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Note

Analysis of data from amino acid and other automated analysers

I. Use of data loggers with magnetic tape cassettes

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We have recently been concerned with the problem of recording a considerable amount of data from analytical instruments for subsequent analysis by a remote computer. Data loggers that record digital information on cassettes of magnetic tape offer many advantages over conventional machines that record on punched paper tape. The advantages are that a large amount of data can be recorded on a relatively compact cassette and the machine is cheap, compact, and quiet in operation. In addition the raw data on magnetic tape are in a suitable form for the limited analyses that can be carried out by programmable calculators that are available in most laboratories.

A current disadvantage of recording data on cassettes of magnetic tape rather than on punched paper tape is that many computers do not have peripherals for handling magnetic tape cassettes. In addition, transfer of the data on to punched tape produces a format often unsuitable for input into the computer.

The present paper is concerned with the modifications and additions that permit the superior features of cassette loggers to be utilized for the analysis of data by computer, with particular reference to that arising from automated amino acid analysers.

EXPERIMENTAL

Amino acid analyses were carried out on a Jeol JLC-6AH Amino Acid Analyser. The output from the 570-nm channel was fed into a Digitronics AL-4 Data Logger with an input range of 0–100 mV. The output was recorded every 8 sec, and scan count was included. A Digitronics ADR-1 replay unit equipped with a parallel output interface was used to drive a Facit 4070 tape punch (75 characters/sec). Data were processed by an ICL 1906A computer.

RESULTS

The Jeol amino acid analyser has separate outputs for recorder and integrator (or data logger). The integrator output (0–100 mV) is taken directly from the detector system, and is independent of the scale expansion setting on the recorder. Thus the data logger can record the output over the whole range of the detector system.

In the cassette logger used, analogue data are converted into binary coded decimals by an integral analogue to digital convertor and recorded in this form. On replay this is extended to the conventional seven bit (plus parity bit) ASC11 (CCITT Alphabet No. 5) code. If every character recorded were extended in an identical way, only the nine digits and characters corresponding to BCD 10-15 (: ; < = > ?) could be generated. To overcome this restriction, the first character of each group of four is extended differently[1] and can give rise to the characters

Space ! " £ S % & ' ( ) * + − , . /

Thus the three digit data can be signed, and an end of record character can be inserted. In addition to output of recorded data, the replay unit can generate carriage return and new line characters, but this facility is not available when using the parallel output option required for driving a tape punch.

Replay of data recorded as described in experimental produces on replay repeating units of eight characters of the form:

*001+032*002+030*003+025.....

The * is the beginning of record character and is followed by the scan count (three digits) and the voltage output from the amino acid analyser (three digits in units of 0.1 mV and sign). The absence of newline characters could be overcome if the computer could recognize the asterisk as the beginning of a record, but although routines for carrying this out exist for many small computers, it cannot be conveniently organised within the George 4 operating system in use with the 1906A. It was therefore decided to modify the replay unit so that all asterisks would be converted into newline characters on replay. Fortunately the ASC11 (and 1900) code for * consists of the two holes corresponding to a new line character plus two additional holes, thus making it possible to suppress the extra two channels by a simple modification of the serial to parallel interface printed circuit board in the replay unit (Fig. 1). The existing interface board had vacant spaces for the two extra digital integrated circuits required (7430 and 7400) and power was taken from the unit. Thus the modified format produced is a single scan count and voltage output on each record. This is suitable for direct input into the filestore of the computer.

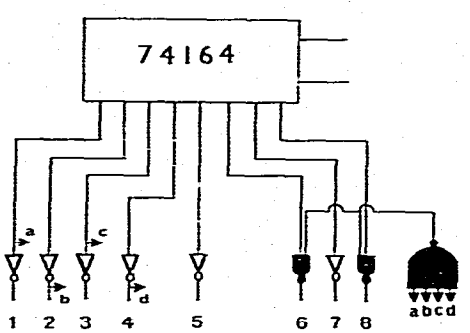

Fig. 1. Modifications (shown shaded) to serial to parallel interface board of replay unit. a–a to d–d are interconnected; 1–8 are output channels to the tape punch.

Design of a start of run indicator

The programmer (process controller) of the Jeol JLC-6AH Amino Acid Analyser comprises a moving paper roll passing through an opto-electronic reading device consisting of eight filament bulbs and phototransistors. On illumination the voltage across the phototransistors falls from 14 V to 0 V. The operation of the first sampler is the first unique programmed event on starting a new run. Thus by attaching leads to both sides of the appropriate phototransistor, the voltage drop can be used as an indication of when each run commences.

The Digitronics AL-4 data logger records, in addition to up to four channels of signed three digit data, a three digit 'scan count', which shows the number of data points recorded. The scan count may be reset to zero manually or by shorting two contacts on the remote control socket on the instrument. Thus, if the fall of voltage across the phototransistor could activate the shorting of these contacts, an indication of the beginning of a run would appear in the logged data. The device designed to carry out this function is shown in Fig. 2. It is based on a 555 integrated circuit timer, which, on being triggered by the voltage drop across the phototransistor remains in an 'on' state for a time determined by the values of C and R (ref. 2) (in this instance about 50 sec). The output from the timer is sufficient to operate the relay (D.I.L. reed relay, R.S. Components Ltd.) that operates the scan count reset. The whole device was built on a small piece of Veroboard and power was supplied by a 9-V dry battery. The high input impedance of the 555 prevents any interference with the correct functioning of the amino acid analyser programmer unit.

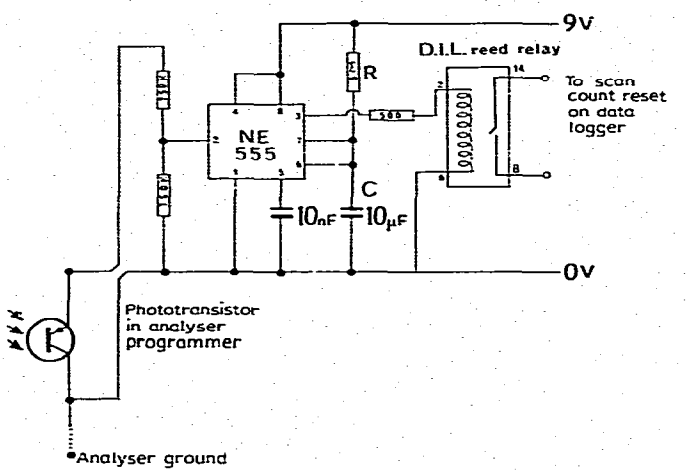

Fig. 2. Circuit diagram of start of run indicator.

Software for the integration of the amino acid chromatograms

The programme we are using is written in Fortran, and is a modified version of an existing general purpose chromatograph peak integration programme[3]. The following major changes were made:

(a) The voltage data are converted to absorbance values and multiplied by 10^6. This large factor enables data values of the same order as expected by the original programme to be provided. (b) The programme is terminated by incorporating an

END = label expression in all READ statements. (c) An error trap routine was incorporated to prevent the programme being halted if a data error occurs[4]. The subroutine called by the error trap assigns arbitrary values to the scan count and voltage reading that will subsequently be rejected as a noise spike by the original programme. (d) A bypass for scan count 000 following 999 was written into the programme to prevent it being interpreted as the end of a run. (e) The end of run signal was taken to be a scan count of 000 not following 999.

DISCUSSION AND CONCLUSIONS

The system described overcomes the problems encountered in processing data from automated amino acid analysers, which have been recorded on magnetic tape cassettes, and consequently has numerous advantages over conventional systems. Use was made of the extra data storage capacity of the cassettes by incorporating the start of run indicator described, thus permitting the sequential evaluation of several chromatograms. Data from other analytical instruments can be recorded and evaluated in a similar manner, using the same modified replay unit and tape punch.

We are currently developing a programme that will identify amino acids on the basis of the retention times of a standard run, analysed as the first of a series of runs. The minor drawback of having to replay data on to punched tape will be overcome when cassette replay facilities are provided at the computer we are using.

ACKNOWLEDGEMENT

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4 *Fortran 32K/48K Disc Compilers*, ICL Technical Publications, Reading, 1970.