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A Microcomputer System for Analysis and Control of Multiple Gas Chromatographs

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Abstract

A microcomputer system for on-line, real-time simultaneous analysis and control of multiple gas chromatographs is described.

The system, incorporating the INTEL 8080 microprosser, is an improved version of an INTEL-8008-based microcomputer system developed by the authors for real-time analysis and control of a gas chromatograph. The new microcomputer system allows many gas chromatographs to share the microcomputer facilities, thus greatly expanding the system capacity at a low cost, without affecting the single-user performance. This new achievement has been made possible by a high-speed central processing unit in the microcomputer and by special-purpose hardware and software developments. A new feature incorporated in the system is a parallel-asynchronous interface for teletype output operations. The interface enables simultaneous analytical and output functions without interfering with the timing of the data sampling process.

Introduction

Gas chromatography is one of the most widely used techniques for quantitative analysis in the chemical industries and laboratories. Recent progress in computer automation has provided the means to solve the problem of automated gas chromatography. Large-scale computer and minicomputer systems for control of gas chromatography as well as simpler, automatic integrators have been previously reported.[1,2,3]

The high cost of the large-scale computer places severe limitations on their use for real-time control of gas chromatography, and limits their use to large laboratories and industries. On the other hand, the development of minicomputers during the last decade has made feasible computer-based gas chromatographic controllers in the medium-sized range, but still at a prohibitively high cost.[4,5] Further reductions in computer size, and recent developments in microprocessor technology have now made available inexpensive microcomputer systems especially developed for local, dedicated process-control applications. These systems have the performance range of the minicomputer-based systems.

The authors have recently developed and tested a microcomputer system for gas chromatography with automatic real-time sampling, data reduction and control features.[6] The present article describes an extension of the single gas chromatograph controller with substantial improvement of that system so as to make possible the simultaneous control and real-time analysis of many gas chromatographs. The new microcomputer system is highly competitive with medium-sized, multi-user systems.[7] New software, at the executive level of control is described for the performance of time-sharing operations of the microcomputer, and augmented hardware components are presented which make possible the multiplexing of microcomputer programs between many gas charomatographs.

System Architecture

The schematic for the microcomputer system for process control and real-time data analysis of multiple gas chromatographs is shown in Figure 1. The microcomputer consists of a series of modular 3" x 5" circuit boards which plug into parallel, multi-pin connectors which are wired to the parallel-wire data and control bus. An INTEL 8080 microprocessor and associated integrated circuits for timing and memory control are located on two printed circuit boards, while random-access memories (RAM) and programmable read-only memories (PROM) are located on other boards for the storage of control programs and special subroutines. An interface board containing a universal asynchronous transmitter-receiver is connected to a standard ASR-35 teletype. A set of digital-to-analog converters (DAC) carry analog voltages to the temperature controllers and column heaters of a series of N gas chromatographs. The detector signals of these chromatographs are individually amplified, selected by an analog multiplexer (MUX), and digitized by a 4 1/2 digit, digital voltmeter which also is connected to a special-purpose interface board. A set of control relays and actuators control the sampling values for each of the gas chromatographs. The relays are operated by a control latch whose status is displayed by a series of light-emitting diodes on the display panel of the microcomputer. The entire microcomputer and power supplies are contained in a volume of less than one cubic foot.

Three of the special-purpose printed circuit boards in the microcomputer are shown in Figure 2. A single analog multiplexer board (Figure 2a) is able to select one of eight analog input signals from different gas chromatographs. The actual analog port selected is set by a signal from the output control board in the microcomputer. Also shown in Figure 2 is the teletype interface board containing the universal asynchronous transmitter-receiver. This circuit board performs self-timed transmission of serial data pulses to the teletype from the parallel-wired data bus of the microcomputer, and allows the data transmission process to occur simultaneously with process control functions in the microcomputer. The 12-bit digital-to-analog converter circuit, also shown in Figure 2, intermittently resets the temperature-controller set-points for each gas chromatograph column.

System Software

The basic software developed for multiple gas chromatograph control and real-time data reduction is shown schematically in Figure 3. The system software is based on a previously described system which acquires data from a single gas chromatograph and which simultaneously performs statistical analysis for noise compensation, start-of-peak detection, end-of-peak detection, peak area integration and baseline skew and scale factor corrections.[6] The program automatically generates a report on the teletype after each peak area integration and correction for base-line skew and scale factor is completed. The input data are converted from BCD format to a three-byte floating-point representation and manipulated in mathematical subroutines in the 3-bytes floating-point representation for high accuracy. The maximum sampling rate with the INTEL 8080 central processing unit (CPU) is 20 Hz, so that ten gas chromatographic signals can be simultaneously handled with a sampling rate of 2 Hz for each. The corresponding sampling rate for the INTEL 8008 CPU is 2 Hz, which limits this CPU to simultaneous control of two gas chromatographs with a sampling rate of 1 Hz for each.

The operating system containing subroutines which control input and output, format, program debug and text editing, is stored on a 1-k PROM board in the microcomputer. The main program, a gas chromatography control program as well as math and statistical subroutines, are stored on two 1-k RAM boards in order to allow flexibility in programming. In addition, one 1-k RAM board is required for data analysis and control of each gas chromatograph connected to the microcomputer.

The software structure of the system is shown in Figure 4.

An executive program controls the time-sharing for different gas chromatographs. This executive program assigns sequential computational subcycles to each gas chromatograph in turn. Process control changes or data analysis for each subcycle is then continued on the memory page assigned to the particular chromatograph. The logic used is the following: The executive program begins the computational cycle by selecting the memory page assigned to the first gas chromatograph (gas chromatographs in Figure 4), then selects the multiplexer channel 1 and the DAC 1 before beginning process control and data computational subroutines. Following these processes is a time period reserved for character transmission to the teletype. Then the executive program switches to the next memory page, next multiplexer channel, and next DAC, and carries out an identical computational subcycle for gas chromatograph No. 2. After completing all subcycles required for N chromatographs, the executive program begins another complete cycle, and continues until an external interrupt signal is received.

A set of control flag values are stored on each data page in order to indicate to the executive program the conditions and subroutines to be used in the next following computational cycle.

Figure 5 shows a simplified timing diagram of the time-share system for sequential control of N chromatographs. The maximum sampling rate decreases with the number of channels monitored. However, the higher speed of the INTEL 8080 microprocessor allows the system to perform up to 20 computational cycles per second even under the least favorable mathematical conditions. This suggests, for example, that up to 20 gas chromatographs could be monitored and controlled at a rate of 1 Hz.

Special Features

The Teletype Interface

The problem of carrying out process control operations and teletype transmission sequentially places a severe limitation on any process controller because of the low speed (12 characters per second) of the teletype. The sampling process is unavoidably interrupted, and useful information is likely to be lost during the teletype transmission time period. When the chromatogram contains merged peaks, or is integrated at relatively high sampling rates, the effect of the time lag for teletype printing could produce fatal inaccuracies in the results. The teletype delay is even more critical in the system described here because of the high computational speed of the INTEL 8080 CPU, with which the sampling period for each gas chromatograph can be as short as 50 ms.

The solution to that problem has been found in the use of a universal asynchronous receiver-transmitter (UART) board (Figure 2) which performs a self-timed parallel-to-serial interface with the TTY. The UART chip is a specialized, LSI integrated circuit which accepts an 8-bit character from the CPU and takes care of the time-consuming (100 ms/char) serial transmission to the teletype (or to a similar serial device. It performs the input function in the same way. In the new software developed for the present system, whenever an end-of-peak condition is detected, the report of processed data is generated intermittently rather than printed at one time on one teletype. The RAM memory board stores the stream of Ascii characters of the data report, and these are transferred one at a time to the output buffer. Whenever the foreground program is idle (waiting for the occurrence of the next sampling time), then the lower priority teletype output routine is called and characters are sent to the UART (while the output buffer is updated), until the ready flag of the real-time clock is raised, as shown in Figure 6. This procedure introduces some delay in the report printing, but continues the sampling process in synchronism with the real-time clock. Note that this feature is strictly necessary while operating many gas chromatographs with the same microcomputer.

Temperature Control

A separate digital-to-analog converter (DAC) is assigned to each gas chromatograph to supply the set-point signal to the corresponding temperature controller, as shown in Figure 1. This method of chromatograph column temperature control has been developed in preference to the more conventional output demultiplexing method to avoid the need of analog signal-hold circuitry and to save the last analog output voltage value while the executive program is serving other gas chromatograph temperature control circuits. Furthermore, it should be noted that in most commercial gas chromatographs the reproducibility of the column temperature control is far more important than its resolution. This fact suggests that a DAC of 8 to 10 bits resolution, now available as monolithic standard dual-in-line package, in the price range of $10, can be efficiently used.

The thermal mass involved in the temperature control of a chromatographic column is generally small, so that the power to be supplied to the heater is also small. The low-power requirement helps to reduce the cost of each temperature controller. Alternatively, with substantially increased software and special hardware, a totally digital closed-loop temperature control can be implemented.[8]

Conclusion

A new microcomputer system based on the INTEL 8080 microprocessor has been developed for control and real-time data analysis of multiple gas chromatographs. The new system incorporates a parallel interface with a universal asynchronous transmitter-receiver for data communication to a teletype, so that input and output operations can proceed simultaneously with analytical calculations and data sampling. Furthermore, additional hardware components and special-function software developments have made possible the real-time analysis of multiple gas chromatograms. The system is capable of simultaneously controlling up to 20 gas chromatographs, each sampled at a 1-Hz sampling rate. This microcomputer system has demonstrated the inexpensive and flexible automation of gas chromatography by microcomputers.

Acknowledgment

The financial assistance of the U.S. Energy Research and Development Agency is gratefully acknowledged.

References

[1] J. M. Gill, "Automation of Gas Chromatography," J. Chromatographic Science, Vol. 7, December 1969.

[2[J. Hettinger, "Comparison of Computing Integrators and Conventional Integrators for Chromatography," Autolab Tech. Bull. 111, 1974.

[3] A. T. Leung and J. M. Gill, "Integration in Chromatography," Research/Development, October 1974, Vol. 25, No. 10.

[4] C. R. Dobbs, C. M. McGinnis and J. G. Peddie, "Interfacing the programmable calculator for chromatographic analysis," American Laboratory, February 1974.

[5] F. W. Karasek, "A Digital Gas Chromatograph," Research/Development, March 1974.

[6] G. M. Bobba and L. F. Donaghey, "A Microcomputer System for Real-Time Monitoring and Control of Gas Chromatographs," Lawrence Berkeley Laboratory, Tech. Rept. LBL-4138, 1975.

[7] J. L. Hendrickson, D. Wallace and F. Baumann, "Multi-User Gas Chromatography Data System with Foreground-Background Processing," Varian-Aerograph, Tech. Bull. 139, 1971.

[8] T. A. Seim, "A Microprocessor Sampled Data Process Controller," Battelle Pacific Northwest Laboratories, Tech. Rept. BNWL-1795, November 1973.

Figure Captions

Figure No.	
1	Overall schematic of the microcomputer systems for control and real-time data analysis of multiple gas chromatographs.
2	Special-function modules of the microcomputer: a) universal asynchronons transmitter-receiver, b) analog multiplexer, c) digital-to analog converter.
3	Schematic flowchart of real-time program for analysis and control of a gas chromatograph.
4	Software structure of the microcomputer.
5	Time sharing for a microcomputer control system with N gas chromatographs.
6	Schematic flowchart of the data sampling subroutine, "Get a sample."

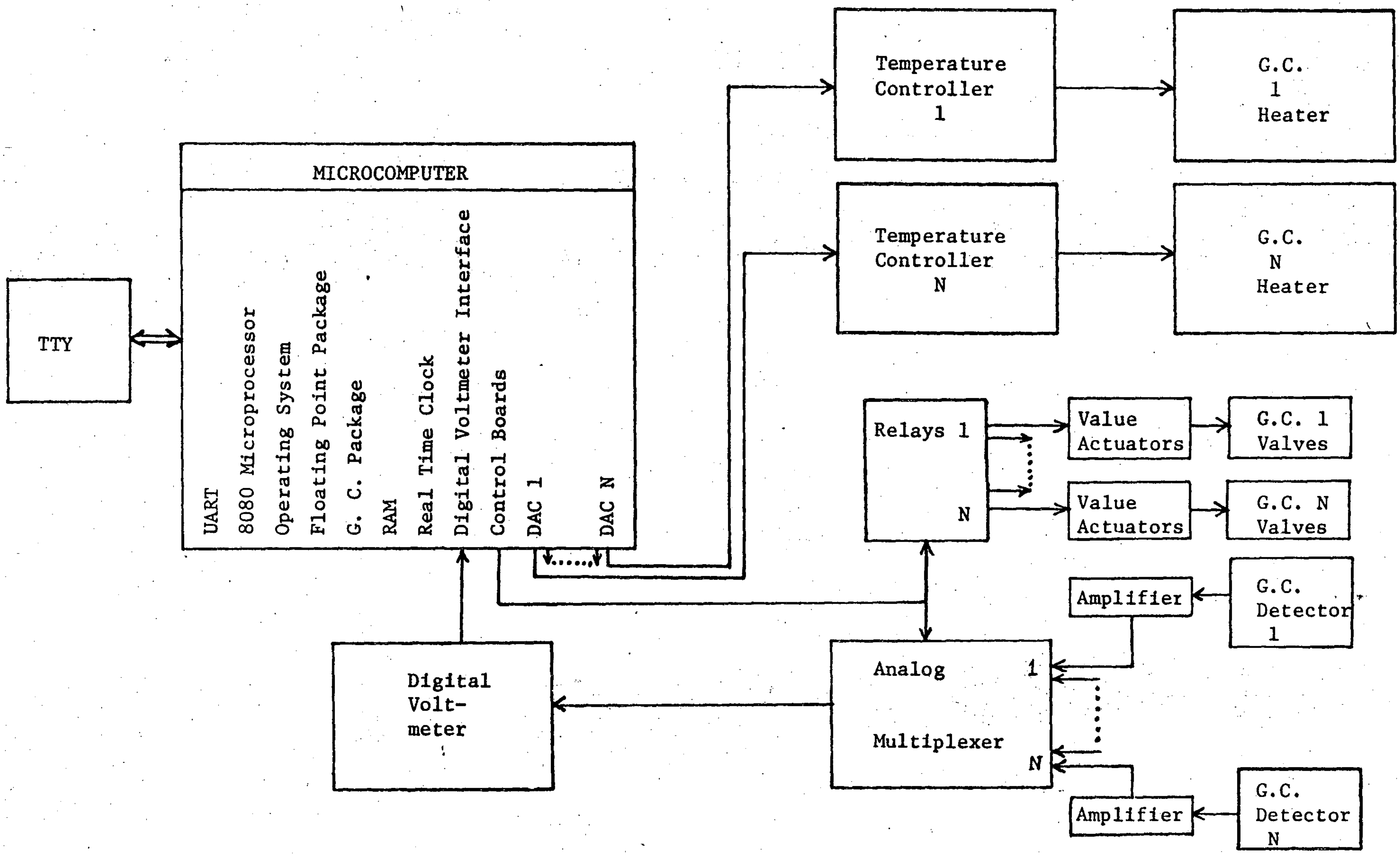

Fig. 1 Overall schematic of the microcomputer system for control and real-time data analysis for multiple gas chromatographs.

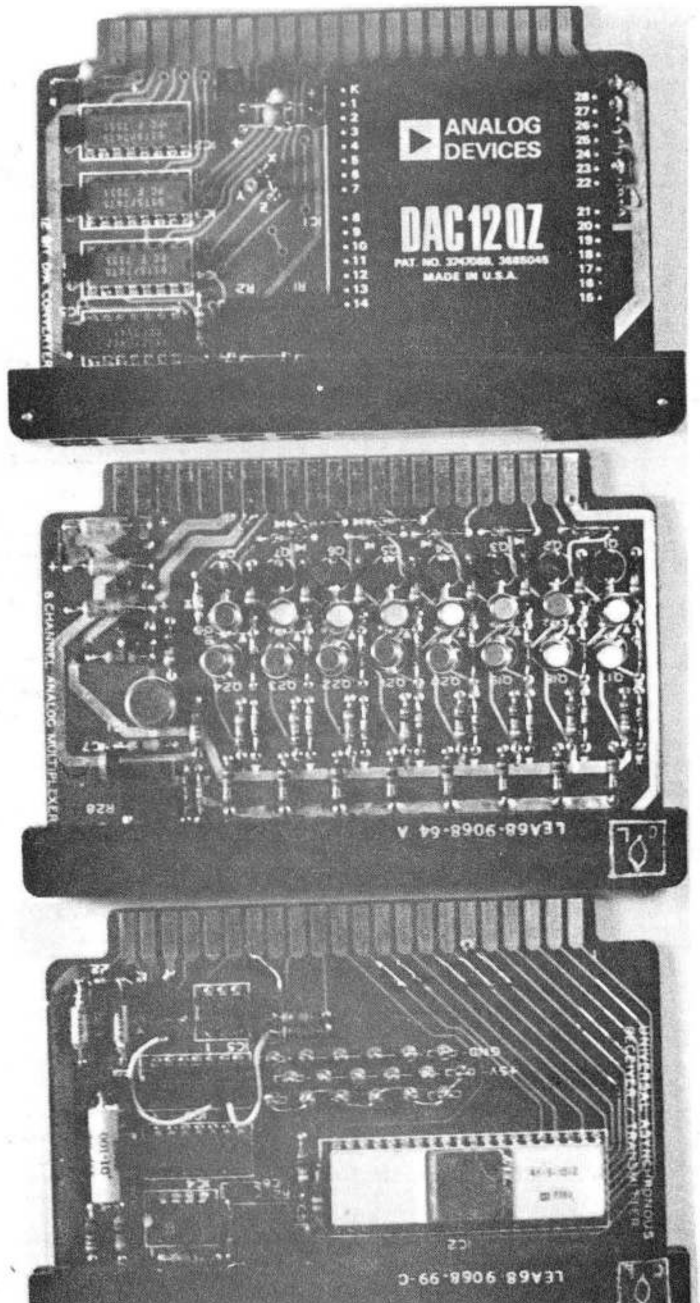

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Fig. 2. Special-function modules of the microcomputer: (a) Universal asynchronons transmitter-receiver, (b) analog multiplexer, (c) digital-to-analog converter.

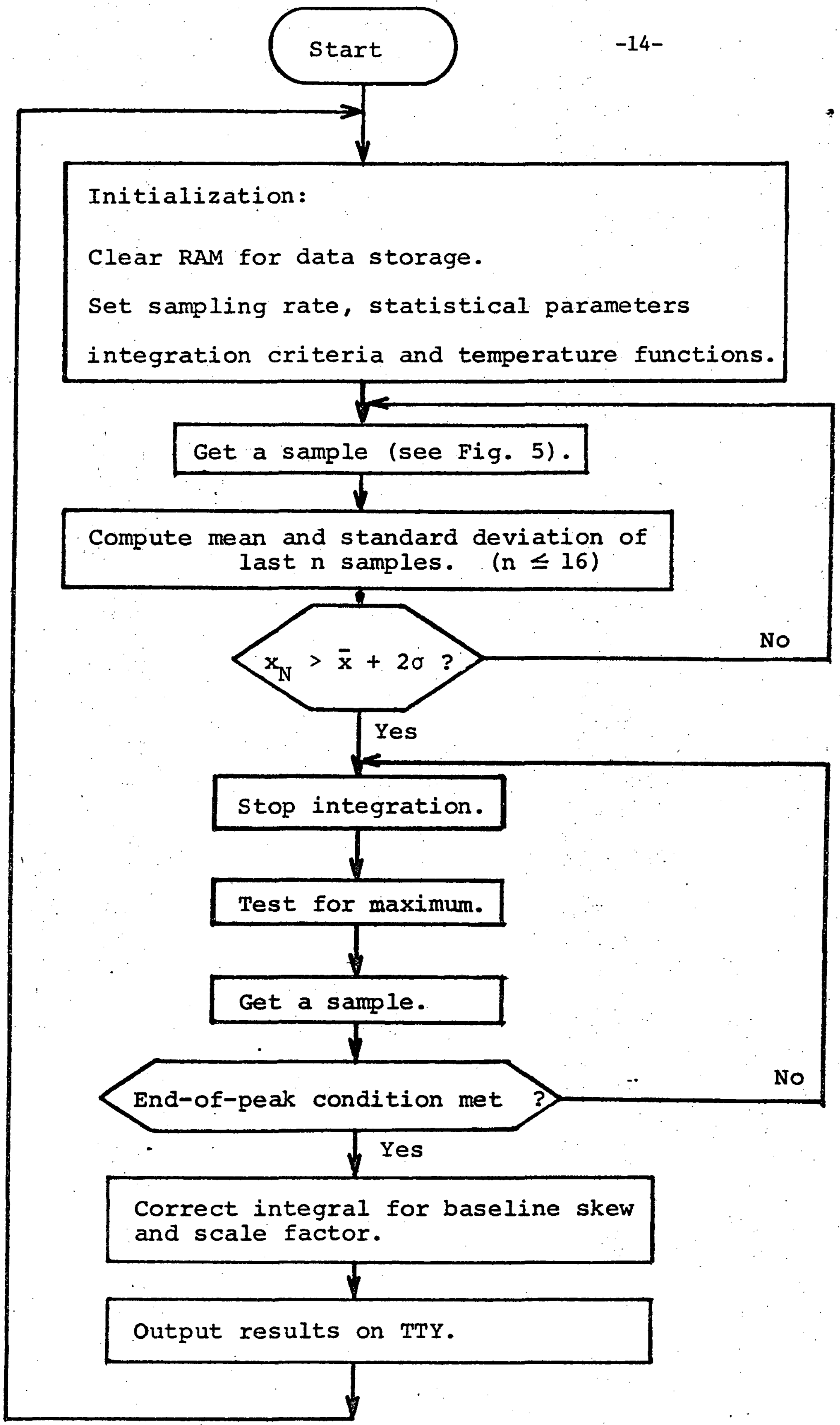

Fig. 3 Schematic flowchart of real-time program for analysis and control of a gas chromatograph.

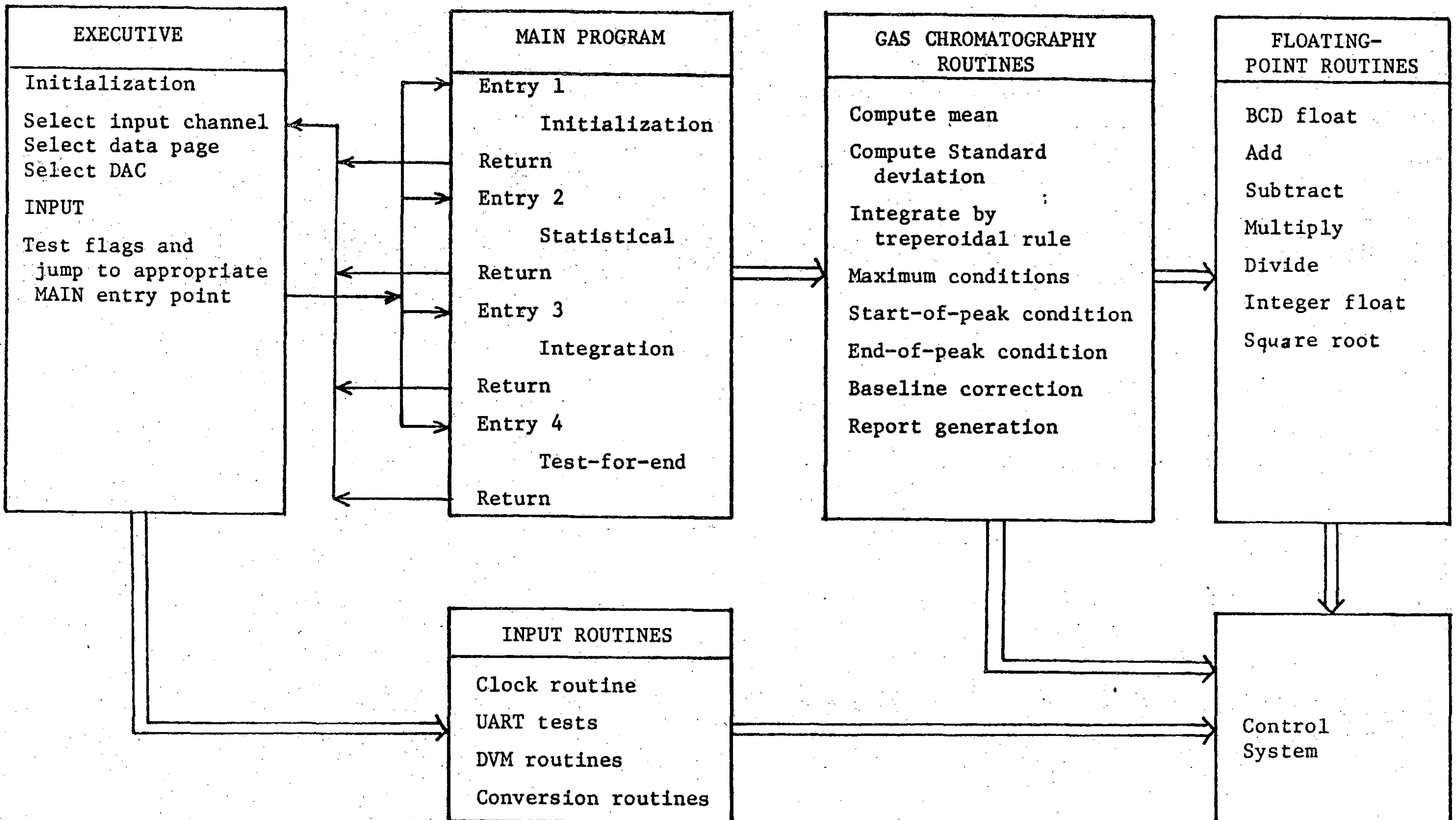

Fig. 4. Software structure of the microcomputer.

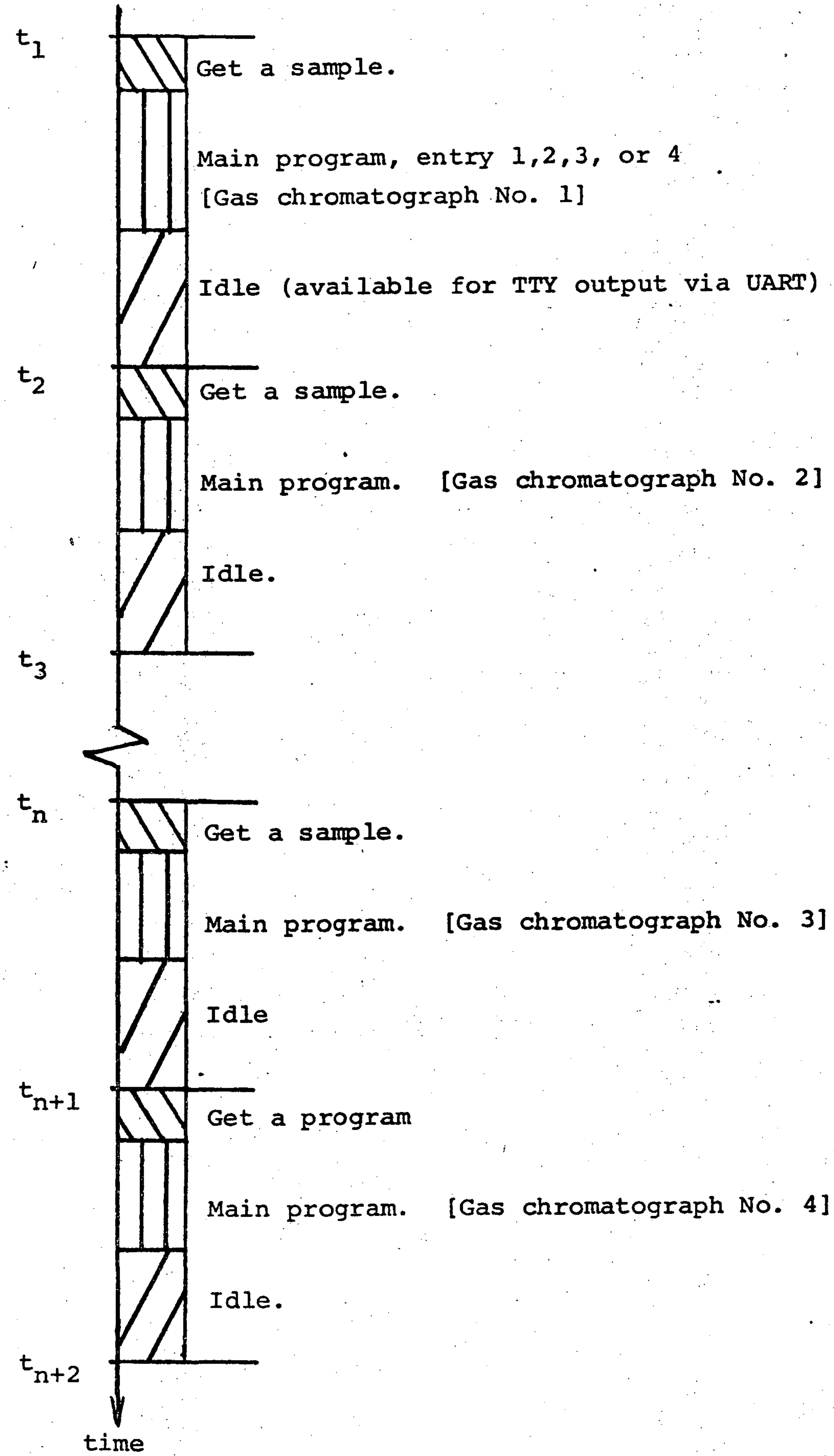

Fig. 5 Time sharing for a microcomputer control system with N gas chromatographs.

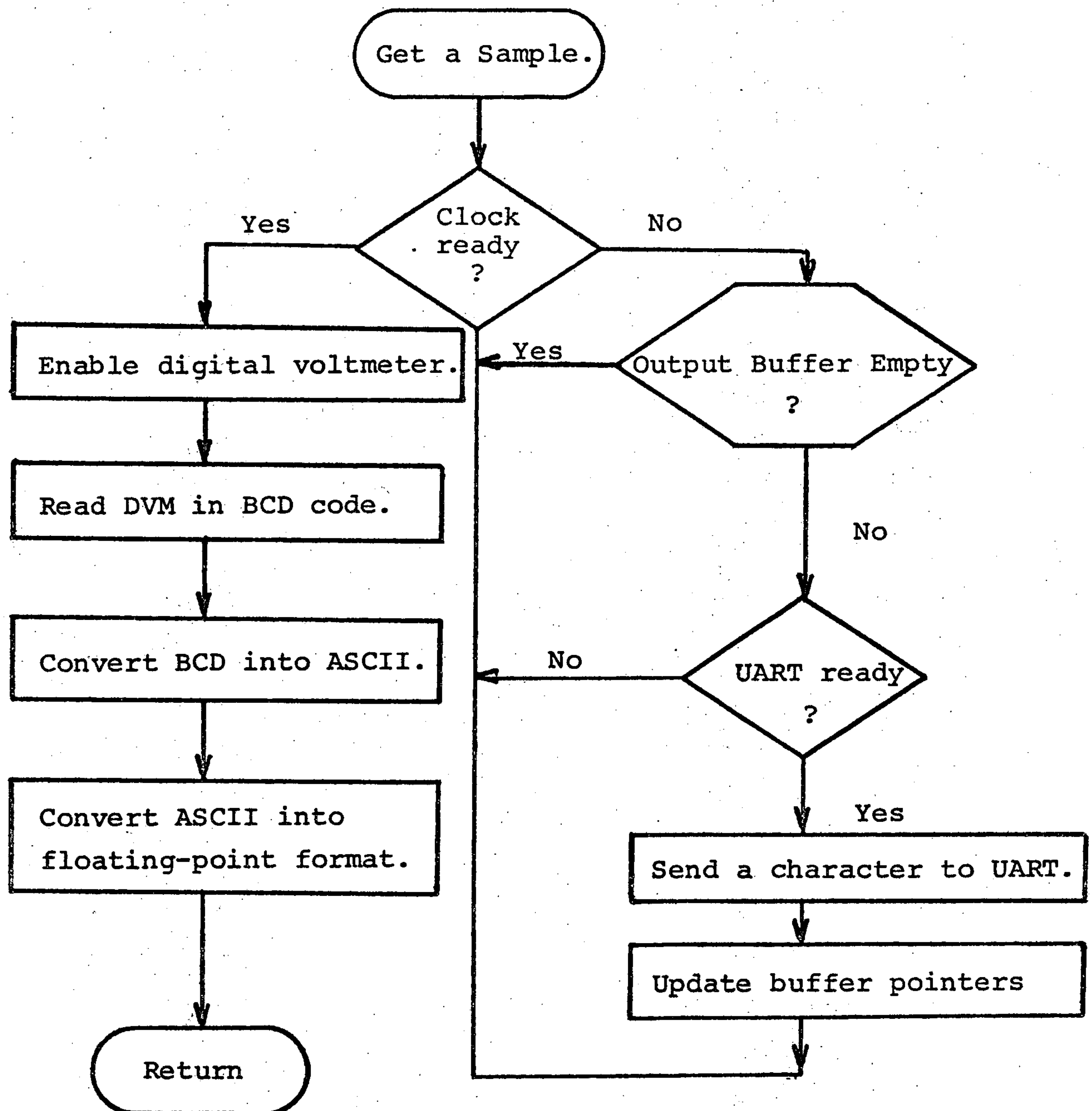

Fig. 6 Schematic flowchart of the data sampling subroutine, "Get a sample."

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