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Note

Analysis of data from amino acid and other automated analyses

III. A magnetic tape cassette data logging system for gas chromatographs

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A system utilizing a magnetic tape cassette data logger for the analysis of data from an amino acid analyser has already been described[1]. The basic requirements of a data logger for use with a gas chromatograph are somewhat different in that there is a large linear range over which a flame ionization detector equipped with a suitable amplifier can operate, and the short duration of many peaks. For this reason the logger must be capable of digitizing and recording voltages over a wide range without loss of accuracy, and at a rate sufficient to record an adequate number of data points from the shortest peaks normally encountered.

DESIGN OF THE DATA LOGGING SYSTEM

The gas chromatograph to be provided with a data logger was a Pye 104 Model 64 equipped with flame ionization detectors and a wide-range amplifier. The latter has a separate integrator output, not affected by the attenuation setting, which gives an output of up to 10 V. At an attenuation setting $\times$ 1, full scale deflection on the potentiometric recorder corresponds to an integrator output of 10 mV. Thus a digitizing device with a resolution of 10 μV would ideally give an accuracy of 0.1 % on the most sensitive range of the gas chromatograph. In practice, stability of the digitizing device and of the gas chromatographic system makes this absolute limit of accuracy and sensitivity of limited practical value, but assures more than adequate accuracy under normal operating conditions. The digitizing system selected on this basis was the Advance DVM5P autorange digital voltmeter with printer output option (Advance Instruments, Bishops Stortford, Great Britain). The output consists of five binary coded decimal (BCD) numbers corresponding to the displayed voltage, one BCD number for range (automatically selected), and a single output for sign. All outputs are positive logic at TTL levels (logic 0 $<$ 0.5 V, logic 1 $>$ + 2.4 V and $<$ + 5 V).

The input terminals of the digital voltmeter were connected to the integrator output of the ionization amplifier. This system displays the output from the amplifier continuously, new measurements being made at the maximum operating speed of the digital voltmeter (5 readings per sec, approximately). The reading rate, and hence the command for the data logger to record the data, must be controlled to make voltage measurements and record this data at a rate which can be selected to suit the chromatographic data being logged. This requires a 5-V pulse of duration greater than 200 msec to be applied, at the selected intervals, to the digitize input on the printer output socket of the digital voltmeter (voltmeter in the hold mode). A simple timer, based on a 555 integrated circuit was designed to perform this function, and the circuit is shown in Fig. 1. The time intervals provided are 0.5, 1, 2 and 4 sec, and the pulse length is approximately 250 msec. The unit was conveniently enclosed in a Type A instrument case together with a 5-V regulated power supply (RS Components, London, Great Britain). The switch for the end-of-run indicator described below was also included in this unit.

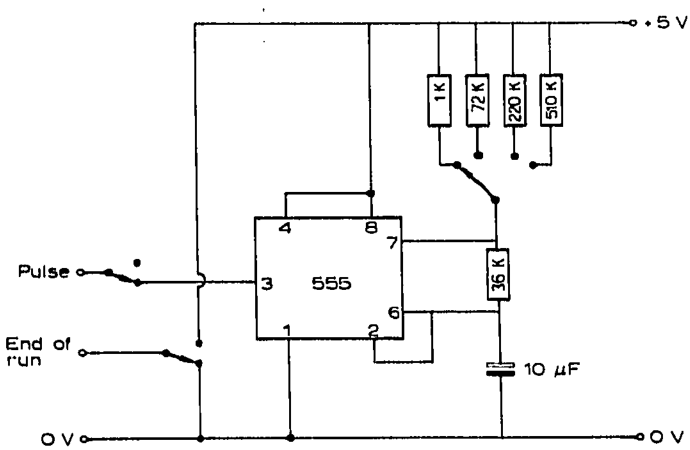

Fig. 1. Timer unit and end-of-run switch. Power supply omitted.

The recording device chosen was a DL1B magnetic tape cassette data logger (Digitronix, Milton Keynes, Great Britain). This will record up to 32 bits of parallel data, *i.e.*, 8 four-bit words[2]. Words 0 and 4 do not give rise to numeric characters on replay[3], and were therefore used for the beginning of record character and the sign. They were connected to produce * and + or − when extended to 8 bit data on normal replay. Of the remaining six words, word 1 was used to record the automatically selected range, and words 2, 3, 4, 6 and 7 the displayed voltage. The recorded data were thus of the form *RDD ± DDD where R is the range and D are the digits displayed on the digital voltmeter. The print command output of the digital voltmeter was connected to the data-true input on the data logger to complete the logging sequence initiated by the pulse from the timer.

When the data from more than one chromatogram are recorded on one cassette some means of including an end-of-run signal in the logged data is required. Although all the available words of the logger are used for each data point, the value of R never exceeds 2 because the maximum output of the ionization amplifier is approximately 10 V. Thus only the first two bits of word 1 need be used (1 and 2 of the 1248 BCD). Thus by providing a facility for changing the third bit from logic 0 to logic 1 by means of a switch mounted in the timer unit, R can be made equal to or greater than 4 whenever an end-of-run signal is required. The interconnections between the three units comprising the data logging system are shown in Fig. 2.

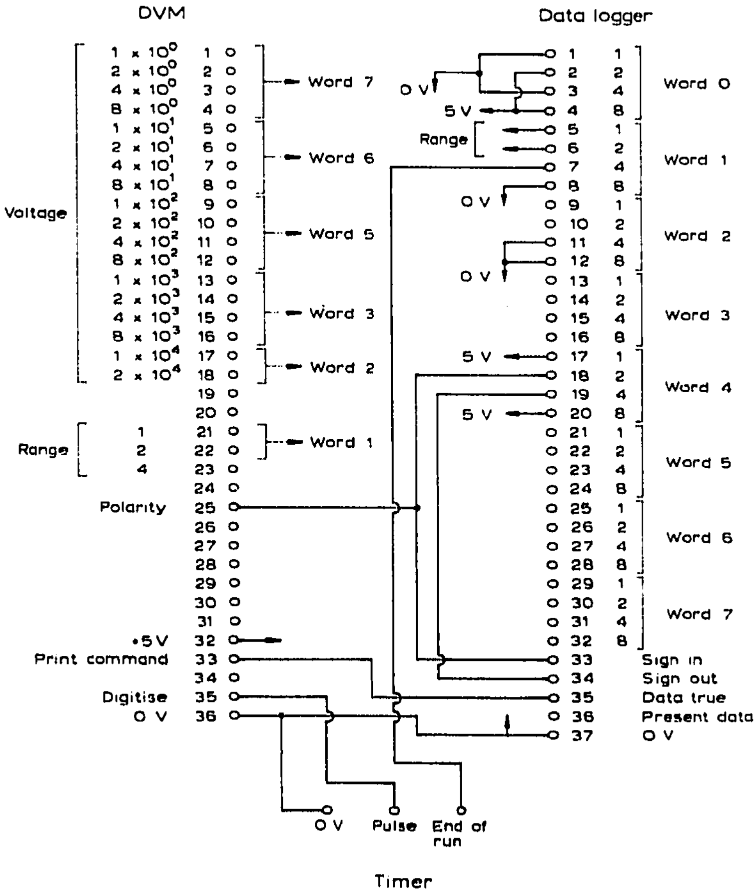

Fig. 2. Interconnections between timer, digital voltmeter (DVM) and data logger.

The data were transcribed to paper tape using the modified replay unit described previously[1]. During the process the * is changed into a new-line character to make the format of the logged data compatible with the computer we are using. This transcription will no longer be necessary when cassette replay facilities become available at the computer.

THE PROGRAM

The program is a modified version of an existing general-purpose integration program[4]. The following major changes were made:

(*a*) The READ and associated statements were changed to take account of the unusual data format dictated by the hardware.

(*b*) The end-of-run signal was taken as two consecutive range values equal to or greater than 4. After the output of results from one run the integration of the next run was commenced, and this process was continued until the raw data file was exhausted (END = label in all READ statements).

(*c*) The first peak with maximum greater than 4 V after the start of a run was assumed to be the solvent peak and all retention times were calculated from the start of this peak. Also the area of this peak was not taken into account in percentage calculations. The value of the total peak area excluding the solvent peak was output. This could prove useful by providing a measure of the total weight of a heterogenous mixture injected, *e.g.*, total fatty acids from a lipid sample and hence a measure of the weight of lipid.

(*d*) An error trap routine was incorporated to prevent the program from being halted if a data error occurs[5]. The subroutine called by the error trap assigns values of zero to the range and voltage reading. This data point will subsequently be rejected by the program as a noise spike if it does not relate to the values of the adjacent data points.

DISCUSSION AND CONCLUSIONS

The system described has all the advantages of the data logging system for amino acid analyses described previously[1], namely low price, compactness, and silent operation. Data recorded on cassettes may be conveniently handled as input into a number of programmable calculators for analysis. The digital voltmeter used can measure wide ranges of current and resistance, in addition to voltage and this makes the system suitable for logging data from a wide range of instruments.

REFERENCES

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