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Data Acquisition and Control Program for Chromatography

M. Keith Hudson
University of Arkansas at Little Rock

William G. Hood
University of Arkansas at Little Rock

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MOSTAFA HEMMATI, Physics Department, Arkansas Tech University, Russellville, AR 72801.

A DATA ACQUISITION AND CONTROL PROGRAM FOR CHROMATOGRAPHY

The recent availability of computers and microprocessors has allowed for considerable improvement in data acquisition and processing from instrumentation. In the last fifteen years, all types of laboratory instruments have been computerized. Initially, dedicated microprocessors were used to control various instrument functions. These early attempts rarely utilized actual data acquisition, normally relying on chart recorders and other data displays common even earlier. However, with the wide availability of more sophisticated microprocessors in the last decade, devices designed to control and acquire data for storage in digital form appeared in the literature and as commercially available systems. Such systems are commonly used with FT-IR spectrometers, mass spectrometers, and gas and liquid chromatographs.

Many instruments available today are the product of recent advances in technology, and represent an evolutionary path which brings together the best components from past and present instrumentation. One such instrument which has recently become available is the Ithaco Model 3981 PC Board Lock-In-Amplifier (Model 3981 Operations Manual, 1989, Ithaco, Ithaca, NY). The 3981 mounts all circuitry onto an IBMPC-AT compatible board which uses the AT bus for all power and data storage needs. This allowed the 3981 to be powerful and have a number of features while being available at low cost. While many instrumental techniques make use of lock-in-amplification, it is of major importance in the field of infrared (IR) spectroscopy due to the inherent noise characteristics of many IR measurements. Many applications in our laboratory are IR spectroscopy based, such as flame infrared emission chromatographic studies, IR emission studies of flames and furnace emissions, and rocket plume IR emissions. While the 3981 LIA worked well with our applications, we found that we needed more advanced software to control, acquire, store, and process data from various experiments. This software had to be generally applicable to all of our projects, rater than be specifically designed for only one application. Having previously written software for a variety of other instruments, including an external LIA (Hudson, Henson, and Hood, Proc. Ark. Acad. Sci., 44:67-70, 1990), the "C" programming language was chosen due to its versatility and speed. Fig. 1 shows data typical of that collected when the LIA and software are used as a FIRE chromatographic data station.

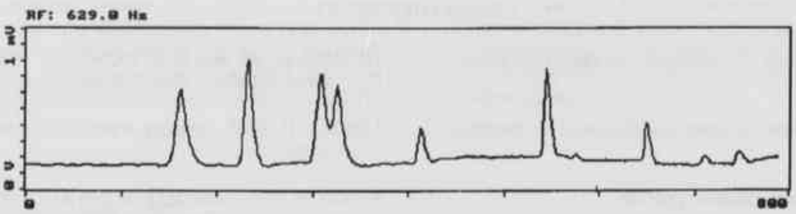
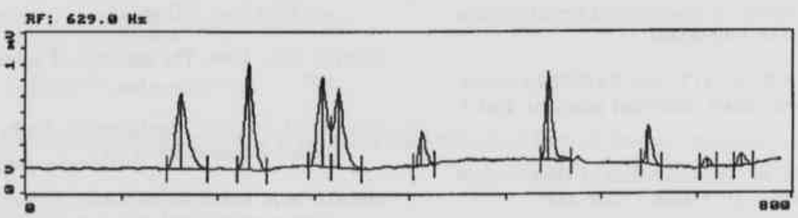


Figure 1. FIRE chromatographic data, emission vs. time.

The 3981 LIA was built to allow the use of up to four separate 3981s in any one computer system. One project of interest to us involves monitoring the IR emissions from two different infrared emission bands, in order to analyze for two elements simultaneously. The use of two IR detectors necessitates two LIAs and software channels to acquire and process the signal. This dual channel feature has been included in the program, and allows the program to be toggled between a one and two board mode. While in the two board mode, data collection is synchronized and data is displayed on the computer screen simultaneously for both channels, in real time. Each channel can be printed, time or intensity scale expanded, or further processing undertaken independently.

After the data have been collected, the software can process the data, automatically finding the location of and the area under the peaks. Fig. 2 shows the previous data after processing for peak location and marked for integration, along with a printed report. The location time of the start and end of a peak is based on the slope of the tangent at each data point. The tangents are approximated by a moving least squares fit of a straight line to segments of the data. The number of data points is user selectable, allowing the use of more points to eliminate noise effects. Integration was accomplished using the trapezoidal rule, as opposed to Simpson's Rule in the previous MBasic program (Hudson, Henson, and Hood, Proc. Ark. Acad. Sci., 44:67-70, 1990). This approach is functionally very similar to that used by commercial chromatographic integrator units, and is comparable in computational time required and equality of results.



Mon Mar 25 09:42:19 1991

Number of samples: 790 Time between samples: 0.10 sec

LIA sensitivity: 1 mV LIA time constant: 333. ms

Reference frequency: 629.0 Hz

Peaks between sample #0 and sample #789: 9

Peak #	Area	Height	Location	Start	End
1	0.0064615	0.00047038	162	148	190
2	0.0065129	0.00065827	233	221	252
3	0.006411	0.00055543	309	295	318
4	0.0057237	0.00048632	326	319	350
5	0.0016025	0.00021317	414	406	427
6	0.0043248	0.00054748	546	537	569
7	0.0016383	0.00023639	650	643	664
8	0.00042138	5.4549E-005	712	705	722
9	0.0006518	7.5709E-005	748	741	760

Figure 2: Processed FIRE chromatographic data showing peak location and integration marking with printed report.

The program offers the user of an Ithaco 3981 LIA a great deal of versatility in acquiring, processing, and storing data. Using the PC bus for data transfer instead of an RS-232 serial line, as is common in other LIAS and associated control programs, allows more speed and greater reliability. Also, the combination of PC, 3981 board level LIA, and this software is economical and easy to use. Those interested in this software should contact the authors.

M. KEITH HUDSON and WILLIAM G. HOOD, Department of Electronics and Instrumentation, University of Arkansas at Little Rock, Little Rock, AR 72204.