And Kenneth L. Kizer of Digilab has found that it is possible to study trace amounts of substances—such as pollutants in water and additives in polymers—in most liquids and in many solids.

Another interesting capability of FT-IR permits measurement of the kinetics of high-speed reactions. Spectrums can be obtained in a few microseconds, so that transient intermediates can be identified by their spectrums and reaction rates can be calculated. William G. Fately of Kansas State University, for instance, cites the demonstration that FT-IR can be used to identify a ketene intermediate in the flash photolysis of acetone, even though the reaction is over in about 100 microseconds. Such reactions can be followed with other techniques, but FT-IR is unique in that it provides a complete spectrum of the substrates and intermediates at each stage of the reaction.

Many of the scientists who have initiated investigations of FT-IR have had to use instrument systems they have put together themselves. Now, however, a variety of high quality instruments are marketed commercially. Four companies were promoting them at the Pittsburgh Conference: Digilab; Willey Corporation; Nicolet Instrument Corporation of Madison, Wisconsin; and Coderg S.A. of Clichy, France. The versatility of FT-IR, of course, does not come cheap. Prices range from about $40,000 for the stripped down models to $100,000 or more for top of the line instruments—a far cry from the $3000 price of a small conventional infrared spectrometer. But for many applications that are possible only with FT-IR, those prices are certainly not expensive.

—THOMAS H. MAUGH II

The Intelligent Instrument: Coming, but Not Yet Here

Envisage a wide array of laboratory instruments under the control of their own internal computers, automatically calibrating themselves, taking and analyzing data from large numbers of samples, repeating procedures that gave questionable results, and warning operators or other machines when certain conditions are exceeded. It is a fascinating prospect, the age of the "smart" instrument, but it is not here yet. Indeed, despite continuing rapid developments in the capabilities and economies of microprocessors—the computer on a chip that makes it all possible—there is every indication that it will be at least several years before many such instruments, even in more modest versions, will be available. Still, a few relatively expensive instruments with impressive microcomputer control and data reduction capabilities are being sold now. More are being introduced with either digital controls that are compatible with computer operation or microprocessors that perform limited data-handling tasks, both roadmarks on the way to a fully integrated instrument. Based on the exhibition at the Pittsburgh Conference, here is an impression of where the action is and what the next few years might hold.

Gas chromatographs are leading the way to more computing power for data reduction and instrument control. Four manufacturers now offer an integrator, built around a microprocessor, for use with the analytical instrument. These essentially separate, add-on devices convert chromatography peaks into concentrations and do similar data-handling chores more rapidly and more accurately than was previously possible. Since most such integrators can be used with any chromatograph, they provide a means of upgrading older instruments. Examples include units manufactured by Spectra-Physics of Santa Clara, California, Columbia Scientific of Austin, Texas, and Hewlett-Packard of Palo Alto, California, and are priced from $3000 to $5000.

The future, however, would seem to belong to microcomputers that are, in a sense, built into the chromatographs, so that they interact with the instrument and provide the programmable controls for essentially automatic operation. The most ambitious experiment in this direction is a completely automated chromatograph introduced last year by Hewlett-Packard. Its design is one in which the microprocessor is integral to the instrument and controls every event in the chromatograph, from turning on the oven to injecting samples. The $10,000 unit (an automatic sampler is extra) prints out and plots a complete analytical report. Additional flexibility in control of the instrument was added this year, making it possible for the unit to change operating procedures or data-handling methods during a run—sample by sample, if necessary. To make use of such flexibility, however, a host of run parameters, calibration and analysis specifications, and control options must be chosen in advance. To avoid repeating this extensive programming, the parameters can be saved on a magnetic card and reentered from it. Despite its cost, the instrument is reportedly selling well, which may be evidence that the cost of laboratory technicians and operator errors is greater still.

A somewhat different approach is evident in a new chromatograph made by Varian of Walnut Creek, California, that can be operated either alone or, coupled with a separate microprocessor unit, as an automated system. Here the microcomputer is used more selectively than in the Hewlett-Packard unit to control or to check most chromatograph functions, as well as to handle data reduction; it can also be operated separately as an integrator with other chromatographs. This interactive but separate approach, Varian spokesmen claim, makes it easier for the user to do such things as locating and repairing simple malfunctions without manufacturer assistance. Both the Hewlett-Packard unit and the comparably priced Varian instrument can transmit data directly to other computers and will sound alarms if certain preset parameter limits are exceeded. They are complicated instruments—so much so that Hewlett-Packard is thinking of establishing courses for operators. All manufacturers contacted expect the computing power and the control logic of chromatographs to increase rapidly.

Atomic absorption spectrometry is another area where microprocessors are beginning to appear. A unit from Perkin-Elmer, Norwalk, Connecticut, incorporates one, but uses it for data reduction only; the instrument itself operates with analog controls. A new instrument from Jarrell-Ash, Waltham, Massachusetts, is completely digital and uses its microprocessor as the control center for the unit—automatically recalibrating itself, finding a designated wavelength, and searching for the most intense absorption peak in that spectral neighborhood. As a result, the instrument is said to be relatively simple to use, even for inexperienced operators, and it can be run remotely from a teletype terminal. At a cost of nearly $11,000, it is more expensive than other atomic absorption spectrometers.

Spokesmen for Jarrell-Ash say the greatest difficulty in developing the instrument was programming the microprocessor to perform all its control functions in real time without delaying the instrument unduly, and still do data reduction. Indeed, manufacturers of all microcomputer-controlled instruments are finding that programming—or software—is a major problem, just as it is with larger computers.

There are no commercial infrared or ultraviolet spectrometers for laboratory use designed around microprocessors, although Wilks of South Norwalk, Connecticut, is introducing an infrared instrument for process control applications. (The user must supply all the programming for the microprocessor, an enormous task for the uninitiated.) But microprocessor instruments are probably not far away. Beckman Instruments, Fullerton, California, is offering an infrared spectrometer with digital data output, for easier linking to a computer, and GCA/McPherson of Acton, Massachusetts, is marketing a new, completely digital ultraviolet spectrometer controlled by a separate Monroe calculator with programs on magnetic cards. New Perkin-Elmer ultraviolet spectrometers are also digitally controlled, and hence compatible with computer operation and data reduction, although no computer or calculator is supplied. A word of warning—electrical compatibility with a computer is not sufficient; logical compatibility, often not provided, is needed too.

In spectrofluorometers, one company offers a unit with a microprocessor that is used only for data processing. Two others that now offer digital instruments controlled by minicomputers expect within a year to offer versions with microprocessor control and data handling.

Fourier transform infrared spectrometry (see accompanying article) is another area where minicomputers, now used with the instruments to handle the large volume of data processing, may well be replaced by the combination of microprocessors and special circuits for some applications before very long. Raman spectrometers, which are now available as digital instruments controlled by minicomputers, also appear to be prime candidates for microprocessors.

All in all, one has the impression that the next few years will see a number of new, more versatile, and more reliable instruments based on microprocessors, as users begin to expect more intelligent instruments and manufacturers come to grips with the power and the complexity of computerized analytical devices.

—ALLEN L. HAMMOND

Fluorescence Spectroscopy: Finally of Interest

Fluorescence spectroscopy is one of the easiest, most sensitive, and most neglected techniques of analytical chemistry. Instruments to measure fluorescence have been available since the 1940's, but only in the past 2 years has the use of fluorescence spectroscopy for quantitative analysis been of significant interest to large numbers of researchers. According to Richard Passwater of the American Instrument Company in Silver Spring, Maryland, researchers have been forced to turn to fluorescence by their needs for more and more sensitive measurements. Instrument manufacturers claim that another reason for the burgeoning popularity of this technique is that their companies' efforts to introduce spectrofluorometers of greater sophistication and reliability at lower prices has, apparently, paid off.

This year at the Pittsburgh Conference, investigators reported a wide variety of applications of fluorescence spectroscopy. Clinical investigators, for example, are using it to detect lead poisoning of children. Other researchers are using it to identify the sources of oil spills and to monitor the presence of hazardous substances in the environment. And food companies are using fluorescence spectroscopy, combined with liquid chromatography, to determine amounts of various nutrients in their products in order to comply with labeling requirements. To aid in these applications, the instrument manufacturers this year introduced on their medium-priced instruments features that were previously available only on high-priced instruments.

J. Julian Chisolm and Dean Brown of Johns Hopkins University and Baltimore City Hospital are standardizing a technique, based on fluorescence spectroscopy, that provides a quick, easy, and sensitive way to screen children for lead poisoning. In conjunction with researchers at the Center for Disease Control in Atlanta, they are in the process of introducing their method to clinicians throughout the country.

When children are poisoned by lead, their synthesis of heme is blocked. This causes zinc protoporphyrin, a precursor of heme, to build up and appear in their blood. Zinc protoporphyrin fluoresces (that is, it absorbs light of a specific wavelength and subsequently emits light of a different wavelength) so it can be detected in trace amounts in extremely small quantities of blood. Brown claims that he needs only the blood obtained when a child's finger is pricked to detect as little as 4 nanograms of zinc protoporphyrin per milliliter of blood.

Two symposiums at the Pittsburgh Conference were devoted to the use of analytical techniques for the identification of oil spills, and many of the results reported were based on fluorescence spectroscopy. The Coast Guard, in particular, is developing a way of using fluorescence, along with a few other methods, to "fingerprint" oil spills. They hope to show that they can identify polluters with such accuracy that their results can be accepted by the courts as evidence. In one case, widely reported by the news media last year, the Coast Guard used their fingerprinting technique to identify a tanker that dumped about 100,000 gallons of oil off the Florida Keys.

A crucial aspect of the Coast Guard's oil technique is the use of double-beam fluorescence spectroscopy. Double-beam spectrofluorometers differ from most other spectrofluorometers, which send all their light to one sample chamber, because these double-beam instruments split the input light and send it to two sample chambers. Janet Sheridan and J. Richard Jadamer of the Coast Guard Research and Development Center in Groton, Connecticut, explained their use of the method at one of the symposiums on oil spillage. They place a sample of oil from a spill in one chamber of the instrument and a sample of oil they suspect comes from the source of the spill in a second chamber. The double beam of light passes through both sample chambers, and the fluorescence of both samples is measured. Then, the light emitted when the oil from the suspected source fluorescences is subtracted, by the electronics of the instrument, from the light emitted when the oil from the spill fluoresces. If the oils in the two chambers are the same, the instrument will register no net fluorescence.

Until recently, no spectrofluorometers that met the Coast Guard's requirements of a medium price (about $20,000) and for double beams were available. Double beams were previously available only on