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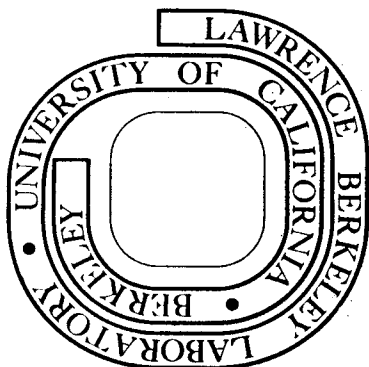
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Microcomputer Systems for Chemical Process Control

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Abstract

Microcomputer systems for application to chemical process monitoring and control are presented. Recently developed modular components are described which expand the utility of 8-bit microcomputers in data-logging and monitoring systems, process-sequence controllers and direct-digital process controllers.

Introduction

Microprocessor-based microcomputers have significant potential for dedicated chemical process control applications. Microcomputer systems are currently capable of making the same impact on chemical process control that large scale digital computers did in the early 1960's [1]. Following the introduction of the PDP-5 and PDP-8 minicomputers in 1963 and 1965, respectively, the cost of industrial computer control equipment has fallen steadily, owing largely to continuous improvements in integrated circuit size and complexity, and in processing cost reduction for semiconductor IC's which have averaged 30 percent per year. Just as the minicomputer has introduced significant flexibility and simplified system design for automatic process control, the microcomputer introduces a unique compactness and modular simplicity to this field, and makes possible a wide range of new applications that previously required a significantly more expensive, dedicated computer.

In this paper the results of the author's current program on microprocessor systems studies are presented to demonstrate and explore the range of feasible microcomputer applications to chemical process control. A primary objective of the author's current program has been to explore applications in technologically important chemical industries, but a secondary objective has been to develop general purpose control systems for use in university-based chemical engineering research. The microcomputer systems described are based on the Intel 8008 and 8080 microprocessors, but interfaces and applications should be compatible and easily extended for use with other microprocessors as well.

Microprocessors

Microcomputer control systems are based on one or several integrated circuits which are the central processing unit (CPU), or microprocessor. The microprocessor is a direct outgrowth of the extensive advances in integrated circuit design and in microelectronic device processing technology. The development of large-scale integration (LSI) of integrated circuits utilizes both metal-oxide-semiconductor (MOS) and novel bipolar technologies. The perfection of n-channel MOS LSI technology has made possible the processing of circuits having higher component densities, lower power requirements and better production yields over the equivalent bipolar circuits [2]. These advances led to the introduction of the microprocessor -- a 4-bit programmable microprocessor on a single silicon chip -- by Intel Corp. in 1971, which, when combined with a memory control, a temporary memory storage and a master clock, constituted an entire microcomputer that originally could sell for less than \$50.00 [3]. During the last four years, over twenty different LSI microprocessors chips, and microprocessor multichip sets have been introduced, with word lengths ranging from 4 to 16 bits [4,5].

Two characteristics of the microprocessor are of fundamental importance in microcomputer control systems development. These are the execution speed or cycle time of the CPU and the word length or number of lines in the data bus. For chemical processes monitoring the cycle time of even the slowest CPU is sufficient since no calculation time is required, whereas for process control applications

with extensive real-time calculations of control algorithms, higher speed microprocessors are required.

The 8-bit microprocessor appears to be a good compromise between bit size requirements for CPU sophistication and data bus size for minimizing the support-system complexity, and a popular choice for use in the development of digital process control systems. The eight-bit word length, although insufficient for the precision required in many chemical process control applications, is a convenient choice for the designer of digital process controllers because of the ease in matching to other available IC components and because of word size-benefits in data transmission applications. An example of an 8-bit microprocessor chip is the Intel 8080 CPU shown in Fig. 1. This chip circuit contains over 5000 transistors, has a 16-bit internal data bus, and a cycle time of 2 μ sec [6].

The current trends indicate that microprocessor-based controllers will soon become more economical replacements for hardwired electronic, as well as electromechanical and pneumatic controllers in many applications [7,8]. Thus, microcomputers have enormous potential for low-cost, dedicated digital process control applications.

Modular System Components

The microcomputer systems currently used by the author in process control studies make use of the bus-oriented, modular design approach developed at the Lawrence Livermore Laboratory [9]. The logic modules are computer elements assembled on 3" x 5" printed circuit boards. These plug into a parallel-wired bin chassis which carries data and control signals in a parallel format between the modules. The basis for the modular design approach was originally set to meet trouble-shooting and service-function requirements of the central processing unit. Because of size and complexity limitations of many microprocessor chips, such functions as memory addressing and input-out controlling must be carried out on supporting electronic circuits. Additional impetus for extending the modular design concept to peripheral functions is the engineering goal of adapting the microcomputer to a large number of specialty applications. The modular design approach makes possible the construction of custom-made, dedicated microcomputers with a minimum of circuit wiring and peripheral control logic design.

The basic 8-bit microcomputer system built around the Intel 8008 consists of the central processing unit and the supporting LSI circuit components on three standard, printed circuit boards. These boards, shown in Fig. 2, are the central processor board, the input-output control board and the memory address board. The three boards supply all of the timing, tri-state buffering and address decoding needed to support the operations of the basic microcomputer.

The central processor board contains the heart of the micro-computer system, the central processing unit, a single bipolar, LSI integrated circuit. In addition, the board contains several low-impedance input driver circuits, two 4-bit input multiplexers with buffers and a 1-of-8 binary decoder. These circuits process and decode the instructions of the central processing unit that are sent to, and received from, other boards in the microcomputer system. The memory address storage board contains four tri-state registers, each with 4 bits, and associated inverters to invert the logic polarity. The memory address storage registers latch and hold the memory address during the memory read and write segments of the timing cycle. This board also contains a programmable read-only memory which stores the lowest numbered page of the operating system program. The input-output control board generates all timing and control signals required by the central processing unit, as well as for the 8-bit memory address bus, peripheral control multiplexers and decoders. The board contains four variable potentiometers for trimming the two timing pulses, which are extremely critical for successful operation.

A basic microcomputer system based on the Intel 8080 microprocessor has been developed on two card modules. The microprocessor module contains the Intel 8080 CPU chip and logic circuits for timing and control signal processing. The 8080 control module contains the clock generator, and generates all timing, control and status signals for the 8080 microprocessor module, and for RAM and PROM memories.

The two card-module set for the 8080 CPU is shown in the lower panel of Fig. 2.

Memory modules have been developed which contain $1K \times 8$ bits of random-access memory (RAM) or alternately programmable read-only memory (PROM). Based on a design developed at the Lawrence Livermore Laboratory, the 1024-word random access memory module contains eight, 1024×1 -bit, silicon-gate, MOS integrated circuits. In the 8008 system up to sixteen 1024-word RAM boards can be separately addressed by the memory address board, while 256 inputs and outputs can be addressed by the 8080 system. Also, by placing a 4-line to 16-line decoder demultiplexer on each memory board to address the eight individual RAM chips, the modules become independent of the slot they occupy in the memory section of the bin chassis. The 1024-word PROM module contains four 256-word read-only memory circuits, each of which can be programmed by a special programming unit which traps charge on the silicon-gate, MOS circuit elements by sending a current pulse through the element. The PROM can easily be "erased" by exposing it to ultraviolet light, which activates the trapped charge and allows it to lead away to ground. A 4-line to 16-line decoder demultiplexer circuit is required to decode the PROM address from the memory address storage board. The decoder is sufficient to access up to eight PROM boards, for a possible PROM memory of 8K of 8-bit words.

Figure 3 shows special purpose modules: a program stack and a dual-restart board are shown from upper left to right; boards containing digital-to-analogue and analogue-to-digital converters are shown at lower left and right, respectively.

The program push-pop stack module has been designed as a peripheral circuit to the 8008-based microcomputer. This module consists of a 16x8 bit read-write memory and an up-down address counter which points to the top of the stack. The module is used in complex, multi-level software applications to store the state of the machine at a program-break point, and to hold the parameters for subroutine calls and returns. The dual-restart board functions as a manual restart of the microprocessors, or as an automatic restart at a stored location in memory. This board is useful in software-debug and also in executing two-level priority interrupts. The analog-to-digital, and digital-to-analog converters (ADC and DAC) are twelve bit resistance ladder-network devices with a sampling time of ≥ 25 μ sec. The DAC has a decoder circuit on the module which sequentially stores the high-order and low-order 8 bits on a tri-state latch connected to the data bus.

Interface Modules

General and special purpose interface modules have been developed for interfacing 8-bit microcomputers to chemical process apparatus. Several circuits were developed to solve typical laboratory interfacing problems [10,11].

A basic problem of interfacing to 8-bit microprocessors, especially those with limited port-addressing capabilities such as the Intel 8008 CPU, is that of bringing a large number of parallel lines to the 8-bit data bus with a limited number of ports used. For interfacing to digital volt meters with BCD output, this problem

has been solved by partitioning the input lines into 8-bit slices, as is shown in Fig. 4. For BCD digital panel meter interfacing, the four lines from each BCD digit are each connected to 4-bit latches. When the interface output line is enabled, the contents of the accumulator is used to selectively enable 8-bit tri-state buffers each connected to two sets of BCD digit lines, thus connecting these lines to the input bus. In this example the lower 4 bits of an output port, OUT 4, are used to control the interface operation. They are latched by D-type flip flops whenever the corresponding output instruction is issued. The bit 0 on the output bus enables the DVM conversion, while bit 1 selects the input of the most significant digit (MSB or 10,000's bit), the sign bit and the "busy flag" bit. The other bits on the output bus select respectively the remaining two 8-bit slices containing the BCD form of the 1000's through the units digits.

This general purpose interface modules has been successful for interfacing the microcomputer to a Newport 2000B 4 1/2 digit panel meter and to a Preston 723A digital voltmeter as well as to a tape recorder for data storage. A module of a similar design enables the transfer of data from the output bus to latches on the input-output module. Software programs have been developed to read the BCD output code of successively latched digits of a digital panel meter, to store a block of data at a rate up to 150 Hz, and to print stored data in several formats on a standard teletype. The digital panel LED's also serve as a status monitoring display [10].

Automatic switch operation is another very typical feature of process control systems, when on-off operation of control equipment such as motors, lights, valves, meters, alarms, etc., are to be under computer control.

A simple switch matrix has been constructed to control six double-throw, single pole reed relays, able to switch currents up to 1 ampere, controlled by a single output port. Two optically isolated solid-state power relays able to switch currents up to 10 ampere are also included. This interface circuit, shown in Fig. 5, also contains 8 LED indicators which indicate the state of the reed relay switches.

Several binary real-time clocks incorporating MOS timing circuits and quartz oscillators have also been developed to provide a time base for process control functions. The designs use 4-bit synchronous binary counters and look-ahead logic for the carry bit, thus assuring fast, simultaneous switching of counter flip-flops and asynchronous read-out of the contents onto the input bus through tri-state buffers. The clocks can be reset using a single bit of an output port [11].

A general purpose keyboard and digital display for manual override of a process monitor is shown in Fig. 6. This keyboard has been used in a digital tape storage system developed for digital data storage. Based on an inexpensive tape deck, this system interfaces to the microprocessor through a general-purpose, 16-bit interface module. Bit errors during the read cycle are reduced by sensing both leading and trailing edges of each pulse. Tape storage is useful

for later statistical analysis or for data storage prior to off-line analysis.

Process Control Devices

Transducer technology is an essential component of automated control [12]. Transducers are needed to convert process variables into digital signals and back again. Schematic forms of a number of input and output devices are shown in Fig. 7.

By far, the primary variables in the chemical process industries are vapor or liquid temperature, pressure, flow rate and quantity (liquid level). Thermocouples produce an analog voltage directly, while pressure transducers and differential pressure transducers are needed to convert strain, or differential strain, respectively, into a voltage, which is then digitized by a thin film resistor -- ladder network and voltage comparator (an analog-to-digital converter).

Output controls most easily implemented in process control are the stepping motor, the solenoid switch, and the solid-state or ac solenoid. These controls are also shown schematically in Fig. 7. The analog output to an electrically controlled valve is representative of control set-points of analog process controllers.

Transmission Links

Cost reduction work in industrial, computer control applications has been centered recently on developing methods of remote digitizing and remote multiplexing of plant variables [13]. Methods of connecting microcomputers to remote equipment has become a concern of the author's present program. Of the many systems developed or proposed for data

"highways," three show the necessary widespread acceptance and standardization needed for industrial acceptance. These are the CAMAC Series Highway [14], the Hewlett-Packard Bus Interface System [15], and the Teletype Interface [16,17]. The Hewlett-Packard transmission path length is limited to 50 feet, making it unsuitable for industrial applications. Also, the teletype system has not gained industrial acceptance in plant use. Consequently, it appears that the CAMAC system, with its major international backing could become the standard for remote data transmission.

Operating Interfacing

Operator interfacing between the process engineer and the computer-controlled process must be present in some form to allow status inspection. The operator interface equipment can consist of display devices, consoles and alarms. The operator-interface equipment available for process monitoring is exemplified by the Automatic Batch Monitor System developed at the Lawrence Livermore Laboratory, the schematic for which is shown in Fig. 8. This system is based on the Intel 8008 microprocessor interfaced to teletype, video display, electronic keyboard, teletype and high-speed reader [18].

Software Developments

A major requirement for implementing microcomputers in process control applications is the development of software programs. Some of the software developments utilized by the author's research group are summarized in Table I. Basic programs for assembling octal coded programs from instruction mnemonics or from a programming language, and for program simulation have been developed by Intel

Table I

Software Developments for Microprocessors
Based on the Intel 8008 and 8080 Microprocessors

<u>Code</u>	<u>Function</u>	<u>Computer</u>	<u>Source</u>
Assembler	Program Assembly from Mnemonics	CDC 7600	1
Simulator	Program Simulation	CDC 7600	1
PL/M	Program Assembly from PLM	CDC 7600	1
Assembler	Program Assembly from Mnemonics	DEC PDP-8	2
Floating Point Math Package	Basic Mathematical Functions	Intel 8080	3,4
ODT	Basic Operating System	Intel 8080	2
ODT-8	Input-Output Oriented Operating System	Intel 8080	4
Research ODT	Research-Testing Oriented Operating System	Intel 8008	4
Assembler	Program Assembly from Mnemonics	Intel 8008	5
Editor	Program editing	Intel 8008	5
Disassembler	Mnemonic Translation of Octal Code	Intel 8080	4
Monitor	Process Monitoring of a Time-Dependent Process	Intel 8008	4
Controller	Monitor and Control Equilibrium Electrochemical Experiments	Intel 8008	4
Titration	Control Electrochemical Titration Experiments	Intel 8008	4
Chromatograph Controller	Control and Real-Time Data Reduction for the Gas Chromatograph	Intel 8008 and 8080	4
DDC Simulator	Direct Digital Control Algorithm Simulator	Intel 8080	4

1. Intel Corporation
2. Lawrence Livermore Laboratory
3. Recognition Systems
4. University of California, Berkeley
5. Control Logic Corporation

Corporation to run on the CDC 7600. The Lawrence Livermore Laboratory has further developed the assembler program for use on the PDP-8, and has developed a basic operating system for the Intel 8080 [19], as well as general-purpose subroutines [20], and a programming guide [21]. Effective operating systems which stress input and output operations have recently been developed at the University of California, Berkeley [22].

A Research-Oriented Operating System

A research and utility operating system has recently been implemented in microcomputer control systems in the author's laboratory [23]. This operating system has special editing facilities for editing and moving program text, for inserting break-points during program-debug, and for listing the contents of all operational registers including the memory address pointers and the accumulator at program interrupts. The system utilizes several operating levels to allow execution of a sequence of program cells by a single teletype keystroke, while performing a different function for the same keystroke in a different operating level.

Floating-Point Mathematical Subroutines

A floating point mathematical subroutine package written by Recognition Systems for the Lawrence Livermore Laboratory has been improved by the author's group. Both 24-bit and 32-bit floating point computation can be performed with input or output in either binary or Ascii format. This subroutine package has been invaluable for statistical and closed-loop process control applications [24].

System Programs

The implementation of microcomputer systems for process monitoring and control requires software programs for input and output device control, for data transmission and control of operator interfaces, and for specialized process control, software programs available to, or used by the author's research group are shown in Table I.

System program packages consisting of the operating system, data processing programs and control programs have been developed for several applications. In general, the program flow chart showing typical process control elements utilization is shown in Fig. 9. Program inputs are the system parameter and structure information values of operational variables and control switch and alarm data. Primary program output functions are data storage, digital and analog signal output. The combination of analog or digital inputs and outputs is required for direct-digital process control. All of these elements are present in several special-purpose microcomputer systems which are described in the following section.

Special-Purpose Microcomputer Systems

The modular approach to microcomputer system design has facilitated the development of special-purpose microcomputer systems for application in chemical process control and in research. Table II summarizes the special features of several microcomputer systems developed in the author's laboratory. All of the specialty modules are functionally compatible with bin chassis for the 8008 and 8080

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Table II

Summary of Special Features of Microcomputer Systems
Developed in the Author's Laboratory

<u>System</u> <u>Features</u>	<u>Process Monitor</u>	<u>Gas Chromatography Analyzer</u>	<u>Electrochemical Experimental Controller</u>	<u>General-Purpose Digital Controller</u>
System				
Hardware:	Tape Deck Control Circuit	Digital Voltmeter Interface	Digital Panel Meter Interface	Digital Panel Meter Interface
	Serial Teletype Interface	Serial Teletype Interface	Serial Teletype Interface	A/D Converter D/A Converter
	Digital Voltmeter Interface	Program Stack	Crystal-controlled Clock Circuit	Real-time Clock Reed Switch Matrix
		Real-time Clock	Control Latch	Control Latch
			Temperature Controller Interface	Solid-State Relays
			Input Multiplexer	High-Speed Reader
Memory:	1K×8 PROM	3K×8 PROM	2K×8 PROM	2 1/2K×8 PROM
	2K×8 RAM	1K×8 RAM	1K×8 RAM	3K×8 RAM
Software:	Input-Output Oriented Operating System	Research-Utility Operating System	Input-Output Oriented Operating System	Research-Utility Operating System
	Tape Drive Control	Floating-Point Math Package	DPM Read Routine	Floating-Point Math Package
	Process Monitor Program	Mean of N Points Standard Deviation	Equilibrium Test Routine	DPM Read Routine PID Control
	DVM Read Routine	Integration; Base Line Correction	Temperature Correction-Reset Routine	Sequential Function Control

microprocessor-module sets shown in Fig. 2, with few modifications, primarily in the backplane wiring of the bin chassis.

Processor Monitor

The process monitor system was designed to record process data and operating status on a continual basis [25,26]. The system requires an operating system which is specially suited to input and output functions. In addition, special subroutines which control read and data store operations are stored on PROM memory, so that no program loading is required, and so that the operating program is not lost in the event of a power failure.

Gas Chromatograph Controller

The problem of operating control of an analytical gas chromatograph for process monitoring has been solved until recently only by manual operation, or by large-scale computer control [27]. A microcomputer system based on the Intel 8008 microprocessor has been developed to perform real-time, on-line data acquisition and analysis of gas chromatographic data, and to control sampling and operation of the gas chromatograph [28,29]. Real-time analysis is achieved by the novel method of interleaving subprograms for the sequential data acquisition and data reduction steps, thereby minimizing memory requirements. The system contains a real-time clock for signal timing, and interfaces to a teletype and digital volt meter. A digital-to-analog converter is used to control the temperature of the gas chromatographic column, while a matrix of relays is able to

actuate sampling values. The system is far superior to the minicomputer integrators [30] in both cost and real-time control capabilities.

The system characteristics are summarized in Table II.

In this control system data acquisition reduction and control are performed cyclically on-line and in real-time, thereby reducing to a minimum the system memory requirements (less than 200 bytes for data storage) [31]. The gas chromatograph detector signal is amplified, then digitized in a digital panel meter at a frequency of 2 Hz for the Intel 8008, or 20 Hz for the Intel 8080. The program cycle is synchronized by the real-time clock, and a research-oriented operating system with special debug programs is stored on PROM. A double-precision, floating-point mathematics package is stored on RAM for statistical measurement of input noise, and for integration. The slowest subprogram is that which computes the mean and standard deviation of sixteen stored values, which requires 0.4 sec with the 8008.

The program flowchart is shown in Fig. 10. In operation, the microcomputer records fifteen readings, then computes the mean and standard deviation of the previous sixteen values for each successive value. When the chromatograph input signal increases by more than 2σ above the mean, peak integration is begun, ending when a 2σ criterion is again reached. The baseline is then corrected for skew, and the peak initiation time, peak and completion time, and the normalized integrated peak area are printed on a teletype. Temperature regulation also is performed after each sampling value. The program is automatically initialized after each peak.

The microcomputer system was experimentally tested in separate process-control and analytical studies. The program behavior was thoroughly tested both by manual input using a special simulation routine and by on-line input to the DVM. The accuracy of chromatographic peak integration was studied with propane-helium and cyclopropane-propane-helium mixtures with known concentrations. Chromatograms were produced with a Beckman GC-2A gas chromatograph with a thermal conductivity detector, whose 0-1 mV output was amplified with an extremely stable, high-impedance differential amplifier. The amplified signal was digitized by a 4 1/2-digit digital volt meter with BCD output. Peak integrals were obtained with the gas chromatographic subprogram, with a normalization factor of unity. The number of data points used in the moving statistical window was 16. Comparison of the real-time analytical method to off-line CDC 6400 computation was achieved by preparing a paper tape storage of the chromatographic data.

The results of the integration of gas chromatographic data are summarized in Table III for propane-helium mixtures. The results show that the present microcomputer integration algorithm gives integrals which are <0.6% lower than those calculated by off-line computer analysis with data smoothing for all samples where the peak area is much larger than the root-mean square integrated baseline noise (denoted by Integral Noise in Table III). Both the microcomputer algorithm and the off-line program are susceptible to interpreting noise peaks as real data, a problem which can be overcome by input filtering.

The differences can be attributed partly to the methods used to detect the integral end-point. In the off-line program with data smoothing, the base-line is computed from the tangent fitted to the smoothed data, whereas in the present microcomputer algorithm the integration is terminated at the first data point where the end condition on slope is met. The tests performed showed that the peak area measured by real-time microcomputer analysis was sensitive to the statistical criteria used whenever the baseline drift was much larger than the standard deviation of the baseline noise.

Table III

Comparison of Analytical Results

Propane Injected (μmol)	Real-Time Microcomputer Analysis			Off-Line Analysis		
	Standard Deviation of Baseline Noise (mV)	Integral Noise (mV-s)	Peak Area (mV-s)	Standard Dev. of Smoothed Baseline Noise (mV)	Peak Area (mV-s)	Difference (mV-s)
856.19	5.99×10^{-4}	0.047	109.740	3.69×10^{-4}	110.075	0.335
369.77	7.03×10^{-4}	0.056	109.980	3.34×10^{-4}	110.658	0.678
321.93	1.51×10^{-3}	0.071	40.852	3.69×10^{-4}	40.958	0.106
0.20	8.80×10^{-4}	0.004	0.003	3.69×10^{-4}	0.196	0.192
0.10	5.78×10^{-4}	0.004	0.009	3.69×10^{-4}	0.010	0.010
Noise	8.17×10^{-4}	0.003	Not Detected	3.69×10^{-4}	0.014	0.014
Noise	5.54×10^{-4}	0.002	0.007	3.34×10^{-4}	Not Detected	0.007

Electrochemical Process Controller

A microcomputer system for the control of electrochemical processes was constructed around the three-module 8008 microcomputer. Shown in Fig. 11; this system has been thoroughly tested over a 15 month period in laboratory-prototype electrochemical processes involving high-temperature galvanic cells.

The features of this system are outlined in Table II. The input-output oriented operating system and mathematics subroutines are stored in 2k×8-bit PROM's while operating programs and data storage are stored in RAM. System data is recorded on a standard teletype.

The system control functions are carried out by means of a control latch and an auxiliary 5 volt power supply. By storing an octal control word in the latch buffer, two-wire transmission lines carry 5V, d.c., control signals from each of sixteen decoded (normally-on and normally-off) control words.

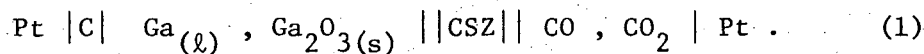
A schematic of the microcomputer system developed for electrochemical studies is shown in Fig. 12. The control-latch output lines are connected to read switches in a temperature controller whose setpoint can be altered by driving a stepping motor. Process control signals from a thermocouple and from a high temperature, solid-state galvanic cell are amplified by high-impedance electrometer amplifiers and connected to a 4 1/2 digit panel meter via a demultiplexer.

A simplified software program for equilibrium, high-temperature galvanic cell studies is shown in Fig. 13. This program has control

subloops for temperature incrementing and control, and for sensing high-temperature equilibrium for automated, experimental control. This control program has been operated successfully

in a graduate research program on the thermodynamics of compound semiconductors [32-36].

Electrochemical studies of the free energy of formation of group III oxides, and of component activities in compound semiconductors were automated using the microcomputer system. The study of the free energy of formation of gallium sesquioxide is representative of these studies. The solid-electrolyte galvanic cell employed in measuring the free energy of formation of $\beta - \text{Ga}_2\text{O}_3$ can be represented schematically as



The equilibrium partial pressures of oxygen in the two electrodes are related to the cell potential E , by the Nernst equation:

$$E = (RT/4F) \ln \{P(\text{O}_2, \text{CO} + \text{CO}_2) / P(\text{O}_2, \text{Ga}_{(\ell)}, \beta - \text{Ga}_2\text{O}_3)\} \quad (2)$$

In this equation, $P(\text{O}_2, \text{CO} + \text{CO}_2)$ indicates the oxygen fugacity of a $\text{CO} - \text{CO}_2$ buffer gas mixture, $P(\text{O}_2, \text{Ga}_{(\ell)}, \beta - \text{Ga}_2\text{O}_3)$ represents the equilibrium partial pressure of oxygen over a $\text{Ga} + \text{Ga}_2\text{O}_3$ mixture, R is the gas constant, T is the thermodynamic temperature and F is the Faraday constant. The $\Delta G_f^0(\beta - \text{Ga}_2\text{O}_3)$ values calculated in the present study from the experimental data

showed excellent internal consistency with a standard error at 1000°K of only $\pm .312$ Kcal/mole, owing to the effectiveness of the microcomputer control program. On comparing the results with those obtained from other emf measurements, however, one finds an apparent discrepancy in both the standard enthalpy and entropy as shown in Fig. 14. In particular, the standard entropy found in this work was well above that reported in several previous studies. On the other hand, the absolute values of $\Delta G_f^{\circ}(\beta - \text{Ga}_2\text{O}_3)$ show relatively good agreement but differ markedly in the temperature dependence from earlier studies, as shown in Fig. 14, as several typical sources of error have the effect of lowering the value of $-\Delta G_f^{\circ}$.

Because of differences in the results of this study as compared to results of previous emf studies and also of the availability of good calorimetric data, a "third law" calculation was carried out. The results of this calculation are shown in Fig. 15, where $\Delta H_{f,298.15}^{\circ}$ is the standard state enthalpy of formation of $\beta - \text{Ga}_2\text{O}_3$. The calculated results for $\Delta H_{298.15}^{\circ}$ are compared to the data of Mah, determined by direct combustion calorimetry, and to the value of Shchukarev, Semerov and Rat'kovskii obtained by isothermal evaporation studies. The close agreement between the data derived from this study and the findings of the latter two different methods tend to support the experimental value for $\Delta H_{298.15}^{\circ}$ of $-261.9 \text{ kcal}_{\text{th}} \text{ mol}^{-1}$. In an early part of the study where microcomputer control was not used, the statistical variations in the data were considerably greater, and there was a lack of agreement with calorimetric data [37]. On the other hand, the direct measurement of $\Delta G_f^{\circ}(\beta - \text{Ga}_2\text{O}_3)$ performed

in this study showed much better consistency with the calorimetric data than did the data from earlier emf studies, when compared with "third law" calculations.

A study of the component activities in the gallium-antimony system was also carried out with and without microcomputer control of the electrochemical experiment [36, 37]. When activities in the liquid phase were measured without microcomputer control, considerable time delays overnight were unavoidable, and the possibility of contamination or oxidation of the electrodes was significantly greater than when the experiments were under microcomputer control. When experiments were controlled by an Intel 8008-based microcomputer, the cell emf was monitored automatically as the microcomputer reset the temperature in increments of $\sim 20^\circ\text{C}$ over a fixed range after complete equilibrium had been reached at each temperature. At least two cycles of the temperature range of interest were completed in order to reveal hysteresis effects in the measurement. After each experiment the absence of side reactions in the electrodes was confirmed by x-ray diffraction analysis [34].

Based on the results of this study, several conclusions can be made. The accepted liquidus temperature in the Ga-Sb system is very consistent with the measured activity data with and the enthalpy data of Predel and Stein and the accepted value for the heat of fusion. Owing to the good consistency of experimental measurements, component activities could be determined with high accuracy. The accepted melting temperature of GaSb is in excellent agreement with the

value derived from our experimental value and with the derived values for the enthalpy of mixing, whereas an ideal solution model gives a large difference between the accepted and calculated liquidus temperature. This finding lends support to the consistency and accuracy of the present results, and to the utility of experiments automated with microcomputers.

General-Purpose Process Controller

The most recent microcomputer system developed by the author is a general-purpose controller for direct-digital control applications. This system, shown in Fig. 16, has digital-to-analog converters and general purpose, external control boxes containing double-pole, double-throw read switches, and solid-state, optically-isolated power relays supplying 115V, at 10A. The system characteristics are outlined in Table II. A photograph of the general-purpose process controller is shown in Fig. 7. The process controller is currently applied to the study of direct-digital control of a tube-and-shell heat exchanger.

Direct-Digital Control Algorithms

Direct-digital control algorithms are currently under investigation as to their performance and limitations in applications of process control by microcomputer. The control system chosen are tube furnace and a tube-and shell heat exchanger, because these are basic, yet a generally representative apparatus of the chemical industry. Also, heat exchanger dynamics, and the performance of control algorithms has been extensively studied [38].

The design of heat exchanger controllers requires that dynamic relationships between fluid flow rates and temperatures be known in order to simplify the analytical equations of optimal control. In this study, transfer functions were based on linearizations of transport equations expanded about the operating point [39]. The control algorithm used is the three-mode, proportional-integral-differential (PID) control algorithm. The time-dependent control signal for a digital control error e_n is given by

$$u_n \approx k_1 e_n + k_2 \sum_{i=0}^n e_i + k_3 (e_n - e_{n-1}) \quad (3)$$

The integral is approximated by the discrete triangular-hold difference equation and the derivative by a two-period average, so that the discrete control response at the n -th sampling interval of length T is now given by

$$u_n = k_1 e_n + 0.5Tk_2 \sum_{i=0}^n (e_i + e_{i-1}) + 0.5T^{-1}k_3 (e_n - e_{n-2}). \quad (4)$$

The sampling rate could be adjusted by factors of two up to 8 Hz with a real-time clock. The control performance is critically dependent on the magnitudes of the coefficients in the above equation, and adaptive control methods appear to be of significant usefulness. Also, for ramp temperature changes, it has been found expedient to remove the integral feature of the digital control algorithm.

Numerous, more advanced direct-digital control algorithms have been developed for the process control of heat exchanges using minicomputers. Unbehauen and coworkers have investigated the memory storage requirements, speed and accuracy of a number of control algorithms [40]. These are summarized in Table IV and compared to the basic proportional-integral-differential control algorithm. The comparison shows that several of the algorithms are far too complex for expeditious implementation with microcomputer controllers. The deadbeat-response control and the adaptive control with linear filtering require significantly large memory storage, while both the nonlinear half-proportional control and the deadbeat-response control algorithms require relatively long computation times, compared to the simpler, proportional-integral-differential control algorithms. Implementation of control algorithms requiring matrix inversion is limited primarily by memory storage and software storage requirements. On the other hand, the proportional-integral-differential control algorithm is found to be relatively easily programmed, has high software speed, and exhibits relatively low overshoot under the application of a step-input disturbance.

Table IV

Comparison of Direct Digital Control Algorithm Performance

Control Algorithm	Continuous Transfer Function, Form or Basis	Special Computational Requirements Features	Relative Memory Size Required [40]	Relative Computing Time Required [40]
Proportional-Integral-Differential	$G_R(s) = K [1 + (T_I s)^{-1} + T_D s (1 + T_V s)^{-1}]$	Integration.	100	100
Cascade Control (PI with inner-loop controller)	$G_R(s) = K [1 + (T_I s)^{-1}]$	Integration: Software complying to an inner-loop controller.	175	100
Nonlinear Half-Proportional	Three-part control based on error trend.	Storage of n discrete control errors.	150	500
Deadbeat Response Control	Discrete control signal of n-th order	Storage of n discrete control signals. Solution of n+1 synthesis equations.	325	1000
Optimum State Feedback	Minimization of quadratic Performance Index.	Matrix inversion solution of the matrix-Riccati equations. Integration of matrix product.	270	100
Compensator Control	N-th order broken rational transfer function.	Solution of a linear system of simultaneous algebraic equations.	290	100
Adaptive Control with Linear Filtering (3rd Order)	$G_S(s) = \frac{K}{1 + as + bs^2 + cs^3}$	Third-order differential equation molding by recursion relations.	650	80

Industrial, Chemical Process Control

Microcomputers have not yet been utilized in industrial plants for direct-digital control applications, as was predicted some years ago. The experience of the recent few years has shown, however, that the microprocessor-based controller is becoming economically competitive with other controllers for direct-digital control applications in chemical plants [41].

One of the first industrial, process control applications of a microcomputer was that developed by Seim, for the control of a brazing process [42]. In this application, a three-mode PID control algorithm was used to control the induction-heated brazing process. Although the control algorithm was initially insufficient for the application, only a software change was needed to meet the application requirements. This experience demonstrates the unique flexibility of a programmable process controller.

Mini-versus Micro-controllers

With microcomputers available with sizable RAM and PROM memories at low cost, there is ample reason to expect the microcomputer to become cost-competitive in the process control applications. Before the development of the microprocessor CPU, it was economically feasible to use computer control only on the largest industrial processes, such as in paper mills and oil refineries. With the recent trends in cost reductions of computer components, the decentralization of computer control becomes possible, with micro-controllers designed for a specific plant operation, while a central terminal overviews the operation of remote microcontrollers.

A basic limitation of the microcomputer controller in complex process-control applications is that software must be developed for each application. One of the most promising new developments which overcomes software limitations is the KD11-F microcomputer module developed by Digital Equipment Corporation for the LSI-11 microcomputer. The KD11-F module requires a four chip microprocessor processed by n-channel MOS technology. A single control chip is used for decoding mechanisms and for generating microinstruction addresses from macroinstructions while two mask-programmable ROM chips allow the microprocessor to simulate the macroinstruction set of over 150 machine instructions in the PDP-11-40 minicomputer. Thus, the LSI-11 microprocessor can utilize the extensive software which has been developed for the PDP-series of minicomputers.

Microcomputers still may not replace all analogue controllers in chemical plants. Most current, large-scale, computer-controlled chemical plants require conventional analogue backup of direct-digital control equipment, so that in the event of a central-computer or transmission-line failure, the plant operation can be maintained by the backup system. As a consequence, it is unreasonable to expect complete replacement of analogue control equipment by microcomputers. Nor can microcomputers completely replace the central computer, for a central computer is still useful for performing the computation of complex mathematical control algorithms, such as matrix inversion, as well as for supervision of highly decentralized, locally dedicated special-function controllers. Thus, it appears that a hierarchical structure of plant automation can be expected to offer the highest reliability for process control in large plants. This hierarchical control structure is anticipated to be the future trend in microcomputer deployment in the chemical process industries.

Conclusion

Microcomputer systems offer the unique advantages of cost-competitive process control, reliability and programming flexibility. The modular approach to microcomputer system structure, utilized in the author's microcomputer systems, makes possible the construction of special interfaces and control circuits which enables custom-fitting of the microcomputer controller to a given process control application. Special-purpose microcomputer systems have been developed for process monitoring, gas-chromatography control, electrochemical process control and general-purpose control applications. The microcomputer occupies a unique place in the hierarchy of chemical plant control, and is anticipated to fill an ever-increasing role in process control instrumentation.

0 0 0 4 3 0 8 5 7 1

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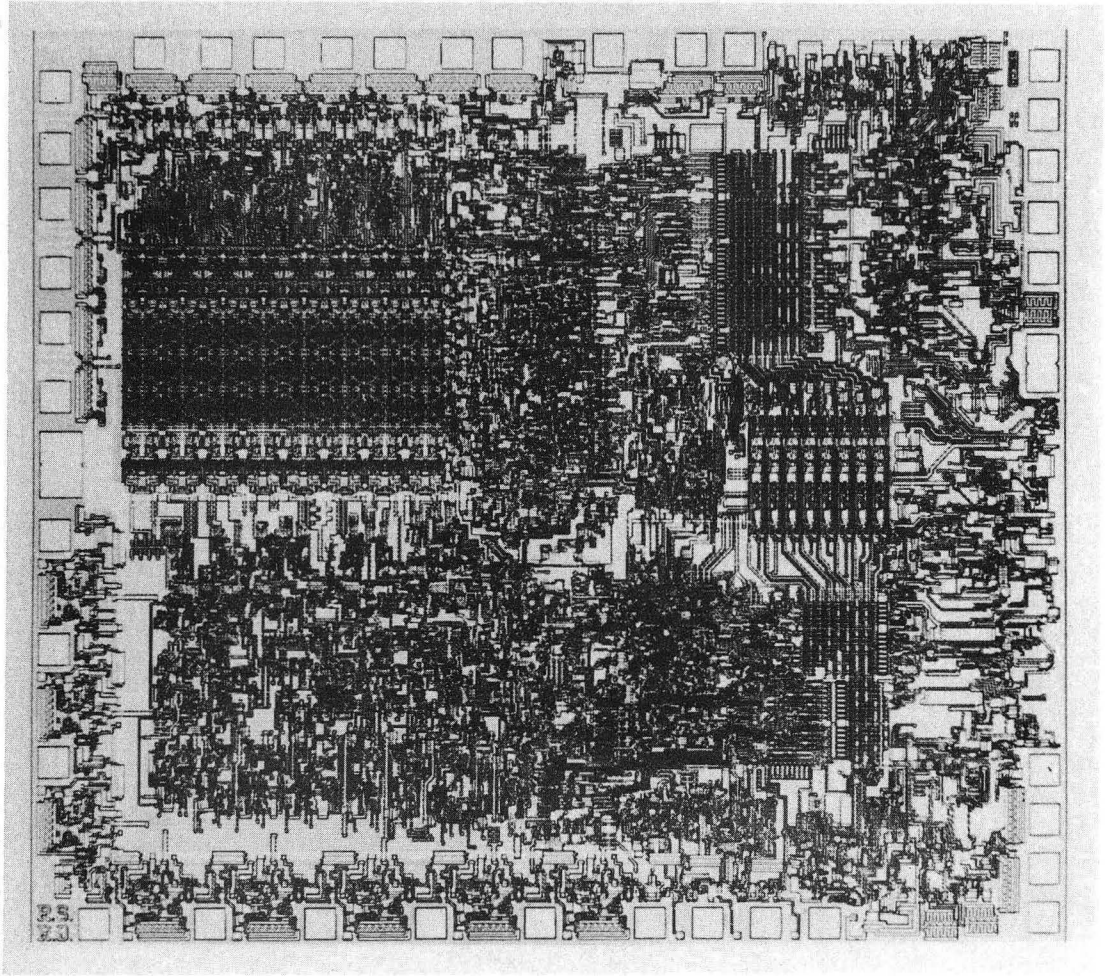
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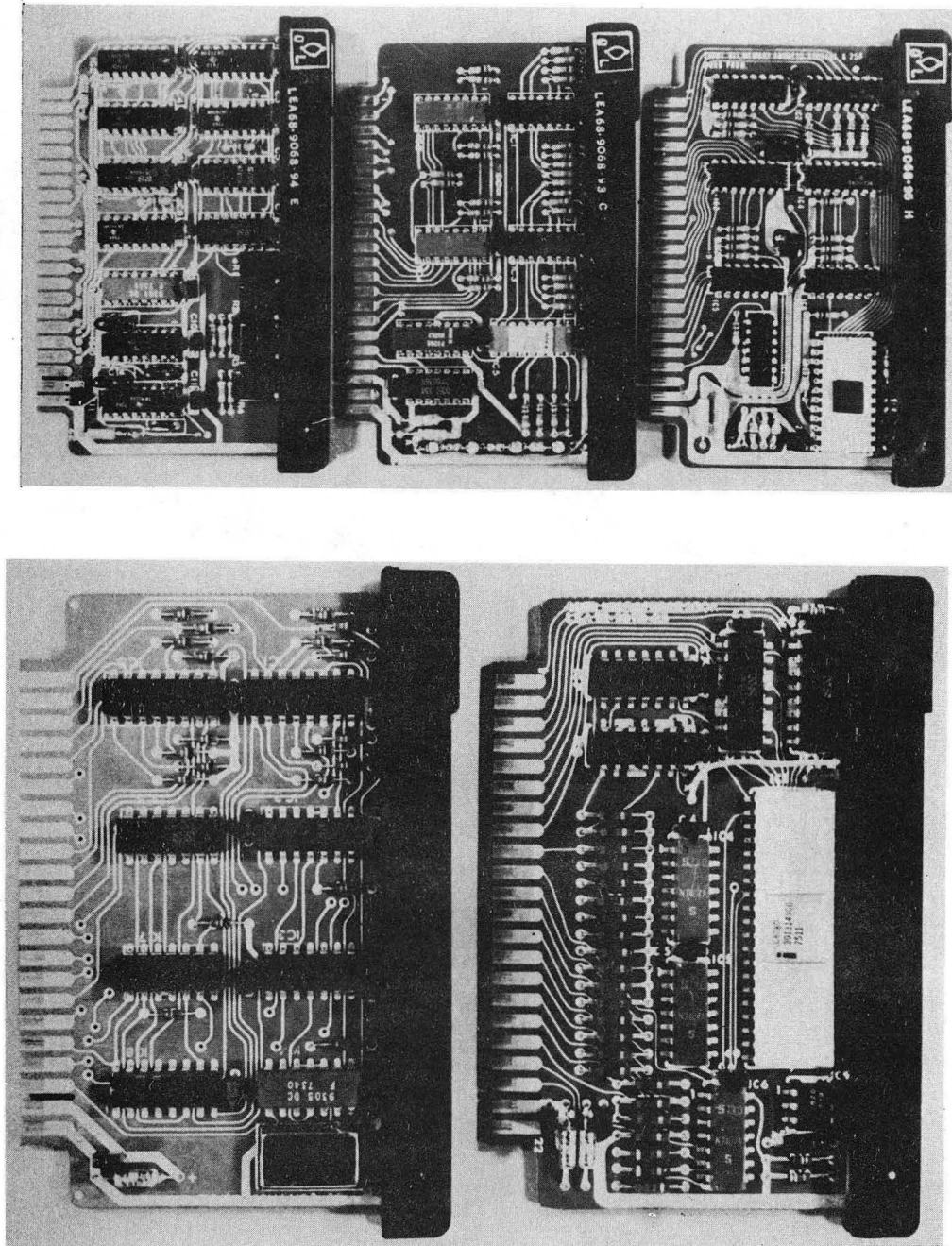
- Fig. 1 The Intel 8080 CPU contains over 5000 transistors on a .164 by .190 inch silicon chip.
- Fig. 2 Modular circuit boards for microcomputers: Upper: Three-board set for Intel 8008-based microcomputers, (left to right: input-output control, microprocessor, and memory address storage and read-only memory). Lower: Two-board set for Intel 8080-based microcomputers, (left to right: control boards, microprocessor).
- Fig. 3 Special-function modules: Upper left: program stack. Upper right: dual-restart board. Lower left: digital-to-analog converter. Lower right: analog-to-digital converter.
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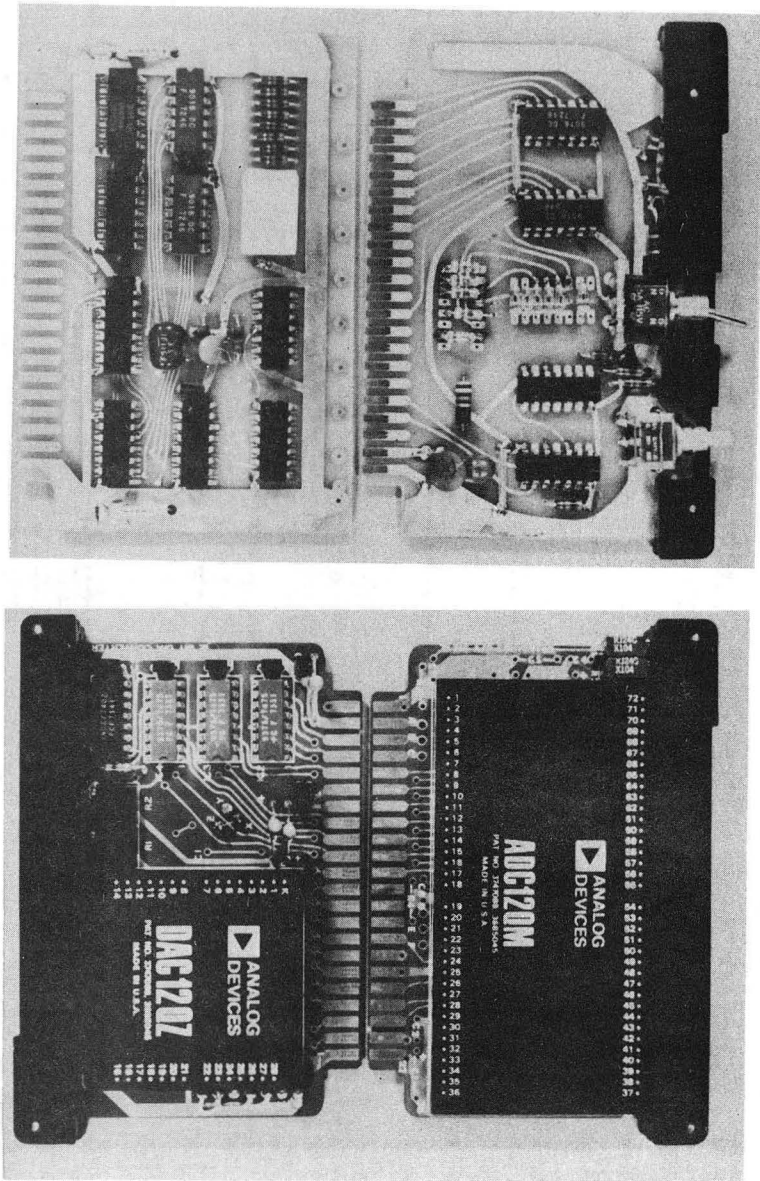
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Fig. 1 The Intel 8080 CPU contains over 5000 transistors on a .164 by .90 inch silicon chip.



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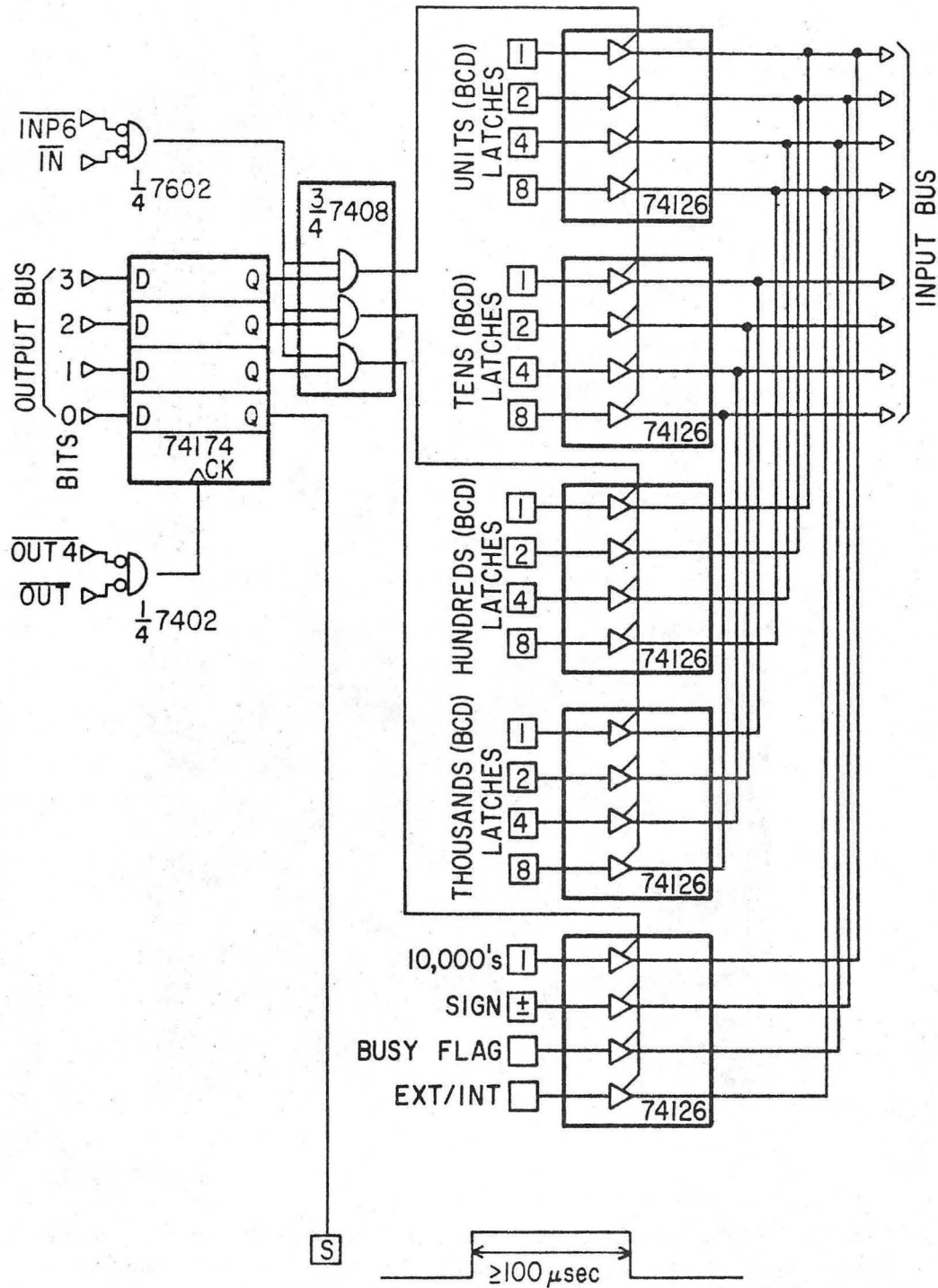
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Fig. 3 Special-function modules: Upper left: program stack. Upper right: dual-restart board. Lower left: digital-to-analog converter. Lower right: analog-to-digital converter

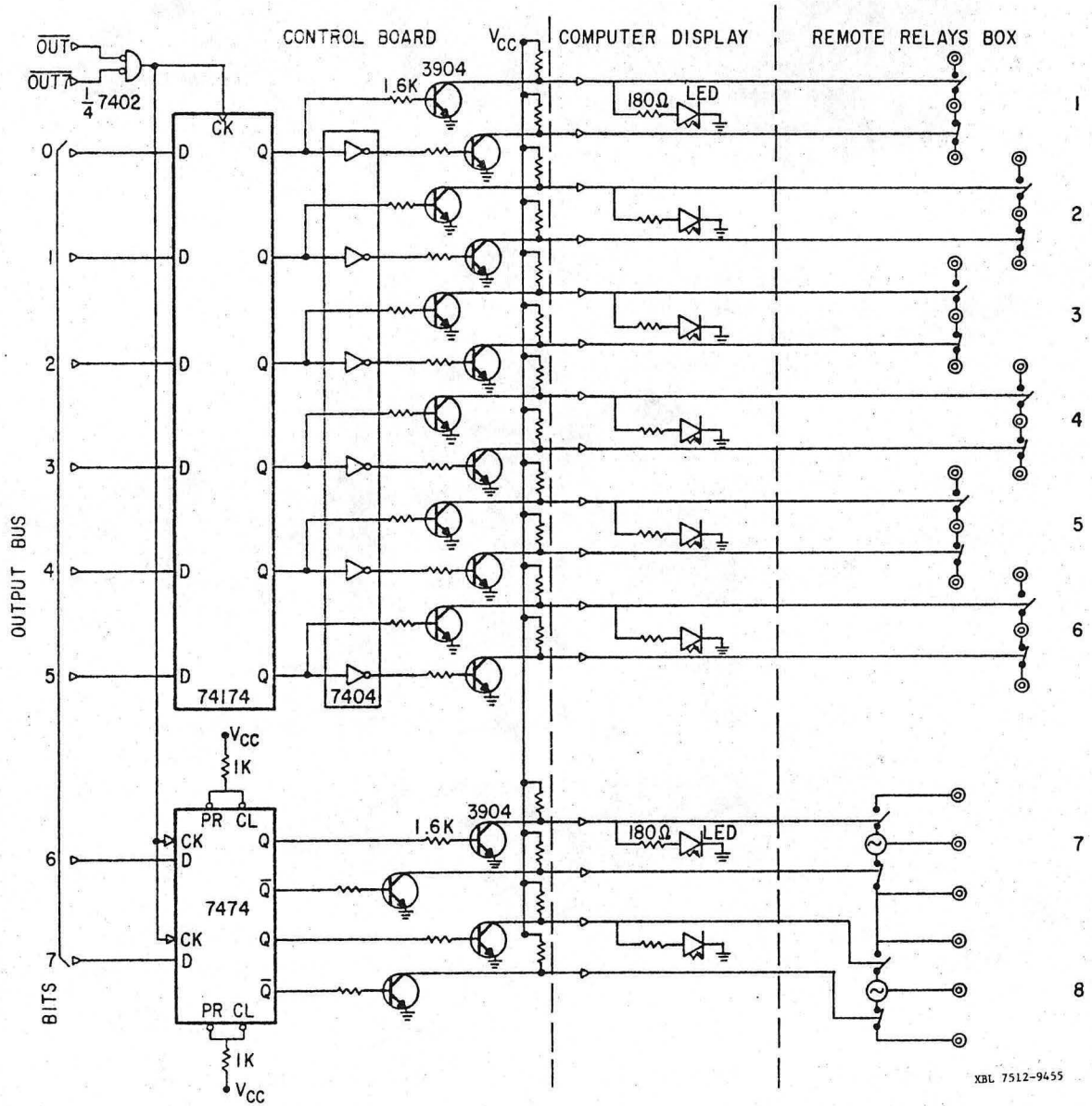
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START CONVERSION WAVEFORM (PRESTON DVM)

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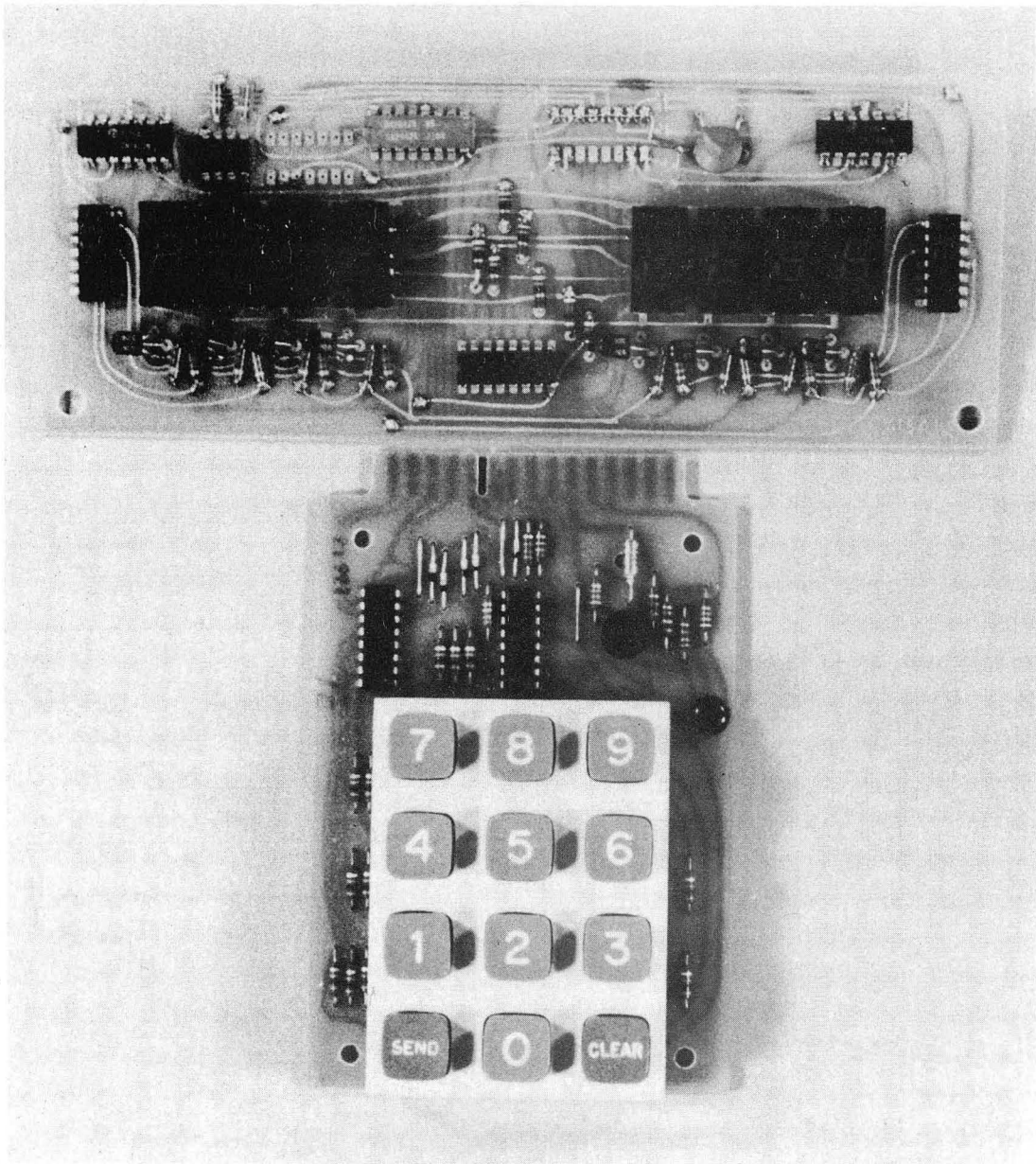
Fig. 4 A general purpose interface for digital voltmeters with BCD output.



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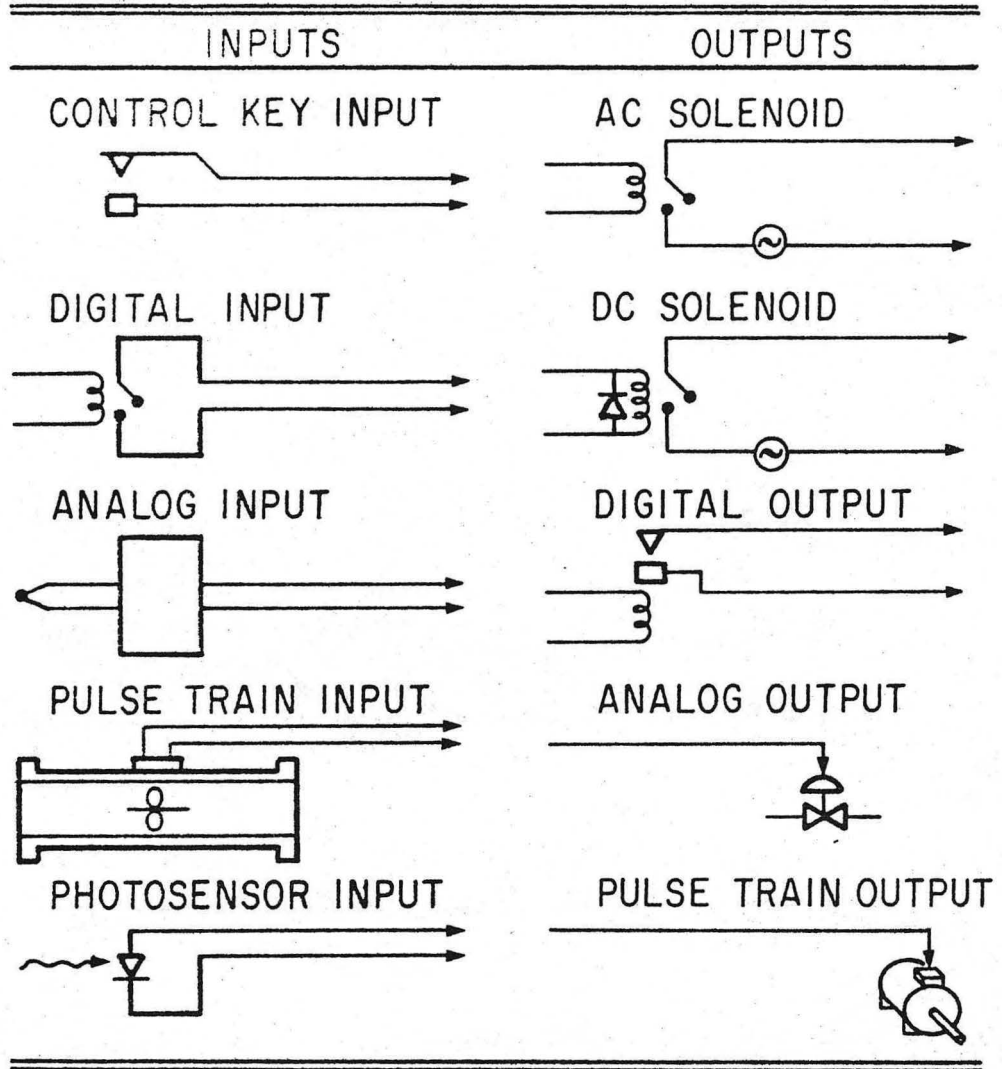
Fig. 5 An interface circuit for reed relay control switches and optically coupled power switches with LED display.

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Fig. 6 General-purpose keyboard and digital display for simple, dedicated microprocessor operation.



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Fig. 7 Process control elements.

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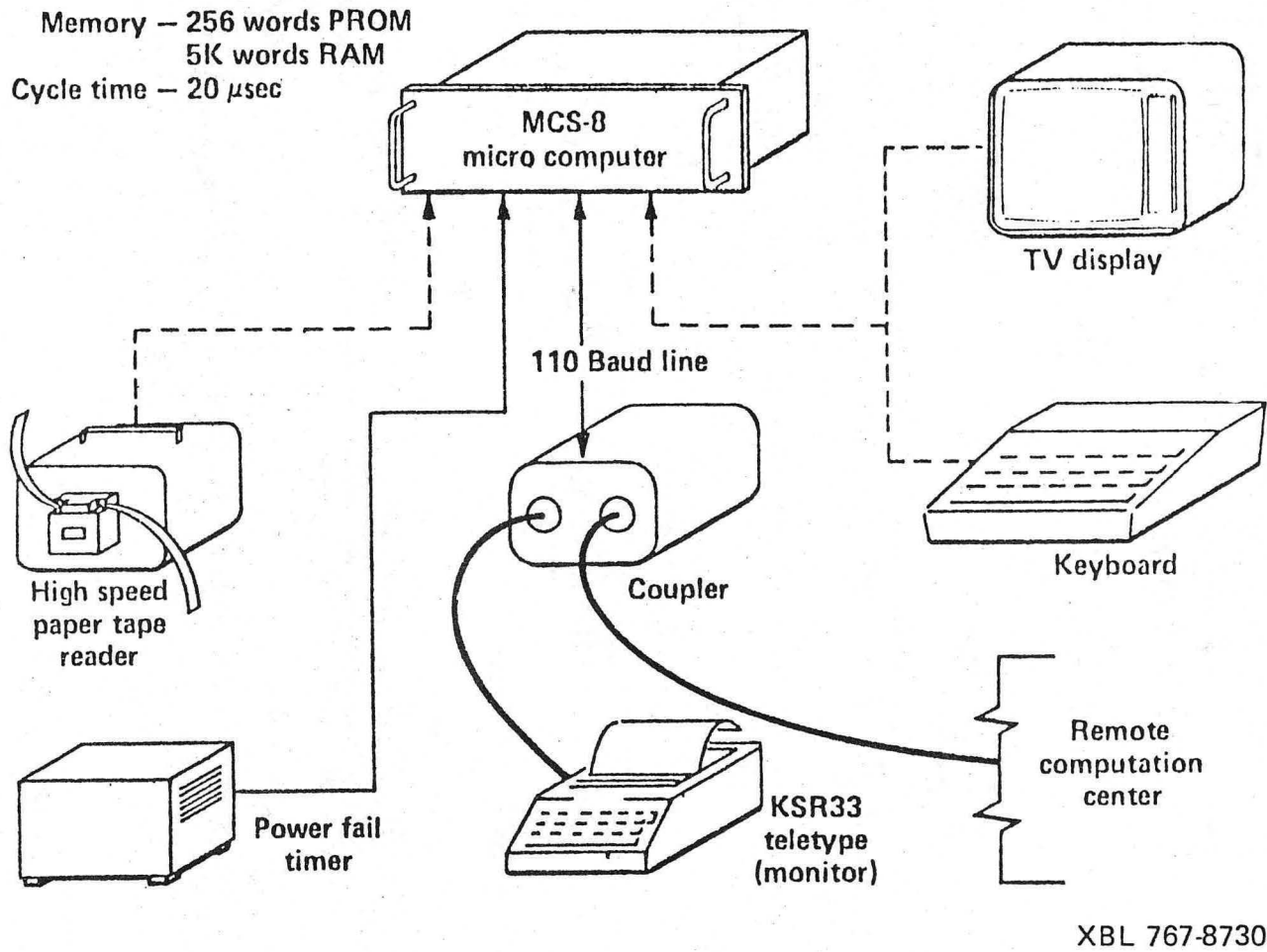
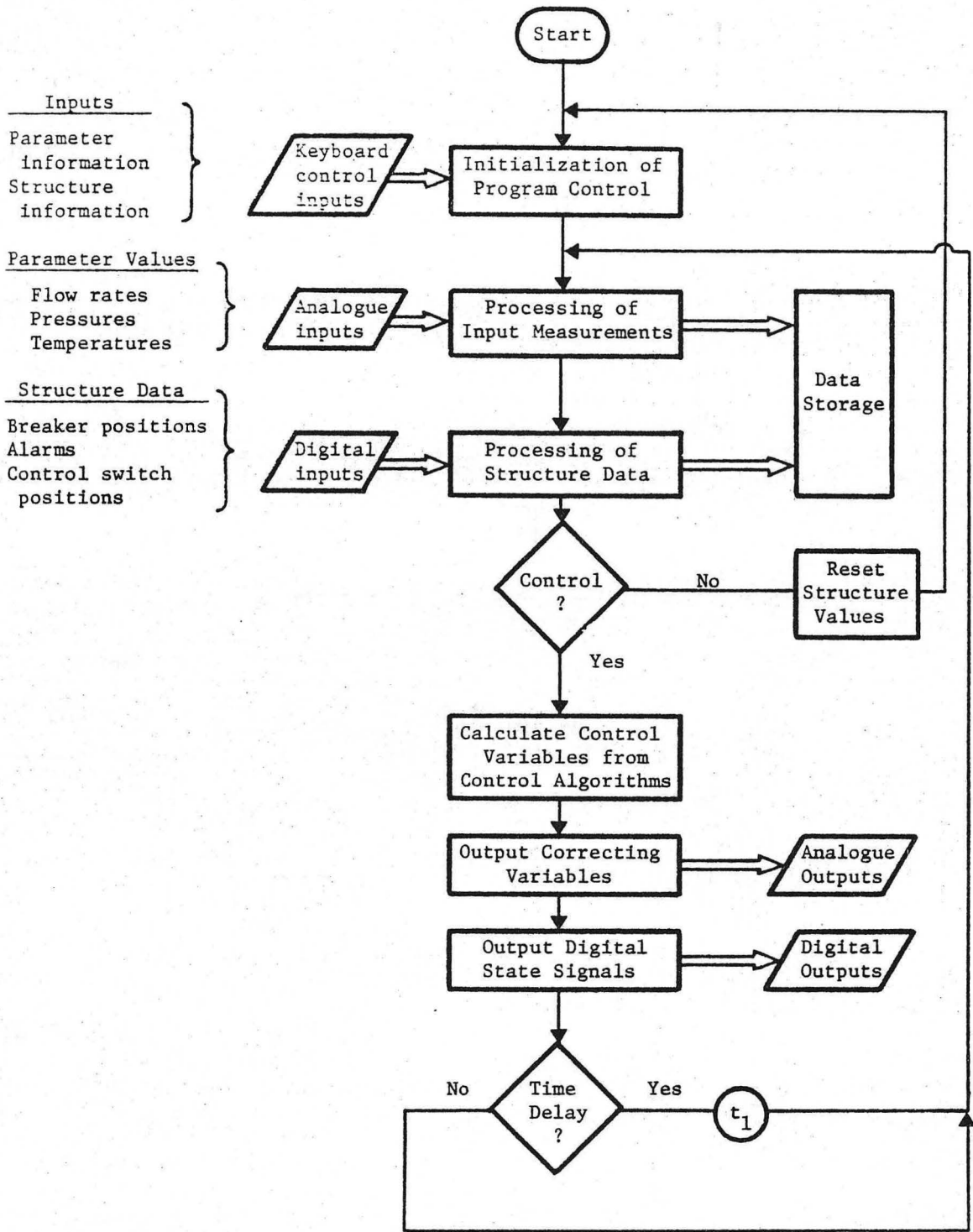


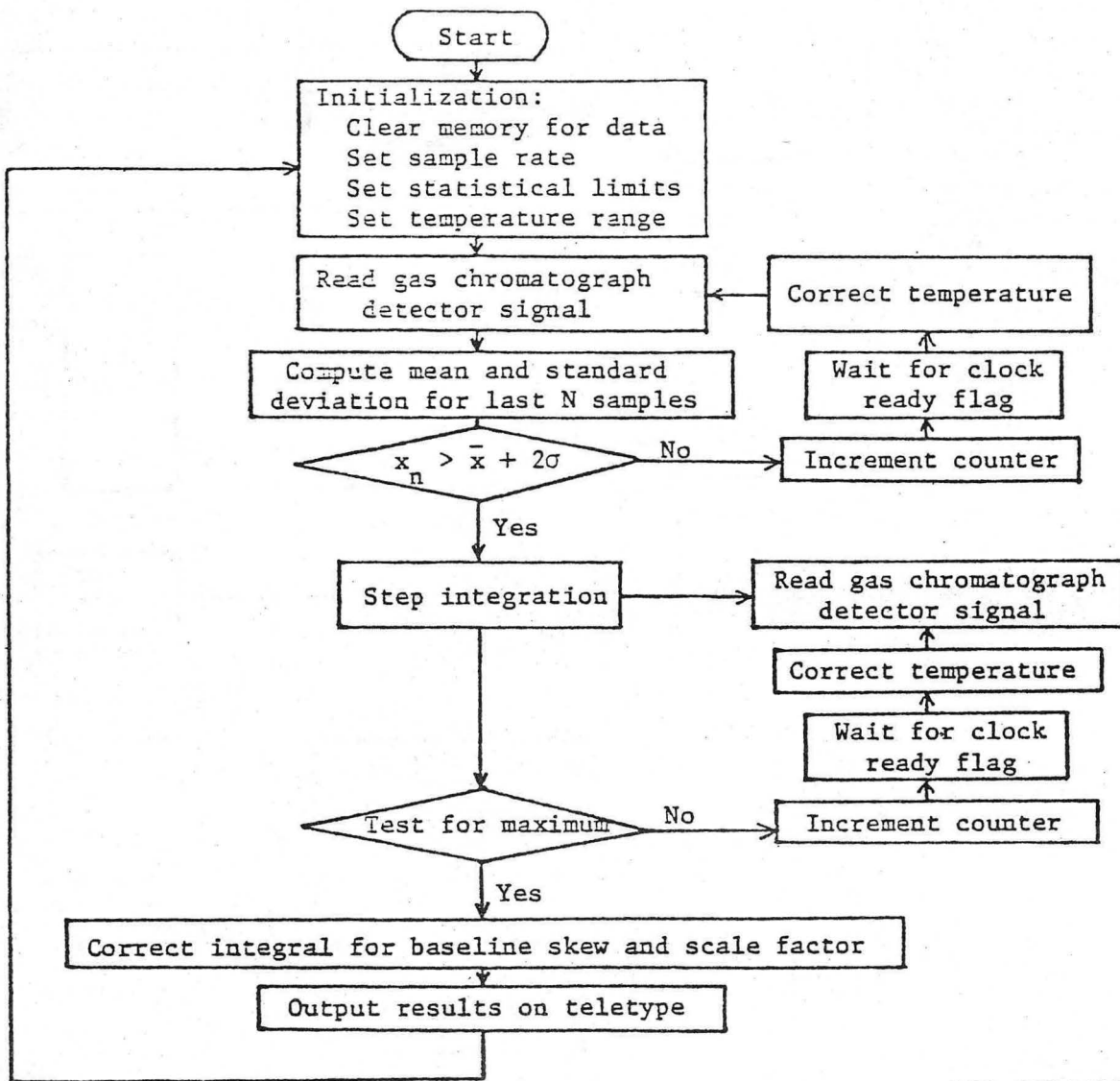
Fig. 8 Automatic monitor system showing interactive display elements.



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Fig. 9 Flow diagram of a general process-control program.

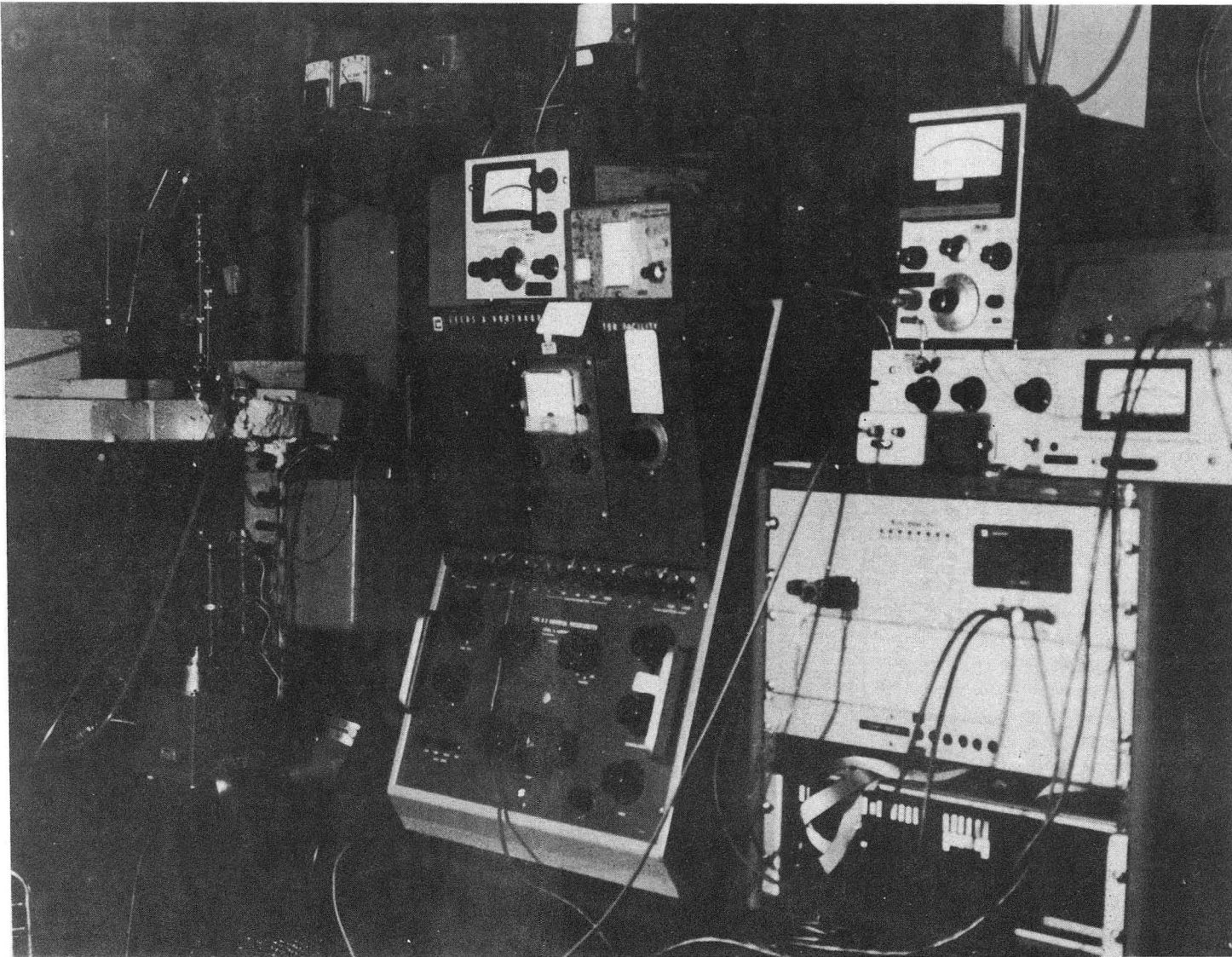
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Fig. 10 Flow diagram for control of a gas chromatograph with real-time integration and column temperature control.

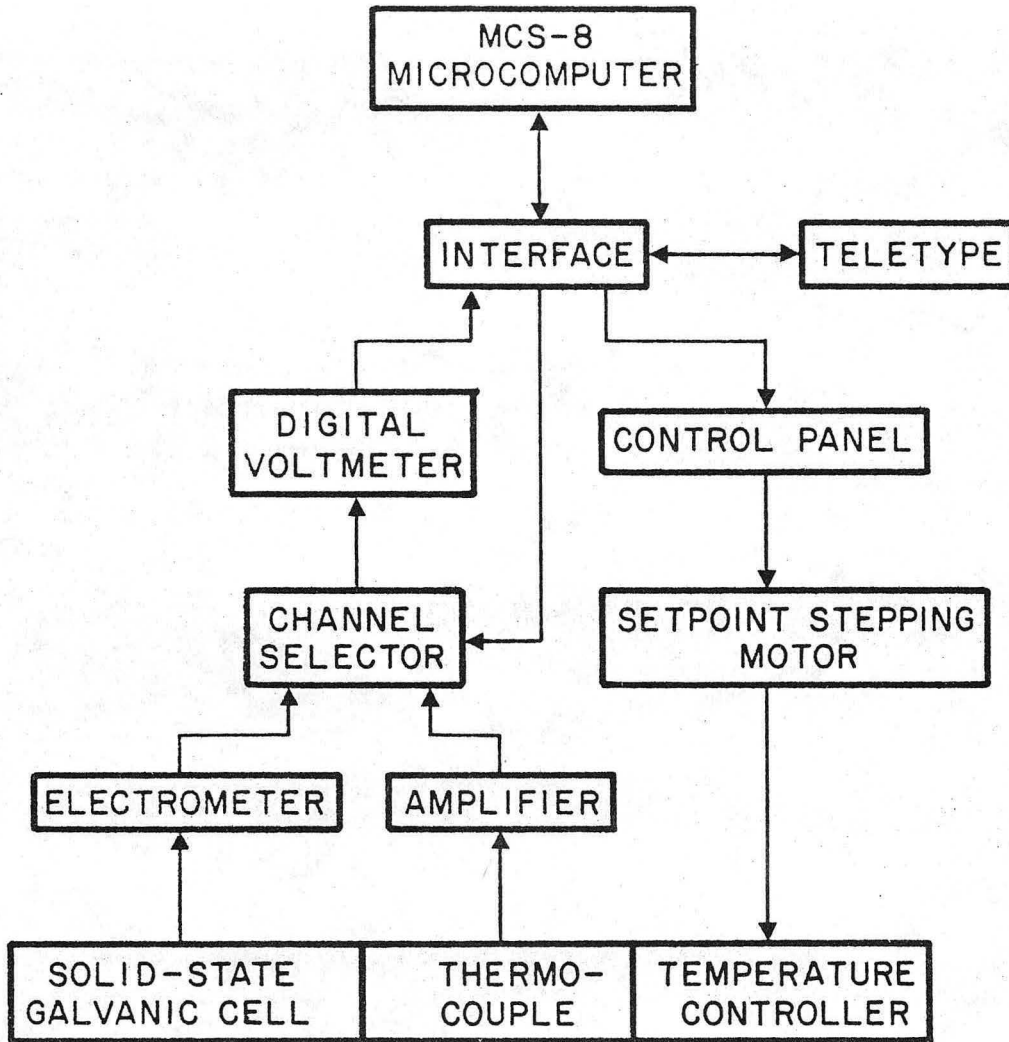
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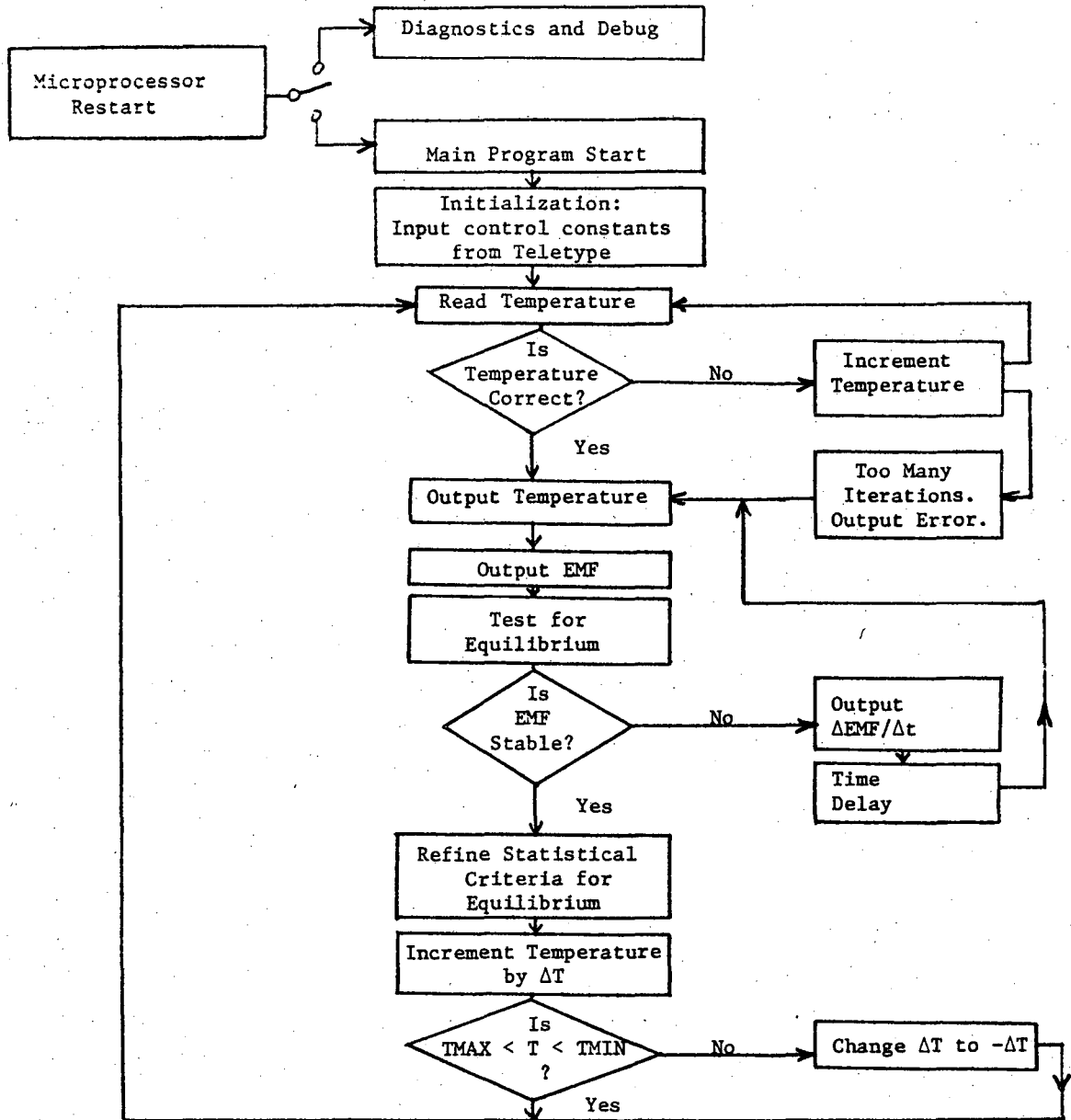
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Fig. 11 Apparatus for a microcomputer-controlled, high temperature electrochemical experiment.



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Fig. 12. Schematic of the microcomputer system developed for controlling high-temperature electrochemical processes

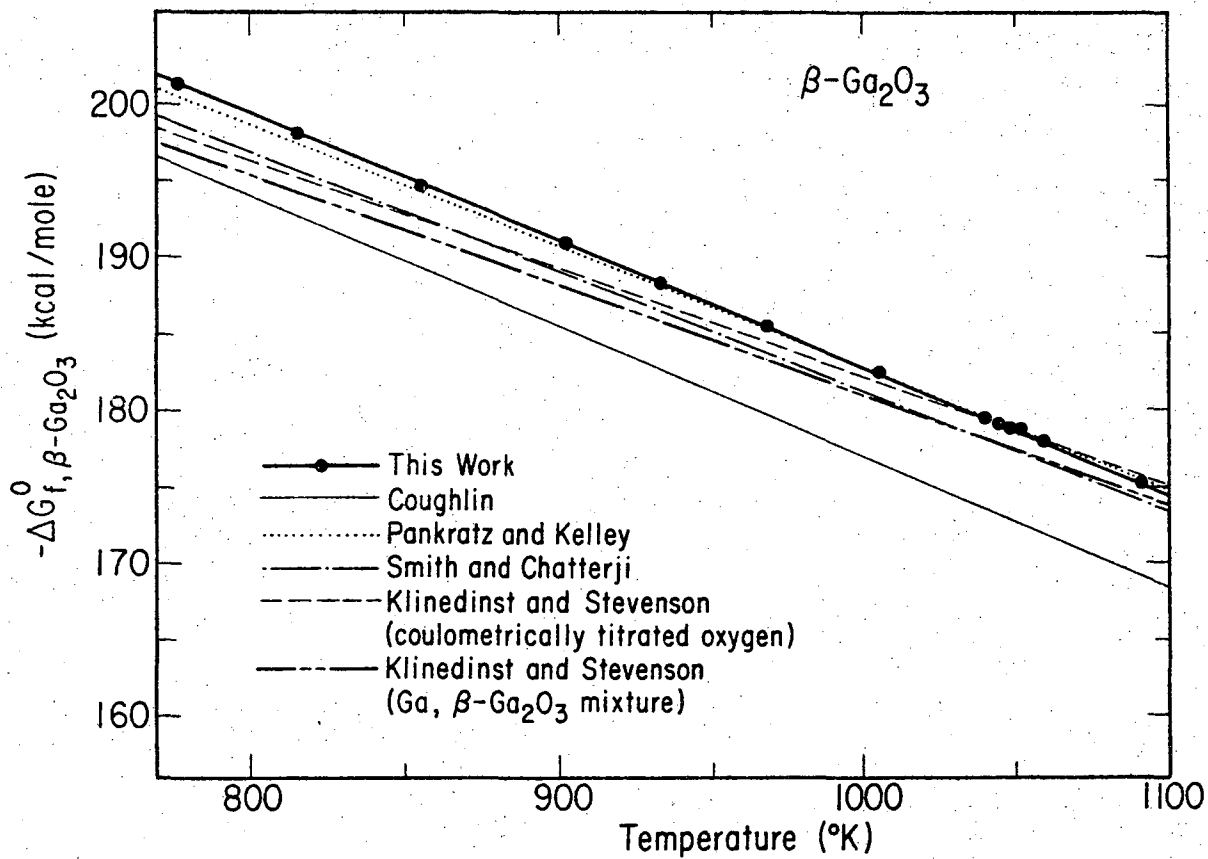


Simplified Software Program for Equilibrium Thermodynamics Studies with Solid State Galvanic Cells

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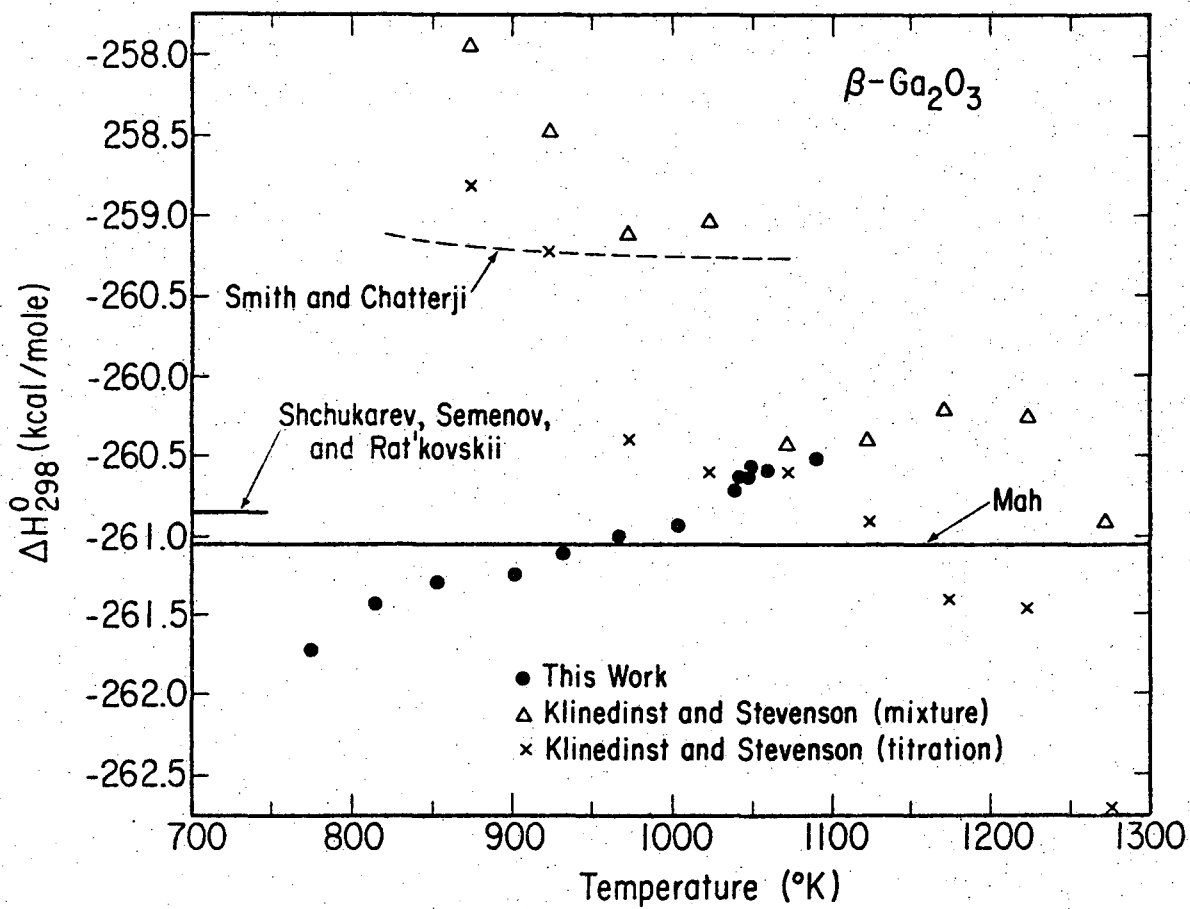
Fig. 13. Flow diagram of a program for equilibrium thermodynamic studies with solid-state galvanic cells.

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XBL 757-6775

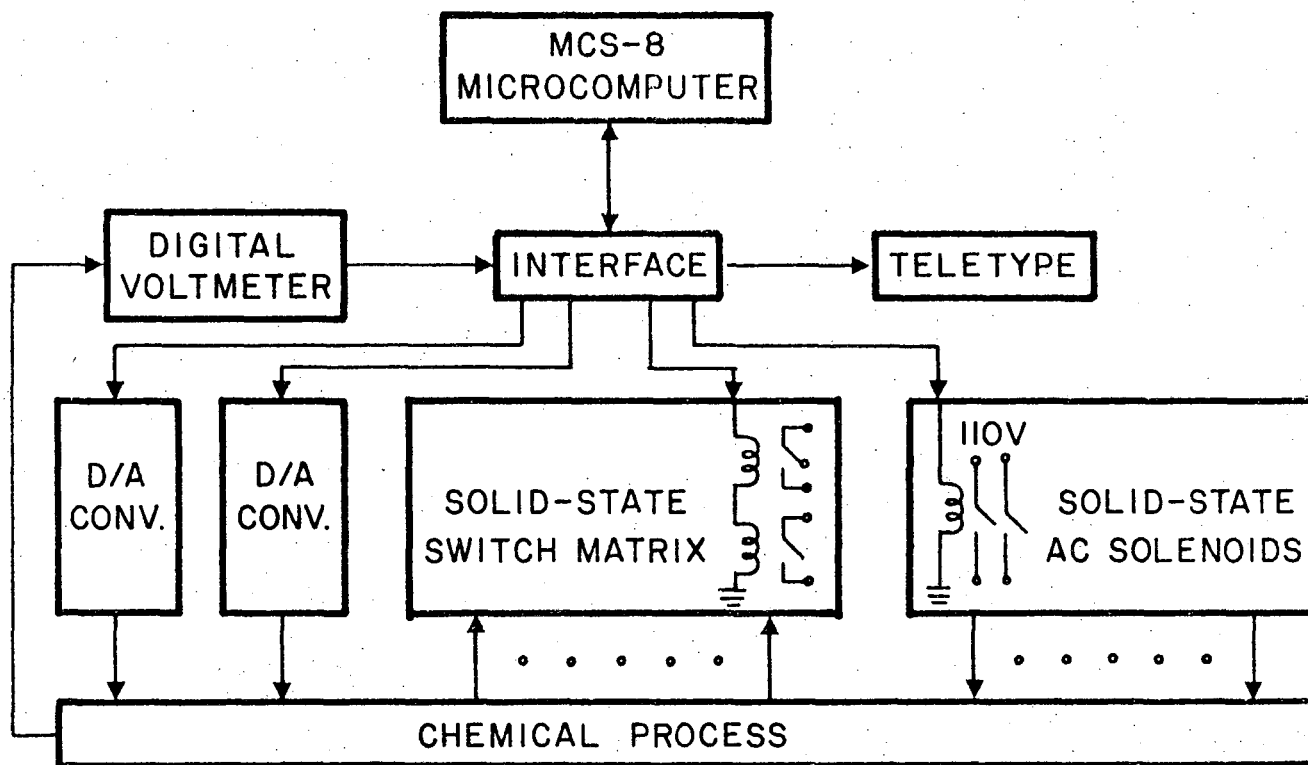
Fig. 14. Measured Gibbs energy of formation of Ga_2O_3 as a function of temperature and comparison to results of previous studies.



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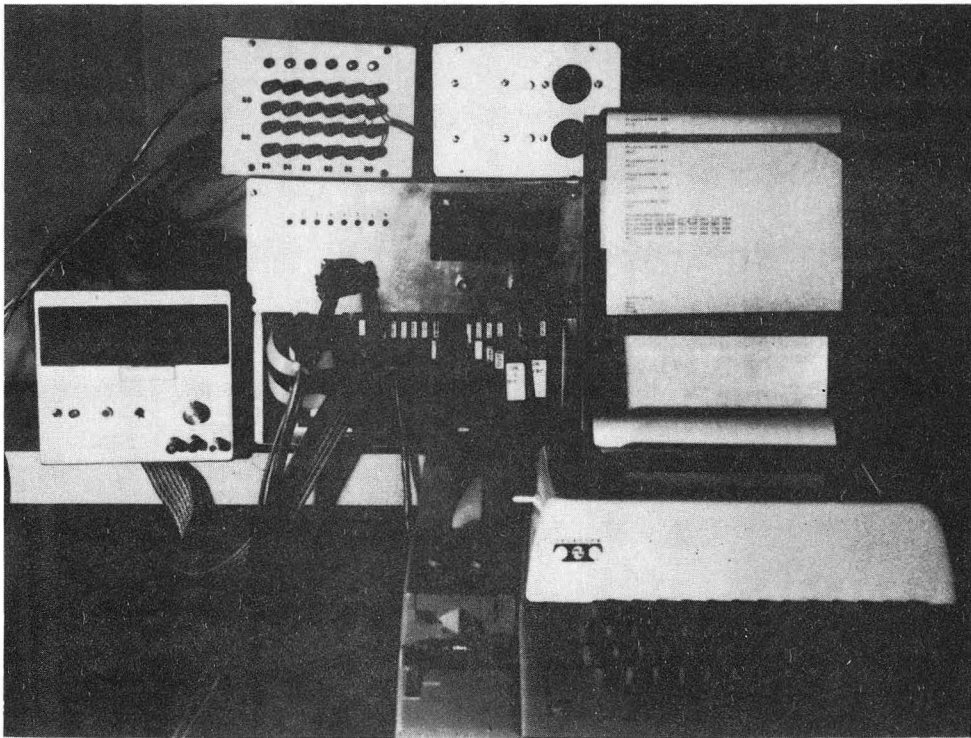
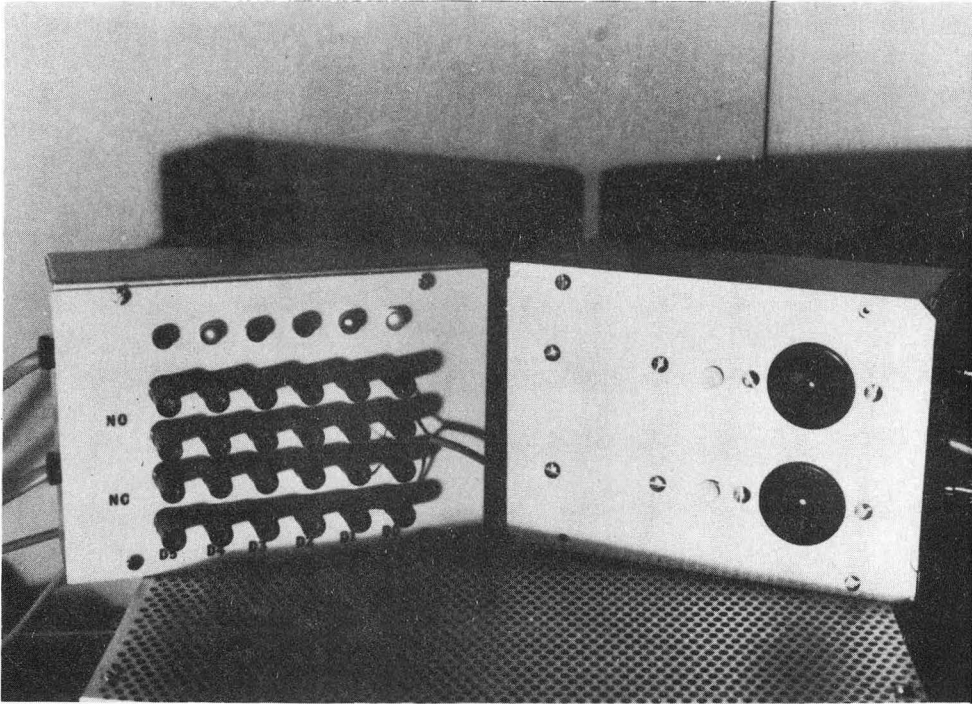
Fig. 15. Calculated values of $\Delta H_{f,298.15}^{\circ}$ determined from a third law analysis of the experimental data.

0 0 0 0 4 3 0 8 5 8 3



XBL 757-6652

Fig. 16 Schematic of the general purpose direct-digital process control system.



XBB 757-5257 A

Fig. 17 A general purpose microcomputer system for direct-digital process control.

0 0 0 0 4 3 0 8 5 8 4

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