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Laboratory Automation

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A number of factors are pushing modern chemistry laboratories to view laboratory automation as a necessity and not as a luxury. The cost of people, government regulations, and making the most effective use of human resources are just three of them. Understanding how we got where we are and the issues facing us are important to making real progress in this area.

INTRODUCTION

Today, the words "laboratory automation" almost immediately bring to mind computers and computer systems. That is a result of the current bias in our thinking and really does not reflect the true meaning of the words. The laboratory is a place to work, and automation refers to things being driven or guided by themselves. It really involves the work place, either all or part of it, functioning without our intervention or supervision. If we go back and reapply that meaning to the chemistry laboratory we will find that laboratory automation is not a recent—given the long perspective of chemistry—development but one that goes back over a couple of decades (some may argue that it dates to the invention of the graduate student, but I will restrict myself to mechanical or electronic means of automation).

Before we get too deeply involved in the topic of automation, let us take a quick look at the environment we are working in—at least those of us that work (or worked) in analytical labs. Our driving ambition is answering questions about samples: What is it? How much of a given component does it contain? Certainly not to be ignored are the problems of method development and the question "is it done yet?". Satisfying those questions involves determining the appropriate method of analysis, preparing the sample, performing the analysis, calculating the results, validating them, and finally preparing and sending the report to whoever submitted the sample in the first place. The goal of real laboratory automation is to reduce the manual effort in repetitive tasks as much as possible. Some day, when computer systems are smart enough, we may reach Lou Mikkelsens' (Hewlett-Packard, Avondale, PA) goal [1983 Pittsburgh Conference symposium: "Solving the Laboratory Data Management Problem" (unpublished)] of a system that will take the sample from bottle to finished result without our being involved at all, at least not for routine tasks.

The drive behind the automation efforts stems from two fronts: the laboratory chemist (predominately the human element) and his management (human element, efficiency, and economics). Both are faced with conflicting requirements: the need to perform more analyses (routine, nonroutine), to develop new testing techniques, and to do it within the facilities budget. The requirements of government regulations are added on top of that to keep things interesting. Manpower is an expensive, but required resource. The trick is to use people where they are most effective and some form of automation where it is effective. The right balance (easier to write than produce) benefits both management and the laboratory worker by reducing the need for people to do routine repetitive tasks and freeing them for more interesting work.

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AUTOMATION BEGINNINGS

Automation in the chemistry laboratory began not with the advent of computer systems but most probably in the late 1950s for commercial systems, with the introduction of the Auto-Analyzer I (Technicon, Tarrytown, NY) and later the Auto-Analyzer II (1969-1970). These systems attacked the problem of automating the analysis. They would take the prepared sample, mix reagents, apply heating and mixing as required, and pass the sample through a photometric detector. The preparation and data reduction were still in the realm of human activities. There were some also systems developed on a one-at-a-time basis for automated work: there was an automated Karl-Fisher titration apparatus at Rexall Drug and Chemical (Paramus, NJ) in the mid 1960s. Automated process chromatographs were made by several companies.

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Again, as in the case of the autoanalyzer, these devices took a prepared sample (a reactor head-space gas sample for example) and injected the sample into the chromatograph. Cam or timer-driven controls actuated event timers and back-flush valves. The Karl-Fisher titrator would automatically add the titrant until the end point was reached and then stop. Chemists and technicians were still needed for calibration and data reduction.

Efforts to relieve the manual work in chemistry came from both the instrument manufactures and the computer system vendors, each for his own reasons. In many cases it was a matter of survival in the face of competition. New methods of chemical analysis (really new, not refinements or variations of existing techniques) are not every day occurrences. The equipment to support basic techniques was augmented with supporting equipment, some of which falls into the realm of automation.

DIFFERENT PERSPECTIVES ON LABORATORY AUTOMATION

(A) Laboratory Automation from an Instrument Manufacturer's View. The development that we will now follow is for a specific piece of equipment—the liquid chromatograph (LC). The path and logic is not restricted to that device but finds parallels in many other devices such as spectrophotometers, thermal analysis equipment, and equipment designed to measure the physical properties of materials. Many of the concepts described below had been developed for the gas chromatograph earlier than the dates noted. On to the liquid chromatograph.

This device was chosen as an example because of the broad acceptance and popularity in the field of analytical chemistry. Those two points have fostered a good deal of competititon between vendors and that has accelerated its evolution over a period of 10 years or so, rather than the longer periods experienced by instruments with less market potential. It is also a device that has been courted by both instrument vendors and computer vendors alike and provides an opportunity to contrast points of view.

In the early days of LC work, the instruments were restricted to single solvents as a carrier and single detectors with the output recorded on strip-chart recorders. The first serious enhancement in its technology was the idea of changing the solvents during the course of an analysis to improve the separation of components (ca. 1976). This was quickly followed (1977) by the advent of pump controllers to govern the transition between solvents. The data—while improved by more sensitive detectors—was still being collected on long strips of paper and reduced by hand. While the technique had improved, the chemists work load had not been lessened. The bottlenecks in the process of LC analysis were the preparation and injection of the samples and then converting elution curves to a finished analytical result.

The first major advance in making life easier for the analyst was the introduction of the autosampler (about 1979), an intricate device that would automatically introduce the sample (taken from a rack of up to 99 sample vials) into the instrument. This piece of equipment would effect both the pump controller (telling it when to restart the solvent gradient) and the sample injection system. It relieved the analyst from the the monotony of watching the elution curve or timing the injection and physically introducing the sample onto the column (all of which could be done unattended and overnight) and left him freer to attend to data analysis and reduction. Considering that the instrument would have 16 h to produce curves and the analyst had 8 h (theoretically) to work with the data and prepare new samples, the autoinjector was sometimes considered a mixed blessing.

This facet of laboratory lore was not lost on the instrument vendors. In order to make the basic LC more attractive and recognizing that solving the data reduction problem would improve their competitive position, they took advantage of the ready availability of low-cost microprocessors and built data stations to collect and analyze the output of the detector (1980 or there abouts). In many cases this portion of automating the LC was made easier by instrument vendors' experiences with gas chromatography. Data stations, integrators, and the like hit the marketplace. In some cases the integrator was mated to a "system controller", which tied all of the components of the "automated" LC together, pumps, autoinjector, integrator, and so on, providing one central control facility.

The battleground for a competitive edge in the market shifted (note the basic LC really had not changed much, people just hung more equipment around it to make it more convenient and easier to use). In some cases the basic technique took a back seat to data analysis and control capability. (In some other instrumental techniques, it appeared that manufactures put microprocessors on things to make them "computerized" whether or not the chip added any real value.) Peak processing algorithms, base-line correction techniques, internal and external standard capability, and stored methods, were the new bones of contention, differentiating one vendor from another. In order to remove some of the redundancy in the controlling subsystems, these were replaced with sophisticated data stations capable of handling the entire instrument (usually more than one) and providing graphic displays, off-line storage, and programming capabilities (1984).

The advantage to the chemist, and the contribution to laboratory automation, was that it removed another bottleneck—data reduction. It made it easier for the analyst to spend time on more creative work, because the routine day-to-day analysis was being handled by automated systems, except for sample preparation; more on that later. For the instrument vendor, it made his basic device—the chromatograph—more acceptable to the chemistry community by reducing the amount of work and effort involved in using it.

(B) A Computer Manufacturer's View. Commercially available computers have been in use in the chemistry laboratory since the mid to late 1960s. Most of its use was in research projects where the computer was part of the experiment and doing work that a person either could not do (high-speed data capture and experiment control for example) or would simply require too much computation. Much of that work fell into the realm of computer-aided experimentation rather than laboratory automation as defined earlier. Computer-aided automation was still some time away.

The computer vendor had what appeared to be the key device in laboratory automation—a programmable controller/data capture/data analysis machine. An examination of the literature during the early 1970s shows the prime focus of instrument manufacturers to be directed toward refinement and exploration of techniques. Those involved in liquid chromatography were still looking at different applications of this analytical procedure. The use of computers in the analytical laboratory was still uncertain. It looked like it should be useful, but how to go about it? Unlike analytical techniques, there was not a large trained pool of people able work with computers, and given its cost at that time, it frequently lost out to laboratory instruments in budgeting. It appeared to be a device with a lot of promise, if people could only figure out how to make it work.

The early 1970s saw some progress in computer-aided laboratory automation. A paper by Charles Walker,[1] published in 1972, gives an overview of a multiprocessor system and includes the use of a distributed approach to data collection and analysis. A 1975 book[2] gives a review of effort toward the development of software systems that are very similar to todays Laboratory Information Management Systems (LIMS).

The October 1975 issue of the *Proceeding of the IEEE* was a special issue on laboratory automation. Of the 16 papers in the issue, four were directed at laboratory automation. The rest were concerned with computer-assisted experimentation (five), data reduction (five), process control (one), and a product description. Some comments of the editors are worth noting in regard to the response to the call for papers (p 1380): "Little information on the use of control in the laboratory automation systems was submitted, leading one to believe that this aspect of automation is still not being utilized on a broad scale.", and "No papers concerned with microprocessors in laboratory automation were receive in a form acceptable for publication in this Special Issue. It is anticipated by the editors that the application of these computer structures will grow at a rapid pace in the next several years. Also little work on distributed computer structure was reported...."

Much of the literature on laboratory computers was not in the reviewed journals but in the wider circulation trade magazines. *American Laboratory* was running a twice-a-year special issue on the subject. In early 1976 it was running a series on microcomputer interfacing (by David Larson, Peter Rony, and Johathan Titus) that continued for quite some time. The topics in that time frame tended toward the use of computers with specific pieces of instrumentation and methods. Much of the workup to that point dealt with computer-aided experimentation, interfacing (how to, how not to). A few addressed real laboratory automation: "Using Computers to Automate a Large Analytical Laboratory",[3] for example and others.[4-6] Computers were beginning to move from the realm of a research tool of the few to a more accepted approach to working in the nonresearch-oriented laboratory of testing and quality control. We were moving from the "let us try it and see if it works" to the beginnings of commercially available laboratory systems.

This acceptance was not lost on the computer manufactures. Where they had been providing systems for research (here are the pieces, you make it go), they now turned their attention to the turnkey solution. Computers are good at calculations—given proper programming—and data reduction is an area that consumes much of a laboratory workers time. A natural fit began to emerge, particularly in the field of chromatography: lots of data points being generated, lots of samples (automatic sample injectors were making themselves known), lots of calculations to be done. Several computer and computer/instrument vendors [Digital Equipment, Hewlett-Packard, Varian, Computer Inquiry Systems (a systems house), and others] began tackling the application in earnest. The 1976/1977 Pittsburgh Conferences saw several approaches to the problem develop. General-purpose computers were providing data acquisition, data reduction, and reporting capabilities for several instruments (8–20) on one machine with several users and offering user programming (usually in BASIC). Microprocessors were dedicated to individual instruments to perform integration and to support internal and external standard calculations (no user programming). The competitive points revolved around peak processing algorithms, base-line correction techniques, graphics, and the cost per channel. Different approaches were taken to handling the data acquisition: successive approximation A/Ds, integrating A/Ds, bringing the signal to the computer, and digitization at the source. So many options were available to the purchaser of a system ("of course you can do it, it's just a small matter of software...") that I wonder how many people really understood what they were getting into. The successful systems did not depend so much on the computer vendor as they did on the ability of the laboratory chemist to work with, extend, and interface the system—in short, to make it work in spite of inherent shortcomings (some things do not change).

These computer-based systems did have some clear benefits to the laboratory chemist and technician. They were relieved of much of the routine day-to-day analysis and computation; the machines acquired the data, analyzed it, and then reported the results—some portion of their work had been automated. Their ability to do nonroutine work improved greatly. Using graphical analysis routines designed for chromatographic work,[7] they could have the machine integrate the areas under the peak and dispense with planimeters and cut-and-weigh techniques. This approach was an improvement of early integrators in that it gave considerable flexibility in handling base lines.

The state of things today in this area has not fundamentally changed. Some centralized (one processor, many instruments) systems are being used. The more popular approach is to put a few instruments, about four, on a single "work station". The need for centralized systems was driven by price; the current cost of microprocessor systems allows us to justify their purchase with fewer instruments attached.

Where does this bring us to in automating the laboratory? The instrument manufactures had automated the instrument (autoinjectors and the like), and computer manufactures and systems houses had tackled the data acquisition, analysis, and reporting end (things really are not that simple, but it holds for an overview).

Judging by the the literature of the late 1970s and early 1980s, the computer became more accepted. The price of systems based on microprocessors dropped markedly, they were showing up everywhere (whether or not they made any sense in an application), and managers were using them for financial and data-base work. People became more familiar with them and were less reluctant to authorize their use in laboratory work. Many of the early workers in the field had moved up in organizations and a new crop of laboratory worker was being introduced to laboratory computers and their use. Laboratory automation through the use of computers was moving from the one-of-a-kind or one-of-a-few examples of successful projects to the point where commercial laboratory automation systems were being marketed and accepted. They were used routinely by people who were not "computer literate" but who treated them as a tool.

Until two or three years ago that was the general state of things. Ray Dessy (Virginia Polytechnical Institute) began a series of articles in *Analytical Chemistry* that presents both tutorials and examples of different aspects of computing and automation in the laboratory. The next major event was the need for and the advent of laboratory information management systems (LIMS). LIMS systems had been produced on a one-at-a-time basis at several installations, but the need for more efficient data storage and management, prodded by the Food and Drug Administrations Good Laboratory Practices (GLPs) and Good Manufacturing Practices (GMPs), made the development of commercial systems viable. To that end, several manufactures, of both instruments and computers, began announcing and producing systems. Among the vendors involved are Perkin-Elmer, Digital Equipment, Hewlett-Packard, Varian, and others. Many instrument manufactures view the ability to offer directly, or the ability to connect to, a LIMS system as a survival issue.

CURRENT TRENDS IN LABORATORY AUTOMATION

There are three key trends in laboratory automation: communications, expert systems, and robotics.

(A) Networks. Communications[8-10] in both local area networks and extended networks is becoming increasingly important. Rather than rely on a single machine to take care of the information needs of the laboratory (including the laboratory bench, and offices), several work stations are being used, with links to one another and to a central host system. This diffusion of resources throughout the facility requires a machine-to-machine communications path to permit data to be moved from one location to another for reporting and analysis.[11]

The speed at which we can move data around a network is going to change our view of the laboratory computer. Ethernet for example, can move data at the rate of 10 megabits/s. This value is the order of magnitude of the data transfer rates within a computer (a PDP-11 can transfer data on the Unibus at 40 megabits/s—both numbers are peak rates). We are approaching the point where commercially available networks can move data between machines as fast as it can be moved within some machines. With this type of architecture available, the laboratory computer system need not be considered as a box containing boards, power supplies, and backplanes but rather as interconnected modules tailored—by their complement of software and input/output hardware—for specific tasks. The analog-to-digital converter board of 5 years ago is now the microprocessor with memory and software to collect and analyze data. Given the speed of data transfer, disks may be optional; operating systems and programs can be down-line loaded to the module. The laboratory computer system could then fill a building and still be worked as a single system.

(B) Robotics. Automation has tackled, at least in the case explored above, getting the sample into the analytical system, collecting, analyzing, and reporting the data—for the routine case. The remaining human intensive portion is sample preparation.

Robotics[12-14] is being used to address this area, taking over the routine manipulative tasks in the laboratory. This goes beyond sample preparation and does include performing analysis where a lot of repetitive, predictable movement goes on. Several pharmaceutical laboratories are exploring the use of robots in dissolution analysis as one application. One clear benefit is that people's time will be better used.

(C) Expert Systems. This is another area in which a lot of effort is being invested.[15,16] Artificial intelligence (AI) applied to chemistry. Its an area that is believed to hold a lot promise, letting properly designed applications guide and assist the chemist in methods development and spectra–structure correlations. The popular literature would extend the capabilities of AI well beyond "guide", but we must be both realistic and cautious in its application. In the mid to late 1970s, a lot of promise was held in computer systems to assist in medical diagnosis. Attempts to develop these systems at that time came up against an interesting realization: medical diagnosis was an art, not a science—the rules in performing a diagnosis were not clearly defined.

ISSUES IN LABORATORY AUTOMATION

Any automation effort, whether it is involved in process control or typesetting raises issues, and laboratory automation has its own set. The comments below are taken from conversations with people active in the field. Given the space limitations of an article, I cannot do more than raise them. A detailed discussion will have to wait to a later time.

(1) Integration of vendor hardware and software. Given the proliferation of hardware and software, too little is being done to make it wasy for the consumer to move data from one system or software package to another. Much of this has to do with a lack of standards for data storage. While needed, the field is too dynamic to wait for a standard to be drafted, reviewed, and used. Some of this has to do with the planning of a laboratory automation project.[17]

A laboratory that is a collection of different microprocessors from various vendors is going to create problems. Another aspect of the problem is the adoption by instrument vendors of RS232 as a "standard" for communications. While it address character-level transfer, it does not get involved with message-level transfer and therein lies the rub. When the message-level protocol is standardized, we will be able to move closer to what is needed in the laboratory: simple movement of data with error checking and correction.

(2) Security and integrity of the computer system and network (this is a topic for a book not an article). This is strongly tied to GLPs and GMPs, but to a large extent it effects any well-run laboratory. The issue involves not only data bases but the programs used to process data. In a completely centralized system, the system manager can put some controls in place to help ensure that either programs used to analyze data have not changed or if they have it has been done in a controlled (why was a change made, what was the change, by who, how was it validated, etc.) manner. When each scientist has his own system, how do you enforce the controls? One way is to have all programs, both sources and executable images, reside on the host and only allow the executable program to be down-line loaded into a satellite machine. This can be enforced by having systems without mass storage (the network link may be fast enough for data storage on the host) or by having mass storage used only for data (how do you protect the data?).

(3) Can computerized laboratory notebooks be used in regulated environments? How do you do the equivalent of signing the notebook? The same applies to work that is done in support of patents. This one will have to be tested in the courts before any approach is accepted. Is there an alternative to the courts for deciding the validity of an approach before it is used?

(4) There is a need for a fourth generation language for laboratory data acquisition and processing. While many chemists can program, a software environment that allowed him to do his work by selecting choices from a menu would be desirable.

(5) A more directed approach by regulatory agencies, in concert with the chemical industry, instrument manufactures, and the computer industry, is needed to set realistic system-evaluation guidelines for automated laboratories. This is particularly important in sites that operate under GLPs and/or GMPs. Of particular concern is the need for source code on data management systems and a list of criteria that a system must meet (backup facilities, audit, design documentation, system tests, and so on). The "wait and see what happens in court" approach does a disservice to both vendors and consumers of instruments and computer systems.

There are also people-oriented issues. While most of what has been written above concerns the state of technology, proper laboratory use of computers (and instruments), and their data, the real issues are people. While economics is a strong driving factor for automation, the approach used has to be guided by a concern for the human element. Any approach that fails to take that into consideration will fail. Among the concerns there are the following.

(1) The reluctance of some to use or work in a heavily automated environment. While the benefits may be clear to management, they may not be to the people they affect. Keeping them involved from the start, with an understanding and agreement of objectives, is the first order of business. Telling people that you are going to do away with the need for paper can raise red flags. Some people find a security in

things written on paper. Implementing a system that does not take that into account is unrealistic (how would you like to deposit your pay check in a bank that had a policy against giving you a receipt?). In one facility I was somewhat surprised to hear that there was no reluctance to work with an automated system. The system designer had done his job right, it did what it was supposed to, and he has a receptive audience for future projects.

(2) Lack of qualified people to design and implement systems. While familiarity with programming in school may prevent someone from going into a catatonic state when faced with a terminal, that does not make him a designer. This needs to be recognized when systems are being designed. The academic community can help this situation by providing for cross-fertilization of computer science people with a bent toward applications with chemistry, the reverse would help equally well. Given the sophistication of the current hardware and software (inside or outside of an instrument), a course or two in Fortran or Basic is not going to suffice. It is also incumbent upon system designers to make sure that systems (a) work and (b) are easy to use, keeping in mind that the end user may be nervous about the use of a system.

SUMMARY

Laboratory automation is beginning to emerge as a discipline of its own. That editorial in the *Proceedings of the IEEE* referenced earlier contains the following statement: "For future laboratory automation systems, there is little doubt that the complexity of the projects will require a considerable team effort....A typical mix of personnel will include instrument experts, persons trained in signal processing and control, and computer scientists or engineers." Every word is as true today as it was then.

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Robotics in the Laboratory

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Laboratory automation has long been an important area where chemistry and engineering have overlapped. Many automated processes now are routine in the laboratory; however, the apparatus that performs these tasks is usually rigid, being designed with only one use in mind. Laboratory robots are flexible automated systems and may well be the scientist's dream of the perfect laboratory technician. Useful laboratory robots are now a reality. This paper will discuss the current state of laboratory robotics in chemistry as well as speculate on the advantages of robots in the future laboratory. The final section will present a project now under way in our research group to produce a flexible robotic system that will be able to design, implement, and evaluate its own analytical procedures.

Laboratory automation has long been an important area where chemistry and engineering have overlapped. Many significant advances have been initiated by analytical and other experimental chemists whose demonstrations have gained the attention of scientific instrumentation manufacturers. These manufacturers have drawn upon the creativity of research scientists and, with their own research and development efforts, produced important instrumentation upon which most laboratory science depends.

Recently, computer data reduction, computer data collection, and computer data interpretation have joined automation as indispensable tools for experimental research. Again, research scientists have pioneered and technologically oriented manufacturers have produced useful systems.

While many automated processes now are routine in the laboratory, the apparatus that performs these tasks is usually rigid, being designed with only one use in mind. A more desirable kind of equipment would be a flexible, automated system capable of performing a variety of laboratory operations including ones yet to be conceived. Laboratory robots are flexible automated systems and may well be the scientist's traditional dream of the perfect laboratory technician. Serious laboratory robots are now becoming a reality and are the topic of this article.

This paper will be divided into four sections. The first will be a brief review of the literature on robotics. Most of that literature will be from areas other than chemistry and often will be references unfamiliar to chemists. The second section

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