manual record-keeping and filing formats are assumed, and the analyses are assumed to be managed in such a way as to minimize paperwork, even though this is not possible if the samples have a limited life. The effort required for the automated reports is assumed negligible, although some manual effort is required to get lineprinter output. All benefits are therefore *net benefits*. Following the detail of the models, the derived benefits are summarized in Table C-1, and carried to Table 3 (in Sec. 6).

The sample effort has been estimated by B. J. Carroll of the LSB to be about level. For simplicity we

*Not including organic, petroleum, or microbiological analyses.

†Calculated as D/S.

**Table C-1. Summary of net benefits derived from a model for the managerial functions.**

| | Net benefit (man-years) |
|---|---|
| Work plans | 0.00 |
| Sample log-in | 0.00 |
| Sample load projection | 0.08 |
| Workload lists | 0.31 |
| Interim reports | 1.06 |
| Query reports | 0.04 |
| Work accountability | 0.11 |
| Update status and results | 0.19 |
| Quality assurance | 0.29 |
| Total | 1.99 man-years |

assume the effort level of the 30,000 determinations a year (that we are considering for automation) represents the mean over the 5-y period of amortization.

## Work Plans and Sample Log-In

The information about the samples and project must be provided to the sample file by keying-in data, whether the sample file is automated or not. The automated procedure should be at least as easy as the manual method in which preformatted sheets and ditto marks ease the entry of data. No net benefit is assumed for the functions of work plans and log-in.

## Sample Load Projections

Assume the following: For every parameter, for one month of planned samples, check four items: date, subelement number, status, and analysis.

| | |
|---|---|
| Number of reports, $N_r$ | 15 |
| Files looked up, $D_s$ | 5 |
| Studies planned, P | 260/12 |
| Items checked, $N_c$ | 4 |

$$\text{Benefit} = [D_s f + P S_p D_s N_c c(\frac{1}{60})] N_r k$$

$$= [5 \times 4 + \frac{260}{12} \times 25 \times 5 \times 4 \times 3(\frac{1}{60})]$$

$$\times 15 \times k = 0.08 \text{ man-year}$$

## Workload Selection

Assume the following: For every active study and every sample, the parameter and status are checked ($N_c$ = 2). If the status is "not done," transcribe the limits, sample, number, and due date ($N_t$ = 3).

| | |
|---|---|
| Mean time to complete study, $T_p$ | 25 |
| Projects active on any given day, P | 26 |
| Samples per study, $S_p$ | 25 |
| Determinations per sample, $D_s$ | 5 |
| Number of reports, $N_r$ | 250 |
| Checks, $N_c$ | 2 |
| Transcriptions, $N_t$ | 3 |

Benefits

$$= [D_s f + P S_p D_s (N_c c + N_t t)(\frac{1}{60})] N_r k/T_p$$

$$= [5 \times 4 + 26 \times 25 \times 5(2 \times 3 + 3 \times 6)(\frac{1}{60})]$$

$$\times 250 k/10 = 0.31 \text{ man-yr.}$$

## Short Reports

Assume the following: For every active study, for every sample, list the sample number and parameter status, transcribe the study and subelement number.

| | |
|---|---|
| Number studies active, on a given day, P | 26 |
| Number of reports, $N_r$ | 250 |
| Files looked up, $N_f$ | 1 (assumes *a special* file) |

Benefit (short report)

$$= [f + P(2t + S_p(t + D_s t))/60] N_r k$$

$$= [4 + 26(12 + 25(6 + 5(6)))/60] 250 k$$

$$= 0.95 \text{ man-year.}$$

## Long Reports

The long interim report calls for a sample description to be transcribed in addition to the foregoing, but fewer reports are needed. Number of reports, $N_r$ = 50.

Benefit (long report)

$$= [f + P(2t + S_p(2t + D_s t))/60]\ N_r k$$

$$= 0.22 \text{ man-year.}$$

Because the daily reports are available and collated, the claimed benefit for the long report will be less. We estimate 50% less, or 0.11 man-year.

## Weekly Reports

Assume the following: The weekly status report lists the subelement, title, and status of each active study. The checking of each sample status is included. Number of reports, $N_r = 50$.

Benefit (weekly)

$$= [f + P(3t + D_s c)/60]\ N_r k$$

$$= 0.009 \text{ man-year.}$$

## Query Reports

For one study, for each sample, check the parameter, for a match; if found, list the result or status.

| | |
|---|---|
| Studies, P | 1 |
| Number of reports, $N_r$ | 500 |
| Files looked up | 1 (the parameter file). |

$$\text{Benefit} = [f + (P S_p(c + t) + D_s c)/60]\ N_r k$$

$$= 0.04 \text{ man-year.}$$

## Work Accountability Reports

During any 1-mo period we estimate 24 studies will have accountability data; of these, twenty studies were begun during the month and four studies carry over. The status of each analysis and the dates started and completed are tallied. The title and subelement of the studies are listed.

| | |
|---|---|
| Number of reports, $N_r$ | 24 (two per month) |
| Studies, P | 24 |
| Files looked up, $D_s$ | 5 |

$$\text{Benefit} = [D_s f + P(2t + 3S_p D_s c)/60]\ N_r k$$

$$= 0.11 \text{ man-year.}$$

## Updating Files for Status and Results

A status is kept for the study, each sample, and each parameter. We assume two updates of each during the course of a study. Six items are transcribed for each parameter: result, units, operator, date done, status, and QC approval. We assume updates are done in batch fashion twice a day.

| | |
|---|---|
| Studies active, P | 26 |
| Files looked up, $D_s$ | 5 (parameter files) |
| Number of days/yr, $N_r$ | 250 |

$$\text{Benefit} = [2 D_s f + (P + S_p + 6PS_p D_s)t/60]\ N_r k/T_p$$

$$= 0.19 \text{ man-year.}$$

## Quality Control Report and Updating Files for QC

This report is not so well defined that modeling is justified at present. From the discussion in Sec. 3 we have estimated that 0.2 FTE would be required to achieve the desired QC accountability.

The rough estimate given by the LSB for time spent in performing the functions in Table C-1 was 1.7 man-years/y. If we consider that a number of the functions are neglected or done less frequently than desired because of a lack of time and personnel, it appears that the 1.99 man-years benefit estimated here is realistic and reasonable.

# APPENDIX D

## ESTIMATES USED IN DEVELOPING MANPOWER COSTS

In Table 2 (Sec. 6) estimates are given for the cost savings expected as a result of automating the LSB. Manpower costs used to estimate these savings are based on the following assumptions and calculations:

- Basic average salary as of September 1976 is about $14,000 to 15,000 per year.

- Assume a salary of $15,000 per year as the average over the first five years of the computer's life.

- Add a payroll burden of 33.5% for pensions, health plans, insurance, etc.

- Add a support burden of 16.3% for secretaries and administrators.

- Add a general overhead of 50% for building rent, custodial care, utilities, travel, etc.

Then, $15,000 x 1.335 x 1.163 x 1.5 = $34,900 per man-year.

This figure checks closely with a best guess of $30,000 per man-year made by B. Carroll of the LSB when projected forward for five years. An estimate of $43,000 per man-year was given by B. Fairless of the CRL Region V laboratory in Chicago, and $35,000 per man-year by O. Villa of the Annapolis Field Office, Region III.

# APPENDIX E

# GUIDELINES FOLLOWED IN EVALUATING AUTOMATION SYSTEMS

## A High-Level Programming Language

We have chosen Dartmouth BASIC (extended) as the most desirable programming language to use in the EPA laboratory environment. Invariably, modifications are needed in the computer programs to meet future laboratory requirements. If such changes are difficult to make, the operator will either live with less than optimum conditions or revert to manual operation, thus undoing many of the benefits that automation was to provide. Of the various high-level languages, BASIC has proven to be the most widely available, and supported by most of the major mini-computer vendors. FOCAL, which was introduced by Digital Equipment Corporation, is no longer supported by them. FORTRAN is a more powerful language than BASIC, and usually faster in execution, but the BASIC interpreter makes program development and modification easier and much faster for the chemist, who can do it while other instruments operate as usual. Modification of FORTRAN programs requires the computer to be stopped and restarted with the new program. This can happen many times as a new program is debugged, and will destroy normal laboratory procedures.

BASIC is now being taught in many high schools and colleges as the language of preference for the occasional computer programmer. Although there are some differences among vendors in the way BASIC is used, these are in extensions to the language and are easily understood. Standards are presently being developed by a committee of the American National Standards Institute. Another strong point of BASIC is that it can be modified on-line and tested immediately. This means that a simple change in calculations or instrument operation can be made directly by an analyst in a very short time on the order of 15 min. Although in most systems interpreted codes like BASIC run more slowly than compiled codes like FORTRAN, speed will not be a disadvantage in the system we propose, because the gain from BASIC's flexibility will more than offset the slower running time.

## Field-Proven Operating System

We feel that there are many advantages to using field-proven operating systems. Our observation is that new systems have many "bugs" in them. Often, too, prototype systems are announced with the promise of early delivery, then the manufacturer finds he cannot deliver them until months after promised. To avoid such problems, only operating systems that have been in the hands of independent users should be considered. The system proposed in this report (Sec. 4) is a composite of the systems now installed at the Environmental Monitoring and Support Laboratory and the Municipal Environmental Research Laboratory in Cincinnati, and at the Central Regional Laboratory of EPA Region V in Chicago. Thus, problems with electronics, operations, and analysis should be minimized. One disadvantage of insisting on a time-proven system is that newer, possibly more powerful systems will be rejected. We are deliberately taking a conservative position. A powerful advantage is that software and hardware are more easily shared between installations.

## Supplier Support of Operating Systems

It is common practice for manufacturers to support their operating systems (if not modified) for periods up to 5 years. Any large software system can be expected to have a few residual bugs in it even after years of testing. By installing a widely used system we increase the probability that someone else will discover the bugs, and that the manufacturer will fix them before they cause problems for EPA.

We also feel that a single system should be designed that will be versatile enough to satisfy the differing needs of users in different laboratories. If EPA were to set up a minicomputer systems group to develop and maintain a unique, special-purpose operating system for its water quality analyses, for example, a faster, more efficient operating system could no doubt be written. It would be very difficult to change, however, and would require the assistance of the systems group for most modifications. Such special operating systems now on the market are exemplified by the Finnigan GC/MS, Hewlett-Packard, Perkin-Elmer, and Varian GC systems. These single-purpose systems work very well but because they are proprietary, changes are impossible without the aid of the original supplier. We feel that EPA should not put itself in the hands of a unique supplier, but rather should adopt systems that can be modified.

In the particular case of the GC and GC/MS systems, however, we feel that EPA should continue with these existing tested systems, most of which have their own built-in computer or integrator and are cost-effective as they stand. When advantageous, the modified output from these instruments could be coupled into the computer system for further data reduction, report writing, or communication to an SFC system.

## Multi-User, Multi-Application, Realtime, Timeshare

There are a number of potentially attractive systems that lack one or more of these characteristics. The operating system must be designed to accommodate several users and several instruments simultaneously while giving each user the quality of service of a dedicated computer. A time-shared system can do this while providing for the sharing of expensive peripherals such as line printers and magnetic tape. A time-shared system also gives the option of adding more instruments to the system inexpensively. If individual computers are used, another computer has to be purchased with each new instrument. A disadvantage of the time-shared computer is that failure of the single time-shared computer forces all users back to manual methods.

## Rapid Response Time

Because of human impatience, worst-case computer response time from the issuing of a keyboard command must be no more than a few seconds. After about 10s, most users become irritated. For automated data collection, worst-case times from the receipt of a "data-are-ready" indication to data-collection action must be less than 200 $\mu$s.

## Instrument Input/Output Handlers

It would be advantageous if the computer vendor provided software to handle data acquisition from instruments, calculation, and reporting functions. No vendor known to us now supplies software for all the particular instruments we have been asked to consider.

Custom algorithms and data acquisition and control programs must be provided. The computer system vendor must allow these algorithms to be simply implemented, with a clear description of how to pass information to and from BASIC, and how to use the operating system for input and output of instrument data.

## String Manipulation Capability

For the simplest and most natural interaction between operator and computer for efficient information flow between data and reports, the system must have the ability to handle alphanumeric strings. If this feature is not provided by the manufacturer, it will have to be added by the system implementer.

## Swapping

To make the most efficient use of core storage, effective program swapping must be available. This implies that run, swap-in, and swap-out areas must be concurrently active. Virtual systems using paging have been proposed as an alternative. For laboratory automation, however, we do not feel that the art of virtual memory has advanced to the same level of effectiveness as program swapping systems. At present, virtual memory systems require careful tailoring of the programs to avoid excessive page swapping. If programs are to be modified by the chemists, the burden of tailoring the programs cannot be placed on the chemists.

## Chaining and Overlays

The ability to chain programs and to overlay segments is imperative. The alternative is to have all programs core-contained, which would require excessive core storage.

## Files

Data files will be stored on the disk for later manipulation and development of new analysis methods by the chemists. These files must be accessible from both the machine language and BASIC level code, because some files will be built by the machine level code and used by the BASIC code.

## Foreground-Background Operation

This feature is desirable for SFC and report preparation. The instrument control programs must run in real time, along with their operator prompts. Calculation routines, summary reports, etc., do not require real-time capability, and so can be run in a background mode using otherwise idle time and increasing the overall system efficiency.

## Multiple Terminals

An analyst's acceptance of the computerized system is strongly influenced by his ability to control it and to know what is happening all the time. There should be either a hard-copy typewriter or CRT screen terminal at each active analytical instrument or group of instruments. This allows initiation of runs, display of data as calculated, and display of diagnostic messages such as out-of-range Concentrations. The operator need not be at the terminal at all times, but he must have immediate access to it so he can verify proper operation.