Overview

The impact of computers on the analysis of metals began with the use of dedicated microprocessors to control analytical instruments and perform calculations on the raw data. These instruments rapidly evolved into multielement analyzers because their computers became more powerful. The large amounts of data they produced had to be accommodated by a laboratory's filing and reporting system. Computerized data management, formerly possible only with large mainframe computers, is now achieved by powerful yet inexpensive personal computers using sophisticated software. Linking personal computers with the computers attached to the instruments creates a network capable of assimilating data, reporting and filing it, and tracking samples.

Installing any computerized system requires goal-setting, planning, evaluating, and training in addition to computer expertise. The purpose of this ASTM symposium on Computerization and Data Management in the Metals Analysis Laboratory was to guide chemists in both selecting the appropriate hardware and software, and using it to interface laboratory instruments, log in samples, process and file data, disseminate information, monitor quality assurance parameters, and generate management reports. The following papers were presented in Nashville, Tennessee, on 24 September 1986. Selected comments, questions, and answers from the presentations are appended to the appropriate papers.

The first paper deals with standards for computerized laboratory systems. Since 1970, ASTM has had a Committee on Computerized Systems, E-31. The author, current chairman of E-31, discusses the history, purpose, and achievements of the committee. They have published a number of standard guides, standard specifications, and a terminology standard relating to computerized systems. The process of developing such systems includes project definition, functional requirements, functional design, implementation design, system assembly, and system evaluation. These are discussed more fully in the ASTM Standards listed in the paper.

One example of a computerized system, described in the next paper as a new automation tool for the metals analysis laboratory, consists of an electronic balance and an atomic absorption spectrophotometer interfaced with a personal computer. Two BASIC programs developed in-house provide a software link to a commercial spread sheet/word processing/data base package. By recording and calculating the data and generating a final report, the system has saved time and reduced errors. Eventually, a robotics system for automated sample dilution and autosampling will be added. The paper describes some of the steps required to structure the software, collect the data from the instruments, and configure the final report.

Linking several computers and peripherals creates a local area network (LAN). As a computerized laboratory management and analytical data management system, a LAN's components include: hardware, software, interfacing, peripherals, and back-up system. The author lists some applications, and evaluates the advantages and disadvantages of various network topologies. The control and operating system is a software program called the utility, while the transmission medium is a physical connection, usually a cable. Criteria for
selecting a network include: availability and reliability, cost, compatibility, expansion potential, speed, response time, documentation, training, logistic and maintenance support, and security. In the second part of the paper, the author describes a real system designed for a specific metals testing laboratory by detailing the hardware and software necessary to interface the scientific instruments and illustrating the actual output.

Using different hardware and software, the next authors developed a local area network in their metals research laboratory. They used a commercial network utility software and twisted pair cabling to connect the nodes, which consisted of scientific instruments, computers, and peripherals. Installation of a powerful but expensive laboratory notebook software on one node of the network allows it to be accessed by various users for plotting graphs, calculating, and reporting. They plan to reconfigure the system using a broadband coaxial cable instead of the daisy chain topology to speed transmission and allow the system to function even when one node is out of service.

The features and applications of a data base software program adopted by a small, independent laboratory are described as an approach to laboratory data management: the application program generator data base. After comparing the laboratory’s existing hardware, personnel expertise, and goals with several commercial software packages, the author selected a relational data base program for use on a personal computer with added memory. Central to the program is a data dictionary. Its unique feature however, is a source-code editor, which guides individual users in tailoring applications programs for specific needs. Files are in ASCII code, easily transferred to separate word processor and statistical programs. The system is used primarily for sample tracking, final report generation, and data query. Other applications include: catalogs of chemicals, standards, and control materials; an instrument service log; an instrument/equipment calibration record; and personnel monthly time tracking.

Developing an integrated, company-wide online laboratory data system helped a company which has locations in several towns and states. The system consists of four modules. The first contains programs for submitting and tracking the test material, then verifying and reporting test results. The second collects data from analytical instruments, some in real time and some in a batch mode, depending on the sophistication of the instrument’s built-in computer. These data are ultimately transmitted to a mainframe computer, but only after review by a laboratory supervisor. The mainframe stores the data in a data base system (module three) and checks the data against specification requirements. Some of the data comes from off-site laboratories, and the final report can be transmitted to a facility or customer in another location. The data base system also permits data retrieval and provides for security. Statistical analysis with graphical representation is provided by module four, a data analysis software package. The entire system has reduced turnaround time and increased productivity.

The two final papers deal with a specific application of computers in the laboratory, using them for quality control. The first discusses the implementation and automation of analytical statistical process control. The author describes the statistical concepts which go into making a control chart. An $\bar{X}$ control chart is a Gaussian frequency distribution plot on its side. Although there is software to generate such control charts, it is still laborious and time-consuming to chart each element tested by a multielement analyzer like an X-ray fluorescence spectrometer, direct-reading spectograph, or plasma spectrometer. The author describes the requirements and advantages of automated multielement control chart software and challenges the manufacturers to build it into their instruments.

As a quality control system for X-ray analysis at a steel mill, three X-ray fluorescence spectrometers are used for process control of the blast furnaces and raw materials. Running control samples periodically furnishes precision data, providing a basis for recalibrating the
instruments when necessary. Exchange of production samples between the three instruments diagnoses possible biases. A third check is the testing of duplicate samples by X-ray and confirming the results by wet analysis. Computers keep track of the data, and will eventually generate the control charts.

One aspect of computerization not mentioned in detail by these papers is the human factors. Computer fear occurs among employees who have not been exposed to computers, especially if they are resistant to change or concerned about the loss of their jobs. Motivating, training, and providing comfortable computer work stations for employees should be an integral part of the planning, installing, and evaluating process.

The amount of expertise, planning, and hard work necessary to computerize is evident in all these papers. Evident, too, are the rewards: reduced errors, increased productivity, solved problems, speeded communications, and improved quality. Computers are changing the metals analysis laboratory, and the full impact of this change will be felt as more laboratories adopt hardware, software, and systems like those discussed in the following papers.

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