2

PERSONAL COMPUTERS IN CHEMICAL EDUCATION

For some chemists, working with computers is their full-time job; a large group uses computers as adjunct to their interest. Computer applications in chemistry education cover an ever broadening range and consequently are difficult to categorise. Nevertheless, an attempt is made to classify and describe briefly the many roles computers play in chemistry curriculum.

COMPUTER-ASSISTED TEACHING

Computer-assisted (or *aided*) *teaching*, CAT, is an alternative to other teaching methods where the computer assumes part of the 'role' of the instructor. Here a student interacts with a computer in direct conversational dialogue, and the computer is programmed to present course material, ask questions that require active response, evaluate and vary its presentation on the student's response. Some authors refer it as *computer-assisted learning*, CAL. Education computing offers, surprisingly a number of other such acronyms, each with its subtle shade of meaning, for example, CAI—*computer-assisted instructions*; CBL—*computer-based learning*; CMT—*computer-managed teaching*. For most educationists, CAT includes all the educational activities in which a computer is used to augment (or initiate) a learning or teaching process. Inclusion of CAT within the curriculum can increase student motivation. This may be due to a number of factors, for example:

- there is a novelty factor which does not appear to wear off
- students are prepared to work hard to gain the satisfaction of obtaining favourable responses, or even 'beating' the computer

COMPUTER GRAPHICS/SIMULATION/MODELLING

One of the impressive features of most of the computers is their graphic capabilities. A computer can draw images of molecular structures, electron densities in atoms and molecules, or plots of one variable versus the other, or spectra of various types, of laboratory apparatus, and many other items that a chemist uses regularly.

Another approach in this area is the animation. A simple animation can be used to introduce a topic, laboratory skill or to demonstrate the moving parts of instruments or chemical reactions.

Computers can also produce models (simulations) of real systems. Programs can be written so that the computer simulates events and conditions that are either difficult or time-consuming to demonstrate practically or such nature that they are not normally investigated. The highly interactive simulation experiments sometimes make-believe the student that he is working with real instrument.

INTERFACING/EQUIPMENT CONTROL

Now that inexpensive personal computers are readily available they are being linked to a wide range of scientific laboratory and field equipment. These links allow the user to establish computer control over equipment, and data collection from the instruments (using transducers or sensors). However, before a link can be made, a suitable interface between the computer and a piece of external equipment must be provided. An *interface* is a device that allows peripheral equipment to communicate with central processing unit (CPU). All computers will contain a number of existing interfaces that link the CPU with its input, output and storage devices.

Most of the equipment interfaced, or used, by the chemists generate an *analog* output. An analog signal produced by scientific equipment will normally be continuously varying voltage or current. Analog signals cannot be directly processed by the computer and must be converted to *digital* format. This conversion can be carried out by and *analog to digital*, A/D, converter. These can be purchased for most personal computers. It is also possible to use *digital to analog*, D/A, converters. These produce analog signal output that can be used to control scientific equipment.

A block diagram of the essential features of a computer-controlled experimental setup is displayed in Fig. 2.1. When one is interested only in tracking and storing experimental data, experiment control interface can be eliminated, and for operations involving just the control, data acquisition interface is unnecessary.

The software for data collection can he written in a high level-language such as FORTRAN or BASIC or in machine or assembly code.

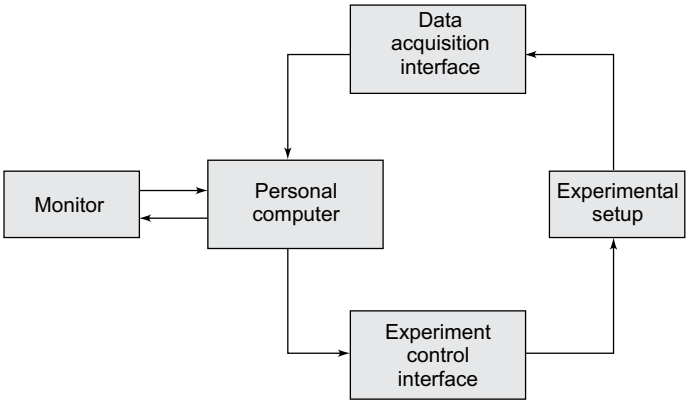

Fig. 2.1 Block diagram of a personal computer-controlled experiment

DATABASE

Storage and retrieval operations are two most important types of information handling procedures in chemistry. A variety of media may be used to store information; however, the most popular is the computer database. A *database* is a collection of information that is stored in the form accessible by computers. A database can be established on several levels, ranging from personal to international, depending upon its intended use. Thus, at postgraduate level, students can be encouraged to replace traditional card-filling indexing of reference with personal computers.

WORD PROCESSING

Personal computers can edit scientific text on a video screen and print the text after all corrections have been made. Further, programs that can check spelling and grammar are now available; besides, speech recognition programs. Such programs may cause a fundamental change in the way reports and assignment papers are prepared and evaluated. Students can be required to submit drafts rather than the final version of laboratory reports and theses, and corrections or addition to these drafts can be made easily, so that the final drafts are well written. Preparation of scientific documents has never been easy. Thanks to the scientific word processors (such as Scientific Word or ScienceWord) or the equation editors (Equation Editor integrated with MS Office, and the stand-alone equation editors such as MathType), preparation of scientific documents is a breeze.

ARTIFICIAL INTELLIGENCE/EXPERT SYSTEM

Artificial intelligence (AI) attempts to build computer systems that possess the characteristics associated with human intelligence such as communication

through languages, reasoning and problem solving. While some researchers are using AI to investigate human reasoning, more pragmatic features of AI programming embodied in expert systems have found application in chemistry, engineering and medicine.

An *expert system* contains organised information covering a specific area of knowledge. The system functions as a consultant for the given area of knowledge and provides an explanation of reasoning on request. Thus these systems are useful in situation where human expertise is not readily accessible. Such systems are currently used to assist in selecting operating conditions for ultracentrifuge and high performance liquid chromatography.

COMPUTER-MANAGED TEACHING

This category concerns the application of personal computers to the 'business' associated with the education process. It includes such categories as the maintenance of students' records, the computer mediated examination of multiple choice answers (question banks), the application of word processing to the preparation of teaching materials and use of graphic facilities of personal computers in the preparation of other audio-visual aids.

A number of journals carry reports on personal computer programs, applications and evaluation including *Journal of Chemical Education* (US), *Education in Chemistry* (UK), *Biochemical Education, Computer and Education, School Science Review* (UK). Several reviews and compilations of articles or list of titles published in educational journals have been published. Besides, the popularity of affordable personal computers has resulted in so called *electronic journals*. American Chemical Society has brought *Journal of Chemical Education: Software*—a publication on DVDs twice a year, compatible with Apple and IBM compatible personal computers.