Computers in chromatography

Richard Patience gives a personal view of how to tackle the growing array of computers being used in chromatography.

How many chemists and biochemists, when faced with a computerized chromatography system, know which button to press and when to press it, but have no idea how the system works? My own first encounter with such a system — a DEC PDPB/e laboratory computer attached to a capillary gas chromatograph/mass spectrometer (GC/MS) — only served to give me a firm conviction that it was all far too complex and that I would never learn to use it. Of course, in time, I did and, what is more, became quite at home with it. But it is one thing to know what to do with a computer keyboard and quite another to know why you do it!

In the mid 1970s, when I first started working with computerized chromatography, laboratory computers were quite rare — and quite large — and generally found only on more sophisticated and expensive equipment, like GC/MS. Temperature and solvent gradients in GC and liquid chromatography (LC) respectively were set up manually. The Pye 104, the Perkin Elmer F17 and the Varian 2700 GCs were all operated in this way, whilst the major LC company, Waters, had the M660 gradient analysis programmer, which has only recently been superceded by the microprocessor-driven M680. 'Data collection' was by chart recorder.

Shortly after I embarked on my research career, there were two major developments. First, in gradient formation, microprocessors began to replace manual control, particularly in GC. Microprocessor-controlled gradients were set up from a small keyboard and parameters such as gradient slope were stored in the memory. Automatic cooling at the end of the run meant that the whole cycle could be preprogrammed and initiated by a single key, but unfortunately you still had to inject the sample.

The second improvement came with the arrival of integrators to calculate peak areas for quantitation. This was a real advantage — both in terms of time and accuracy — even though some early models produced only a numerical strip print out and no chromatogram.

One of the main advantages claimed for microprocessors was an improvement in reproducibility of repeat analyses, in other words an increase in retention times. I have no reason to dispute that, but in my opinion there were, and still are, two disadvantages to microprocessors. The problem with many systems was that, unlike manual units, once started the programme could not be altered without aborting the whole run. This gives a degree of inflexibility that is fine for routine analyses but can frequently be inconvenient when dealing with less well defined samples. What is more, gradient controllers and integrators originally had to be programmed and started separately. The poor user needed three or four hands — one to inject (two for the less steady-handed), one to initiate the gradient programmer and one to start the integrator.

Now, of course, all this has changed and often the whole analysis sequence is completely automatic. The computer boom has reached even HPLC — slower to benefit than GC but rapidly catching up. So, faced with the present array of chromatographic systems, how does the practical biochemist or chemist decide which best suits his or her needs? The mechanical aspects are relatively easy; from practical experience of dismantling pumps and setting up equipment it is possible to assess the mechanics of an HPLC system. But computers — particularly software — are much harder to evaluate without actually using them. If this be the case, then where does one start?

Choosing a system

One tactic is to begin with an assessment of the facilities available from the present generation of computers. Fig. 1 shows a stylized configuration of a hypothetical HPLC system. The controller can be programmed to initiate and control a number of events at preselected times. Furthermore when remote computers or terminals are linked up, the system can be controlled remotely and data can be generated and sent to distant units.

The range of functions offered by individual manufacturers varies considerably, of course. More sophisticated systems include the Varian Vista 402, the Spectra Physics Labnet, Waters' M721 and associated units, the LDC CCM system, Perkin Elmer's Series 4 + Chromatographics 2, Pye Unicam's 4850, Hewlett Packard's 1090 + HP85, Dupont's 8800 and Sentinel, and Gilsen and ACS, which use Apple IIe computers.

Why, though, should such sophistication interest a typical chromatographer? One advantage of microprocessor-based systems has already been mentioned — increased reproducibility of retention times of repeat analyses. However, to me the main advantage lies in the ability to coordinate different units and events from a single keyboard. Gone is the need for three hands to start a run; with fully automated instruments one finger may be enough for dozens of analyses. Of course there are always disadvantages. One of these is cost — around £7,000 to £10,000 at present on top of the HPLC cost. Another is simply the level of complexity of the system itself, which can be confusing for non-specialists, and inevitably introduces a degree of redundancy to the system. Nevertheless, I am sure that the use of computers in chromatography will continue to increase, particularly as they become cheaper. □

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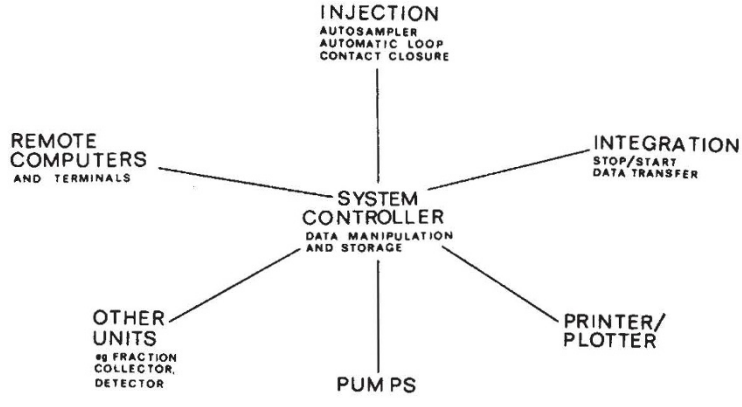

Fig. 1. Stylized configuration of a computerized HPLC system. The controller regulates; (1) injection, which may be by autosampler, automatic loop (user loads loop, controller injects it) or contact closure (user loads and injects, which closes electrical contact and starts controller program); (2) pumps: gradient formation preprogrammed; (3) integration: stop/start or integration and transfer of data to the controller for manipulation, storage on disk or tape, or plotting; (4) printer/plotter; (5) other units, such as a fraction collector or detector; (6) remote computers or terminals.