COMPUTERS IN THE LABORATORY
by Joseph G. Liscouski (ed.)
American Chemical Society, Washington, D.C.
1984, hardcover, $34.95

Reviewed by Harry E. Pence*

The interfacing of computers and microprocessors with modern analytical instruments has produced the capability to generate large amounts of data very quickly. Unfortunately some chemists have found this new power to be a mixed blessing, for it is often difficult to identify the information content in the resulting array of observations. Equally important, many government agencies, such as FDA and EPA, are requiring more stringent record-keeping standards. The obvious solution to this "data explosion," as it is sometimes called, has been to further expand the use of computers for analyzing, reporting, correlating, and storing laboratory data.

At the fall national ACS meeting in 1984, a symposium was presented on applications of computers in the chemical laboratory. This book is based on ten of the papers from that conference. The various authors discuss a broad range of uses for computers, not just data collection and analysis, and the result indicates the current areas of interest as well as the new developments that can be expected.

These papers suggest that computers will play an increasing role in the laboratory of the future. Analytical instruments will be connected to computer networks and computers will analyze the data that these instruments generate by comparison with standard databases and interpret it with Artificial Intelligence (AI) systems. Robots will be used to perform tasks that are tediously repetitive or especially dangerous. Graphics, simulations, and mathematical analysis will identify data correlations and also model the results of alternative decisions; a procedure already familiar to those who use spreadsheet software for business. Even though no single institution currently integrates all of the applications described, many companies are already using one or more of these techniques. This indicates that such an ideal laboratory may be well on the way to becoming a reality.

As might be expected in a symposium, there is considerable variation in focus and approach from article to article. For example, several of the articles deal with various aspects of instrument networking and Laboratory Information Management (or LIMS) Systems, but the result fails to give a balanced view of this vital area of development. These articles are concerned with specific commerically available systems, and general principles are presented only as they deal with the system under consideration. Thus some significant topics are well covered but others of equal importance are neglected.

The longest article is a discussion of graphics. This article is perhaps one of the most useful for many readers of this journal, The treatment assumes little specialized background and should be excellent for someone who wishes an overview of current graphics techniques. Some presentations seem so short that they only whet the appetite for information, such as a paper on robotics, although one of the shortest articles was perhaps the most prophetic, a description of computer use by chemists in the Corps of Engineers. For the Engineers, their "laboratory" is the entire Ohio River, and computers are used to operate an automated water quality laboratory, assess water quality, and simulate the effects of possible water management decisions. In both cases an expanded treatment would have been both justified and welcomed.

The last three papers in the book deal with organizing and extracting information by means of computers. Clustering methods are demonstrated by showing how they are being used on data from the Merck Index to find structure-effect relationships among various compounds that are used for medicinal purposes. Another paper describes the use of information enhancement techniques to establish optimum conditions for obtaining structural or activity information from voltammetric electroanalytical analyses. The final paper argues that linearity and determinism are often assumed with insufficient justification in data analysis, and since computers allow scientists to develop more realistic models, this freedom should be used more often.

The foreword of the book notes that the individual articles were not typeset but were provided by the authors in camera ready form. In some cases this produces more than the usual number of typographic errors and one article did copy rather poorly, but these problems are only a minor irritation. The index is adequate, but the individual chapter bibliographies are often rather brief and in several cases nonexistent. Few of the authors are associated with academic institutions, an indication of the high level of interest in computer applications found in industrial and governmental laboratories.

Overall, the volume suffers from the typical drawbacks that might be expected from the symposium format; the papers tend to be rather narrowly focused and different authors assume that the reader has varying levels of prior expertise. Most readers will gain some useful information from the book, but it fails to provide the well-integrated survey that is needed. Aside from journal articles, such as those in Analytical Chemistry and the Journal of Chemical Education, there are too few attempts to present an integrated perspective on the current status of computer applications in chemistry. It is regrettable the book cannot be enthusiastically recommended. On the other hand, the articles describe areas where current interest is high, and the book might be considered for purchase on that basis.

*Department of Chemistry
SUNY-Oneonta
Oneonta,NY 13820