On-line pulse radiolysis data handling program

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pages + tables + illustrations

Abstract

The report describes a program for PDP8/E, 4k for the initial handling and presentation of pulse radiolysis data. The data are displayed on an oscilloscope or printed on a Teletype typewriter. A variety of algoritms for different kinetic types is available. A data reduction is obtained as only the accepted data are read out by means of the Teletype punch for further data handling.

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Hardware background

A simplified diagram of the hardware system is shown in figure 1. The data transfer from the data collection equipment to the 'on-line' computer is started by depressing a pushbutton.

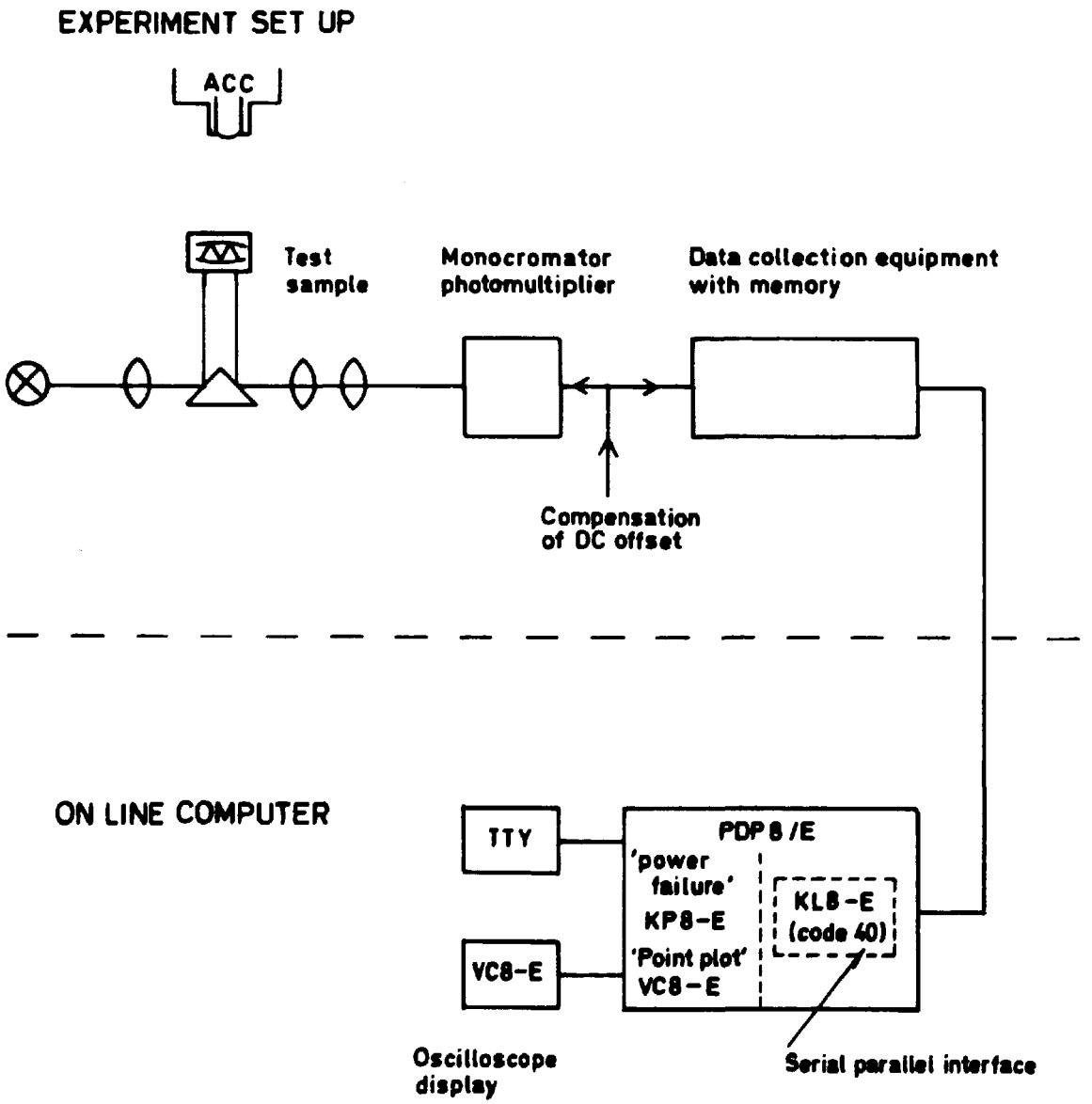


Figure 1. Hardware block diagram.

Principles of data handling

Definitions are given in figure 2 together with a sketch of a central part of the data collection equipment. Note that the curve shown is ideal. The actual curve is divided into three sections (figure 3). The basic calculations in the program are carried out as follows:

The average current delivered at zero absorbtion in the sample (100% light) is

$$J_o = J - \frac{J'}{G} \tag{1}$$

The photomultiplier current is

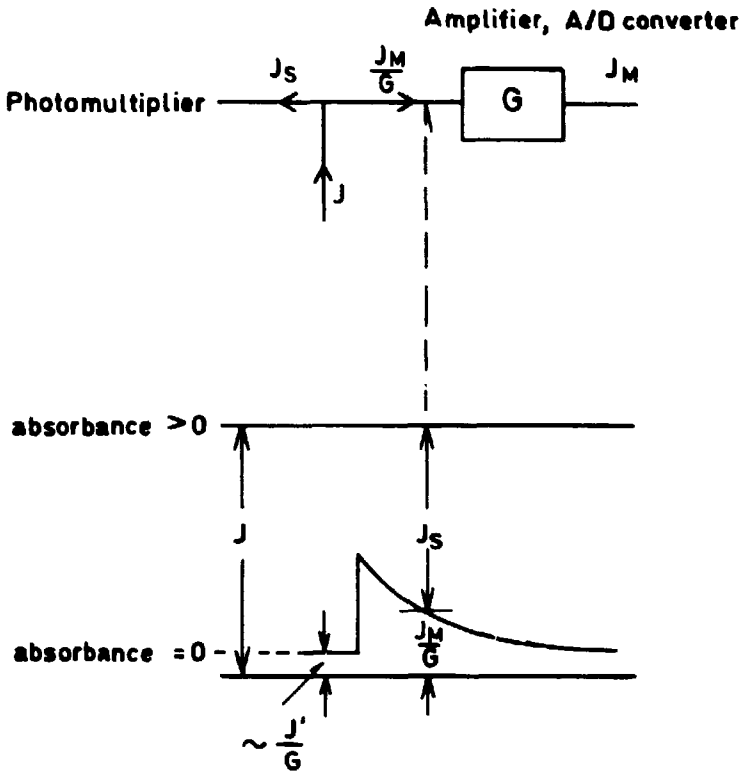
$$J_s = J - \frac{J_M}{G} \tag{2}$$

The absorbance is

$$D = \log \frac{J_o}{J_s} \tag{3}$$

or

$$D = \log \frac{J - \frac{J'}{G}}{J - \frac{J_M}{G}} \tag{4}$$



J_M measured data number 0 ... 511
G "current to number" gain (manual adjustm.) 1 ... 100
J compensation current (manual adjustm.) 100 ... 500
$J' = (J_M(1) + J_M(2) + \ldots J_M(8))/8$
J_s photomultiplier current

Figure 2. Central region of data collection equipment. Hardware and definitions.

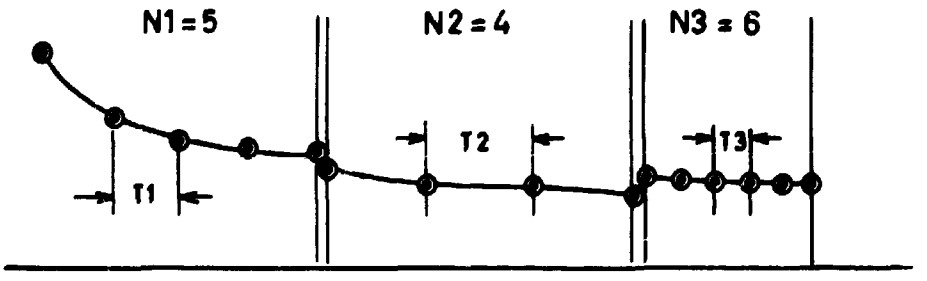


Figure 3. Definition of point number and interval time for the curve segments. ● = collected experimental data. N1, N2, N3 is program output (IN the equipment N2=3,N3=5).

The data handling program

The flow diagram of the pulse radiolysis data handling program (Risø-8-13-U) is shown in figure 3. One main programming problem was the limitation due to the core memory size, which is only 4k (4048, 12 bit words). For this reason 'destructing operations' were allowed. That is, only one table area x is reserved, and this is first used for the initial data, which are then spoiled when the calculated data are stored. The data collection memory however is used for back-up storage. Thus the initial data may be restored by repeated use of the read-in botton.

Another basic problem was the communication with the operator. It was decided to use in general a conversational method. For decoding economy the answer is typically a single digit with up to four values. Some of the constants are often unchanged during a set of experiments. For those constants two levels of questions may be read out. At the first level, changes or no changes are decided. If no changes are wanted, the second level questions are omitted.

Noise produced in the initial part of the curve figure 2 can give a negative signal J'/G, which is below the 'absorbtion = 0' line. In this case the analog to digital converter produces zero output. An error message is printed and the operator can stop the program or force it to go on.

Scaling of the logaritm of noisy data J_M introduces special difficulties. When J_M approaches J', equations (1) and (2), D in equation (3) approaches zero. Then log D and 1/D go to infinite. At high log D and 1/D values (numerical) a serious compression of the corresponding curve will take place. For that reason the limitation of the density data D (figure 4) was introduced.

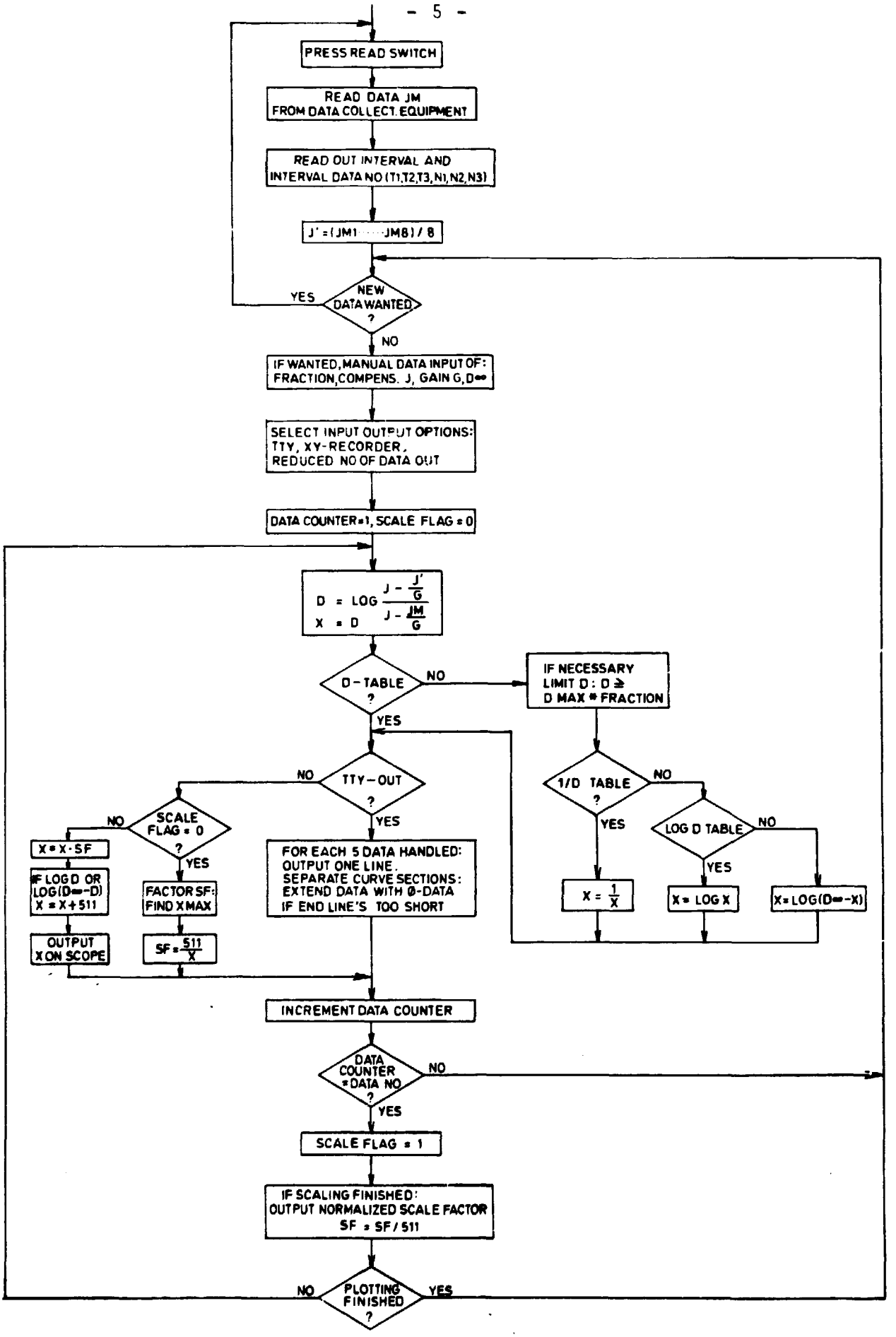


Figure 4. Flow diagram.

A typical Teletype record of the operator communication (with authors comments) is shown in table 1. An abbreviated version of the output table is included. Figure 5 shows a typical oscilloscope display (light emitting diode test input).

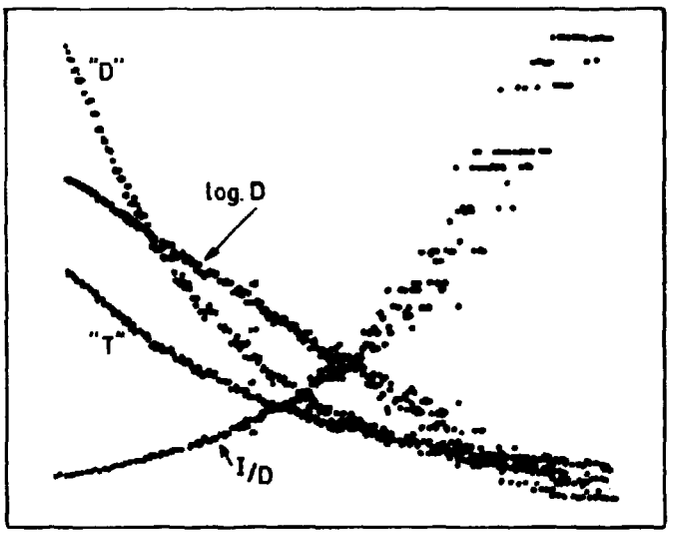


Figure 5. Display output example.
Ordinate 8 cm: 1 machine unit (number range = 511)
Abscissa 10 cm = 270 µsec
T = original data (transmittance)

/Communication (computer output underlined)	/ Comments
PRESS READ	/INPUT DATA FROM EXPERIMENT
SET SWITCHES	/INPUT/OUTPUT OPTION SELECTION (SCOPE)
N1, N2, N3	
7Ø 1Ø1 1Ø1	/NUMBER OF POINTS IN EACH
I1, I2, I3	/CURVE SEGMENT
16 16 16	/SAMPLING INTERVALS = 1.E-6 sec = 1 μsec
N?	/NEW CONSTANTS?
1	/YES
26Ø.	/DATA LIMIT VALUE (Ø...511)
.Ø5	/FRACTION OF ABOVE LIMIT (see fig.1)
255.	/OFFSET Ø...511
G?	/GAIN CONSTANT?
1	/YES
2.	
1=D,2=1/D,3=LOGD,4=LOGDU	
1	/DISPLAY ON SCOPE.THEREFORE SCALING.
SCF= .36ØE Ø1	/SCALE FACTOR = 0.036.
N?	/(0.036 D) IS DISPLAYED.SCOPE RANGE=1.
G?	/INPUT/OUTPUT OPTION SELECTION (TTY)
1=D,2=1/D,3=LOGD,4=LOGDU	
1	/FIRST CURVE SEGMENT (N1,T1)
.277E ØØ .272E ØØ .266E ØØ .266E ØØ .264E ØØ	
.259E ØØ .253E ØØ .251E ØØ .253E ØØ .245E ØØ	
⋮ ⋮ ⋮ ⋮ ⋮	
.125E ØØ .119E ØØ .119E ØØ .115E ØØ .119E ØØ	
.111E ØØ .111E ØØ .1Ø6E ØØ .111E ØØ .115E ØØ	
	/SECOND CURVE SEGMENT (N2,T2)
.111E ØØ .11ØE ØØ .11ØE ØØ .11ØE ØØ .1Ø2E ØØ	
.1Ø2E ØØ .1Ø1E ØØ .1Ø2E ØØ .1Ø2E ØØ .1Ø1E ØØ	
⋮ ⋮ ⋮ ⋮ ⋮	
.336E-Ø1 .3Ø7E-Ø1 .3Ø7E-Ø1 .346E-Ø1 .356E-Ø1	
.336E-Ø1 .ØØØE ØØ .ØØØE ØØ .ØØØE ØØ .ØØØE ØØ	
	/THIRD CURVE SEGMENT (N3,T3)
.3Ø7E-Ø1 .375E-Ø1 .298E-Ø1 .3Ø7E-Ø1 .298E-Ø1	
.259E-Ø1 .336E-Ø1 .336E-Ø1 .336E-Ø1 .259E-Ø1	
⋮ ⋮ ⋮ ⋮ ⋮	
.452E-Ø2 .1Ø9E-Ø1 .725E-Ø2 .361E-Ø2 -.1Ø7E-Ø1	
.114E-Ø2 .ØØØE ØØ .ØØØE ØØ .ØØØE ØØ .ØØØE ØØ	

Table 1. Teletype. Communication and output example.