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Scientific Originals

Hugo Guterman and Sam Ben-Yaakov

Application of Personal Microcomputers in the Analytical Laboratory

Part II: Long Term Monitoring and Control

Keywords:
AIM-65 microcomputer; Apple II microcomputer; programmable monitoring system

A novel general-purpose data acquisition system has been designed and applied in long term monitoring of temperature in evaporation vessels. The system is operated by a general purpose microcomputer in conjunction with a BASIC program and a short machine language subroutine which were stored in a read only memory (ROM). The interface controller, which is based on an earlier design, permits measurements and control of up to 128 channels but can be easily expanded to 256 channels. It was used in the present application to measure temperature by an array of thermistors. Conversion of the thermistor resistance to temperature was carried out by the microcomputer program which applied a curve fitted equation. The temperature data along with other data were recorded on a standard magnetic tape cassette for processing at a later stage. Experience has shown that the programmability of the proposed low cost monitoring system makes it highly versatile in field use.

1 Introduction

The commercial availability of small yet powerful microcomputer devices and the steady decrease in their cost have created a unique situation in which the ongoing process of applying these devices in science and industry seem to lag behind the technology by which they are developed and produced. Consequently, there is an urgent need to develop new ideas for simple and low cost methods that will permit the implementation of these powerful devices in the research and industrial environment. Lacking, in particular, are methods for interfacing popular and hence low cost microcomputers to instrumentation systems and programming techniques that will allow quick and straightforward translation of data acquisition and control requirements into a working system.

In a previous paper [1] we proposed an approach for applying a personal microcomputer in potentiometric analysis. The system comprised a low cost microcomputer and a novel interface-controller that facilitate communication between the microcomputer and analytical instrumentation. The general purpose interface was successfully used in a number of applications such as automatic titration and ion analysis. Each application was implemented by interfacing the microcomputer with auxiliary devices such as specific ion electrodes, and a motor driven buret which were controlled by a program written in BASIC.

In the present study we extended the basic concept as put forward previously [1] to include a class of applications which call for routine, long term monitoring and control of a multi data point system. The basic requirements in this class of applications are different in many aspects from the requirements in other applications. Such a system should have the capability of serving a large number of units which may include an array of sensors as well as a large number of measuring and control devices. Secondly, the system must be protected against power failure as it may be required to work unattended. Another requirement is that the

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Hugo Guterman and Sam Ben-Yaakov*
Department of Electrical and Computer Engineering, Ben-Gurion University of the Negev, Beer-Sheva, Israel 84120.

microcomputer program which controls the operation will be firmware implemented, *i.e.* it should reside in a read-only memory (ROM) so there will be no need load it each time operation is commenced. Such a system must also include human interface facilities such as a display and a printer to permit simple and quick checks of its operation as well as means to announce possible malfunction, along with a display of error messages. And finally, the problem of communication with other computers must be solved beforehand so that the large data mass to be collected can be easily transferred to other, more powerful processing systems.

Here we describe the approach taken by us to realize a data acquisition and control system that answers the basic requirements mentioned above. A decision to develop such a system rather than to purchase it commercially was made after it was realized that the cost of a commercially available system meeting all requirements would be prohibitive. It is believed that the general approach followed in developing the present monitoring and control system could be adopted by other researchers, even if the specific applications are different from those addressed here or if different hardware is chosen.

2 System Configuration

The basic configuration of the proposed data acquisition and control system (Figure 1) includes all the necessary features to permit operation along the lines suggested above. It comprises a general purpose microcomputer and a multi-input interface which permits selection, under computer control, of any of the inputs and reading of its value via a digitizer. Also included are control relays which can be used to operate external devices such as solenoid valves, pumps, heaters, and the like, under program control.

The system is powered by a rechargeable battery which is continuously charged or trickle charged by mains power. Battery capacity is chosen to ensure operation for the largest expected AC power interruption.

The data collected by the system is stored on a magnetic tape cassette mounted on a cassette tape recorder which is in turn controlled by the microcomputer. In normal operation, all inputs are sampled at a predetermined rate and the information, along with the real time and date of sampling, is recorded on the cassette. Between sampling stops, the microcomputer displays the real time on the built-in display. This serves as a simple visual assurance that the system is alive. While sampling and recording, the microcomputer displays the current datum that is being handled and prints the sampling time as well as error messages on the printer. These printouts are used to check the proper operation of the system and to spot gross malfunctions such as a damaged sensor or improper supply voltages. A more extensive check of the system can be performed by the operator by initiating simple diagnostic routines such as sampling and printing out any selected channel.

The operation of the monitoring and control system is controlled by a BASIC program which is stored in a ROM and started automatically by pressing one of the microcomputer function keys. Otherwise the microcomputer can be used in the normal way. Once the monitoring and control program is in command, the microcomputer can be considered as a "black box" instrument dedicated to a specific task. As such, it does not require any manual intervention except for cassette replacement and routine service.

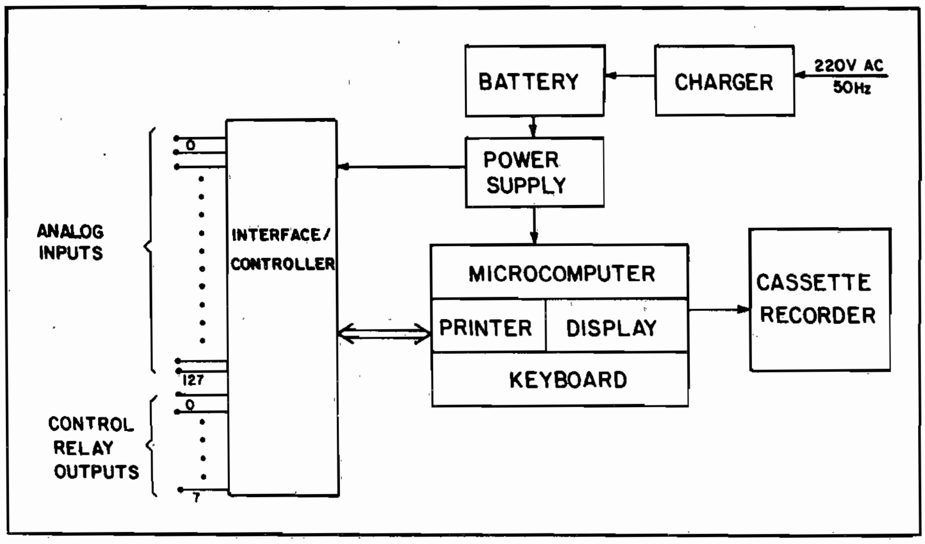

Figure 1: Block diagram of proposed data acquisition system.

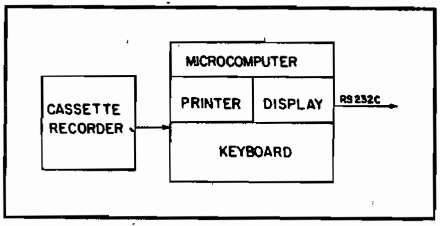

Figure 2: Block diagram of magnetic tape cassette readout system.

The magnetic tape cassettes recorded by the system are read back into the same or a similar microcomputer (Figure 2) and the data can be sent out along a standard RS232C serial communication line [2]. The data is thus readily available to any micro- or minicomputer with the common RS232C standard communication port.

The system that was built by us and is described in detail below is but one possible realization of the general concepts outlined above. The specific hardware items mentioned here were selected to meet a specific application and their choice was affected by many non-technical and often arbitrary decisions. They include: availability in stock of various elements, previous experience with a given microprocessor family, availability of certain memory devices and EPROM programmers, *etc.* Consequently, the mention of any specific commercial unit does not constitute endorsement or recommendation of a given product or manufacturer.

3 Design Details

The design details given here describe the system that was built by us to meet a specific requirement: *viz.* long term monitoring of temperature in a large number of reaction vessels in which evaporation experiments were conducted. The temperature was measured by immersion type thermistor sensors which were wired to the system described here. However, trivial changes in hardware along with a relevant BASIC program will permit utilization of this system for a wide range of applications.

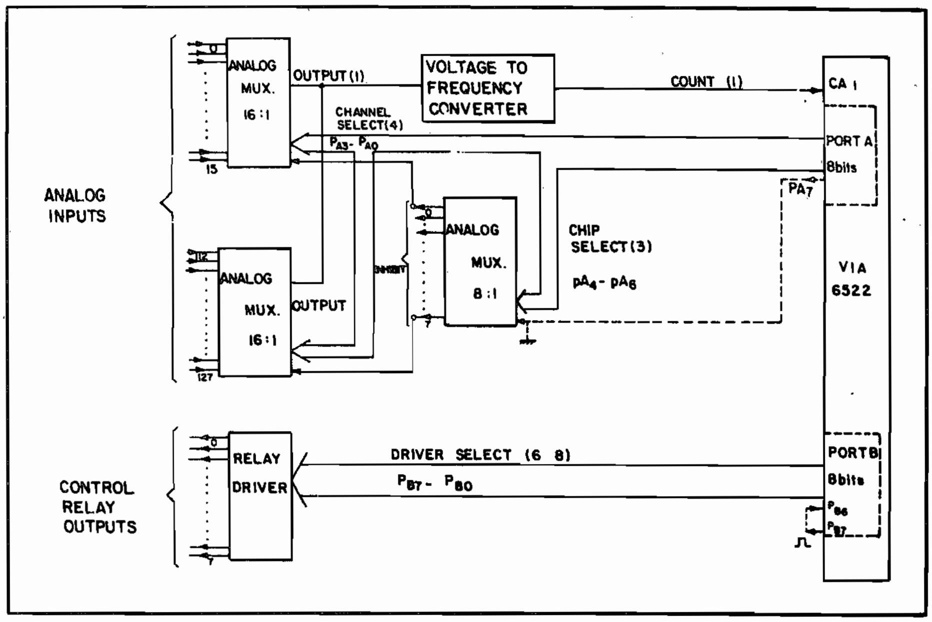

Figure 3: Circuit diagram of interface controller.

3.1 Microcomputer

The microcomputer used in the present study was an AIM-65 (Rockwell International, USA) [3]. The unit includes an 8 bit CPU (6502) a residence monitor and BASIC interpreter, 4 Kbyte RAM and two user expandable ROM sockets. The unit also includes as standard items a one line LED display (20 characters) a small printer (20 characters) TTY and audio cassette recorder interfaces and an input/output port with 2 x 8 bit lines and four handshake lines. Is should be reemphasized that the design concepts outlined here can be implemented with a number of commercially available microcomputers of which the AIM-65 is but one example.

3.2 Interface

The design if the present interface unit (Figure 3) follows the general concepts of the interface that has been described previously [1]. The main differences are in the number of input channels which were extended here to 128 with an option to expand them to a total of 256. The number of control relays is eight or six if two lines of the port B are used for real time clock operation as described below. If required, the number of control relays can be increased, by using the multiplexing scheme described earlier [1]. Since our specific application called for a limited number of control relays, a simple one-to-one decoding scheme was deemed sufficient.

The multiplexing of 128 inputs was achieved by using eight 16-bit CMOS multiplexers (RCA, CD 4067B) which were controlled by one of eight selector (RCA, CD 4051). As the number of bits required to decode 128 inputs is 7, the eighth bit of port A (Figure 3) can be used to control another bank of 128 input multiplexer, extending the total number of inputs to 256.

Digitization was carried out by counting the pulses of the voltage to frequency converter over a fixed period of time. The advantage of this simple and low cost digitization technique in low sampling rate applications was discussed previously [1]. The full range frequency used here was 10 KHz which provided a 1:10,000 resolution when a one second counting time was applied.

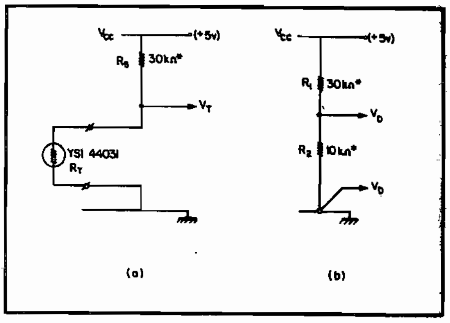

Figure 4: Thermistor voltage divider (a) and reference divider (b).

3.3 Temperature Sensors

Temperature was measured by commercially available immersion type thermistors. No attempt was made to linearize the response by hardware methods. The thermistors were connected in a simple voltage divider circuit (Figure 4a) and the output voltages were fed to the data acquisition system. These voltages were compared to the output voltage of a reference voltage divider (Figure 4b) from which the resistance of the thermistor was calculated. The measurement was made independently of the conversions factor of the voltage-to-frequency converter [1] and the supply voltage to the thermistor and divider network, by an autocalibration procedure which preceded the temperature measurement. The procedure commenced by first evaluating the response of the digitizer by using it to measure the ground potential and the output voltage of the reference divider (V_0 and V_D in Figure 4b). Assuming a linear relationship between the output frequency, f, and the input voltage V, the frequency should follow the function:

$$f = A + K_f \cdot V \tag{1}$$

where A and K_f are the (unknown) conversion constants. The constant can be evaluated from the two reference measurements to yield

$$f = f_0 + \frac{f_D - f_0}{V_D} \cdot V \tag{2}$$

where f_0 and f_D are the measured frequencies for 0 volt (V_0) and V_D respectively.

The output voltage of any thermistor divider V_T can now be expressed as a function of the measured frequency f_T by:

$$V_T = \frac{f_T - f_0}{f_D - f_0} \cdot V_D \tag{3}$$

Since

$$V_T = \frac{R_T}{R_S + R_T} V_{cc} \tag{4}$$

and

$$V_D = \frac{R_2}{R_1 + R_2} V_{cc} \tag{5}$$

one obtains

$$\frac{R_T}{R_S + R_T} = \frac{f_T - f_0}{f_D - f_0} \cdot \frac{R_2}{R_1 + R_2} \tag{6}$$

from which

$$R_T = \frac{R_s \cdot F}{1 - F} \tag{7}$$

where F is the expression on the right hand of equation (6). Hence, the proposed method of relative measurement is independent of V_{cc}, A, and K_f as long as they can be assumed to remain stable between the calibration and measurement stages.

Conversion of R_T to temperature was carried out by using a curve fitted equation which relates thermistor resistance to temperature. The fitted equation was of the form [4]:

$$R_T = A \exp\left(\frac{B}{T} + \frac{C}{T^2}\right) \tag{8}$$

where T = temperature (K)
R_T = resistance (ohms)
A,B,C = constants.

Hence, the temperature can be calculated for any given R_T by:

$$T = \frac{2C}{-B + \sqrt{B^2 - 4C(\ln A - \ln R_T)}} \tag{9}$$

The numerical values of the constants A,B,C of equation (8) were evaluated by a least-squares fitting procedure [5] which fitted the equation to tables supplied by the manufacturers [4]. The tables list the resistance of the specific thermistor used as a function of its temperature, over the useful temperature range.

3.4 Software and Firmware

Real time clock indication was achieved by using internal counters of the AIM-65 (located in the 6522 VIA) in conjunction with a microcomputer program. An external connection was made between PA_6 and PA_7 (Figure 3) to obtain a pulse wave with a period of 65.535 msec. This basic period was then translated into elapsed time by a BASIC program.

The computer program which controlled the operation of the monitoring and control sequence consisted of a short machine language routine and a main program written in BASIC. The machine language program was used for counting the pulses of the analog-to-frequency converter [1]. It was written in mnemonic and assembled by the resident assembler of the AIM-65 [6]. The BASIC program was first keyed into the AIM-65 and stored in the RAM of the microcomputer in the usual manner. Following the debugging stage both the machine language program and the BASIC main program were programmed into an Erasable-Programmable Read-Only-Memory (EPROM) which constitutes the basic firmware of the monitoring system. It operated with the standard firmware of the microcomputer used: a monitor and a BASIC interpreter [7]. EPROM programming was carried out by a PROM Programmer & CO-ED (Rockwell International, USA).

4 Experimental

An AIM-65 microcomputer was used as the controller and was operated with the interface described above. The data were recorded on a CN13 cassette recorder (Commodore Inc., USA). The thermistors were type YSI44031 (Yellow Springs Instrument, USA) which are interchangeable to within 0.1°C. The system was powered from a 12V, 80 Ah sealed, lead-acid battery (Gould Inc. USA) which was charged by an in-house built charger. Total current drain from the battery was 3 A. Hence, the battery could sustain continuous operation for a period of 26 hours.

The monitoring and control system was installed in the experimental station of the Mediterranean Dead Sea Co. of Israel located in the Dead Sea area near Beit Haarava. The system was used to continuously monitor the temperature of evaporation vessels located at that experimental site. The thermistors were wired through an electrical cable network with distances up to 75 meters between the thermistors and the monitoring system. The system has now been in use for about five months (as of Jan. 1983).

The BASIC program of the monitoring sequence consisted of two main parts (Figure 5): a) recording of all inputs on the tape along with real time and date, every hour and b) printing the reading of any channel on the built in printer in response to an operator's command. On operating in the standby mode the system displays the running time on the built-in LED display.

The data cassettes were read back by an AIM-65 microcomputer (Figure 2) and transferred to a dedicated data processing system (Figure 6). It consisted of an APPLE II microcomputer (APPLE, USA), model IPS-5000A (Data Royal, USA) printer, and a model DMP-3 (Houston, USA) *x-y* plotter. The data processing system was used to tabulate the data collected by the present monitoring system along with manual fed data, and to generate various plots.

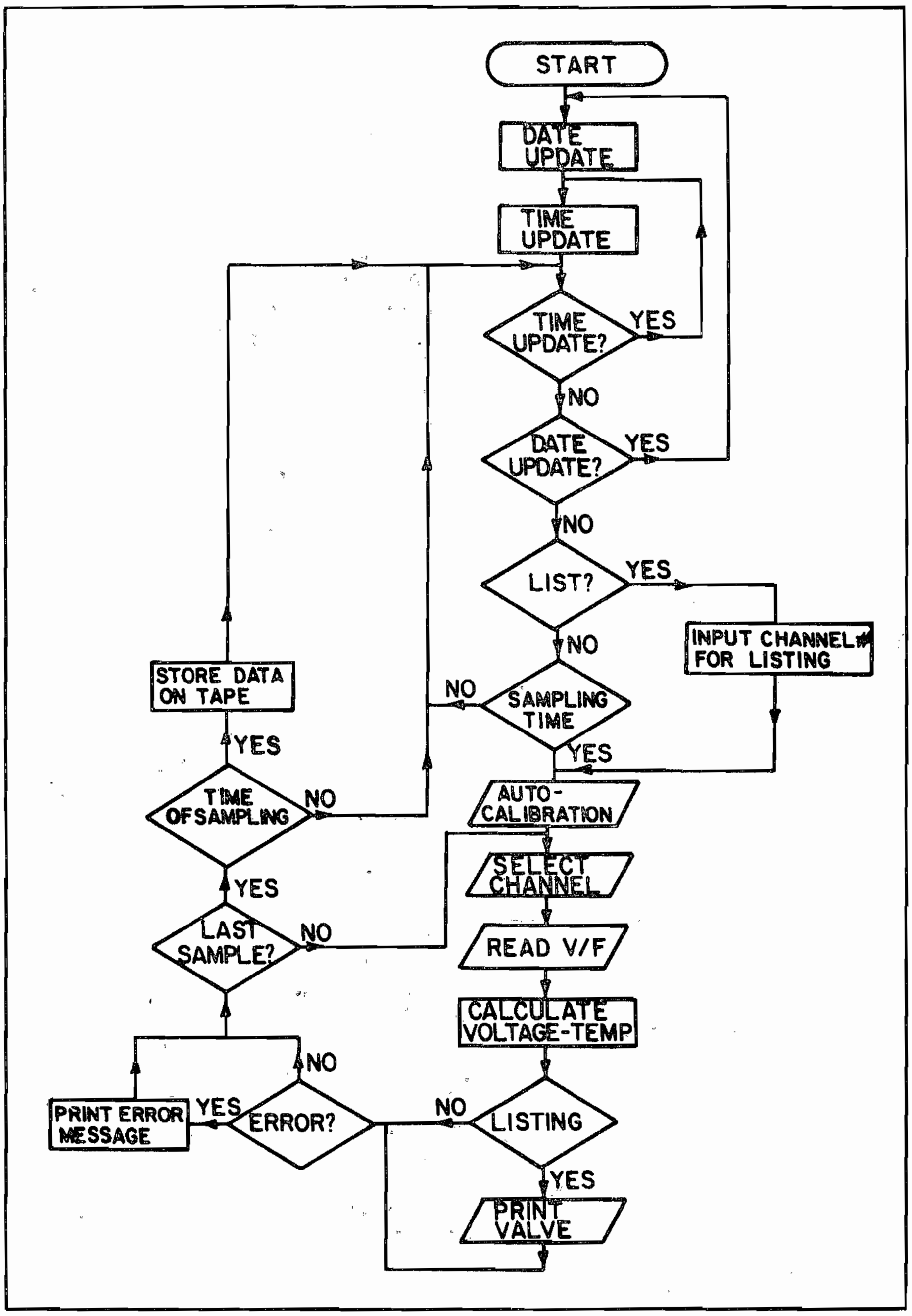

Figure 5: Flow diagram of microcomputer program of the present data acquisition operation.

5 Results and Discussion

The constants of the curve fitting equation [eq. (8)] to thermistor data were found to be:

A = 6.65225 x 10^{-3} ohm
B = 4896.9622 K
C = 19568.496 $(K)^2$

The agreement between the curve fitting equation [eq. (9)] and the manufacturer's tabulated data [4] was found to be very good (Figure 7 and Table 1). The maximum deviation between the temperature calculated from the curve fitting equation and the temperature tabulated for a given thermistor's resistance was found to be less than ± 0.02°C for the temperature range 0 – 100°C. Consequently, the limiting factor in the accuracy of temperature measurement by the thermistors is the guaranteed interchangeability (± 0.1°C) and not the curve fitting approximation. Another factor that must be taken into account is the accuracy of the resistors used in the measuring and reference divider (Figure 4). Since the accuracy limits of these resistors was ± 1%, the corresponding error in evaluating the thermistors' resistance R_T could have reached ± 3%. This corresponds to a maximum temperature error of about 0.75 °C at 25 °C and about 1 °C at 40 °C. Comparison of the

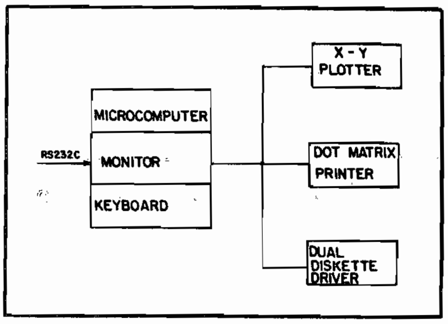

Figure 6: Block diagram of data processing system.

Table 1: Comparison of original tabulated response of thermistor to reconstructed response as calculated from the curve fitted equation.

Tabulated data (T_T)		Fitted temp. (T_F)	Error
Temp. [°C]	Resistance [kΩ]	[°C]	$T_T - T_F$ x 10^{-3} [°C]
0	29.4900	– 0.005	5.510
10	18.7900	9.996	3.351
20	12.2600	20.014	−14.287
30	8.1940	30.007	−7.004
40	5.5920	40.009	−9.245
50	3.8930	50.005	−5.558
60	2.7600	60.003	−3.116
70	1.9900	70.003	−3.833
80	1.4580	79.996	3.622
90	1.0840	89.989	10.681
100	0.8168	99.993	6.976

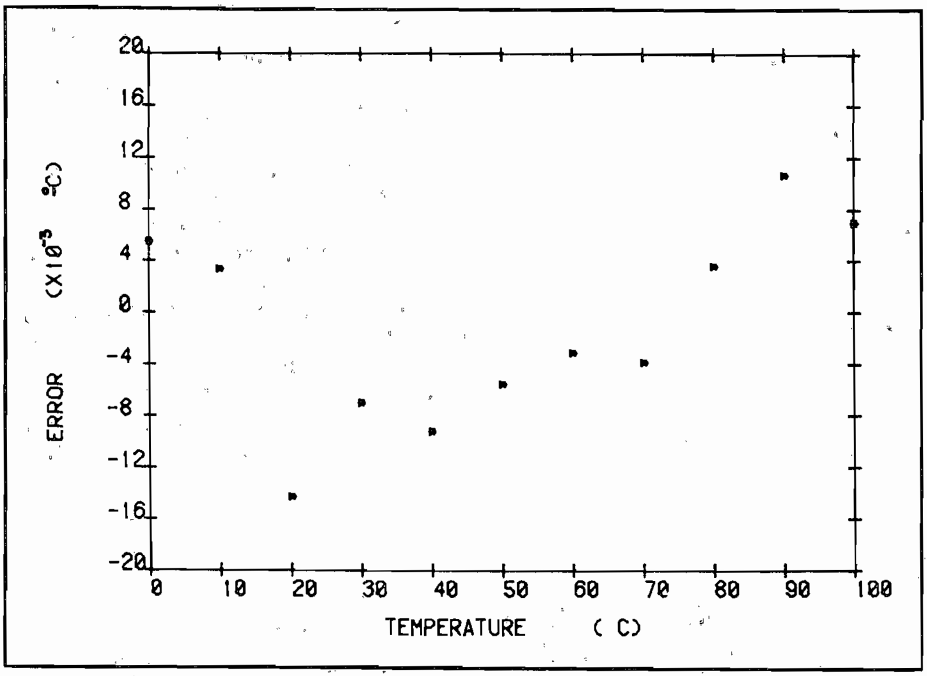

Figure 7: Deviation of curve fitted equation from tabulated resistances of thermistors.

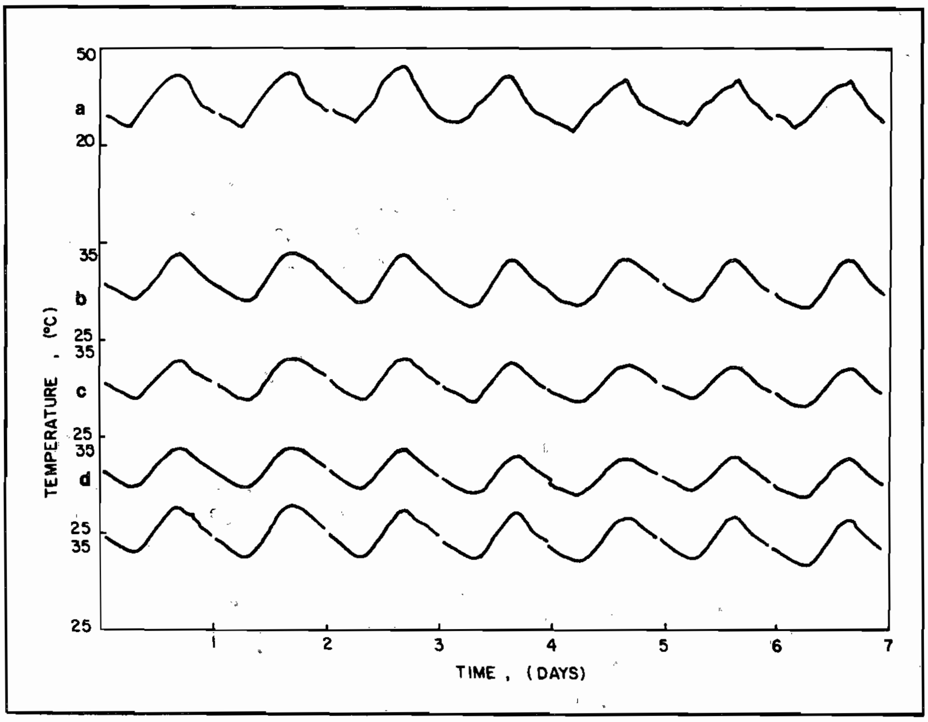

Figure 8: Reconstructed temperatures from data recorded by present monitoring system in Dead Sea experimental station. (a) Air; (b) de-ionized water; (c) Mediterranean Sea water; (d) Dead Sea water.

temperature measured by the present monitoring system and that measured by a hand-held thermometer (Thermic, West Germany) specified to ± 0.1 °C revealed that the maximum error in the field was below ± 0.7 °C at 40 °C, *i.e.* well within the expected range.

The total number of data (channels) recorded on the cassette, per scan, in the present application was 96. Each record was identified by the date and time of recording. The number of records that could be recorded on one side of a standard C-60 audio cassette was found to be 52. This required, in the present application, replacement of a cassette every two days. The maximum number of data points recorded on each side of a cassette was thus approximately 4,992 or about 25,960 digits. This information was read to the APPLE II system (Figure 2). The total time required for transferring the data of one cassette was 45 minutes when using a communication data rate of 1200 band.

Typical plots generated from the data collected by the present monitoring system are shown in Figure 8. It depicts air temperature, and temperatures in three evaporation vessels in which deionized water, Mediterranean Sea water, and Dead Sea water were exposed to solar radiation. Clearly seen are diurnal temperature fluctuations as is the effect of solution salinity on the temperature attained. This salinity dependence is probably due to a lowering of the water vapor pressure, and hence of the rate of evaporation, as the ionic strength increases. Thus the rate of loss of heat by the evaporation process is lower at higher salinities so that a higher solution temperature is reached for any given solar radiation.

Continuous round-the-clock temperature monitoring of the evaporation vessels in the experimental station of the Mediterranean Dead Sea Co. would have been impractical without a data acquisition system. The advantages of using the system described here were found to be not only economic but also functional. The total cost of the present system is for below that of any commercial system including all the required features such as magnetic recording, battery backup, communication with other processors, *etc.* Another advantage is the flexibility of the system stemming from its programmability. This enables one to tailor its performance so as to meet specific requirements of a given application. The specific program can include many features such as curve fitting to a given sensor's response, conversion to physical or chemical units, setting of alarms and switching from one mode of operation to another according to predetermined criteria. The simplicity of the interface unit described here, and in particular the simple digitization method with a built-in noise integration feature, simplifies the construction of the unit. It does not require any special precautions when preparing the layout of the printed circuit, and does not call for elaborate noise filtration, shielding or earthing even though the basic resolution (with a one second counting time) is 1 part in 10,000, *i.e.* equivalent to a binary resolution of *ca.* 13 bits.

The accuracy of the present digitization method can be markedly improved by an autocalibration scheme. In the present application, a built in computer-controlled procedure was used to calibrate the thermistor's resistance measurements. The procedure yields a resistance value which is independent of the excitation voltage, and the conversion factor of the analog-to-frequency converter. A similar approach was successfully implemented for voltage measurements. In that case, a stable reference voltage and ground (zero voltage) were used for evaluation of the response of the analog-to-frequency converter prior to each set of measurements. This simple two-point calibration technique can be implemented because the linearity of the analog-to-frequency converter is very good (RC4151 Raytheon, Inc.). All these procedures of self calibration would have been impractical, of course, if not for the programmability of the monitoring system.

The main disadvantage of the present digitization scheme is the low sampling rate that can be obtained. This restricts the range of application to relatively slow processes in which a sampling time of one second can be tolerated. In such cases the application of the approach suggested here could be very effective and economical.

Acknowledgment

We wish to thank Mr. A. Yechiely for assistance in the construction of the present monitoring system. The temperature data (Figure 8) are reproduced by permission of the Mediterranean Dead Sea Co. which supported the present research and development activity.

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An on-line data capture and data reduction system consisting of an APPLE II microcomputer interfaced to a gas chromatograph is described. The advantages and disadvantages of this approach as against that of a dedicated microprocessor/integrator system are discussed. The microcomputer system is described in detail. A description is given of a wide variety of software, both for general application in the field of gas chromatography and specifically for the calculation of statistical moments and retention indexes.

J.B. Wagener and T.S. Buys

A Microcomputer Sys
Gas Chromatograph

1 Introduction

A microcomputer system consisting of an APPLE II with supporting hardware and software was assembled for on-line data capture and data manipulation in gas chromatography. It was decided for several reasons to use a non-dedicated system instead of the many dedicated systems available today. This approach has both advantages and disadvantages.

Probably the biggest advantage is that the system can be tailored to a specific application with respect to both hardware and software without losing the ability for more general applications. This system can therefore even be used for laboratory administration with applications like word processing and database management. Existing software can easily be adapted to specific applications while new software can be added — a feature which is not available on most dedicated commercial systems.

Another advantage of a system as discussed in this paper is that the raw data, *e.g.* a chromatogram, can be stored on a floppy disk, while with commercial integrators or dedicated microprocessors the raw data is usually lost and only the results of calculations are stored. The availability of the raw data allows for the possibility of human intervention when an unusual chromatogram causes the programs to make incorrect calculations.

It is also possible to use much higher sampling speeds than is possible with commercial integrators. This is useful if very fast peaks (like inlet peaks) have to be measured accurately.

A disadvantage of an average eight-bit microcomputer system, like the APPLE II, is that core memory and disk storage space are limited. The number of points that can be sampled for one chromatogram depends on the complexity and size of the program used for sampling. In the programs used in this study the maximum number of points for one chromatogram ranged from 1000 to just over 4000. The number of chromatograms that can be stored on one disk are also limited to about 50 chromatograms of 1000 points each if stored as 12-bit integer data. It is however possible to expand the APPLE II microcomputer's internal memory to more than 64 kilobytes (although this is expensive) while a hard disk drive with megabyte storage capacity can be added (also expensive and the operation with such a drive is less than ideal because of limitations in the APPLE II's disk operating system).

The operation of an eight-bit microcomputer is usually slower than that of a dedicated system, because no real-time integration programs are yet available, but this is a price that has to be paid for greater flexibility. Operation is also less "user friendly". Both the last two limitations can however be overcome by writing more sophisticated software.

J.B. Wagener and T.S. Buys, Department of Chemistry, University of Pretoria, Hillcrest, Pretoria, South Africa.