



On-line pulse radiolysis data handling program

Højberg, Kristian Søren; Pagsberg, P.; Hansen, K.B.; Jacobsen, G.

Publication date:
1973

Document Version
Publisher's PDF, also known as Version of record

[Link back to DTU Orbit](#)

Citation (APA):
Højberg, K. S., Pagsberg, P., Hansen, K. B., & Jacobsen, G. (1973). *On-line pulse radiolysis data handling program*. Risø National Laboratory. Risø-M No. 1643

General rights

Copyright and moral rights for the publications made accessible in the public portal are retained by the authors and/or other copyright owners and it is a condition of accessing publications that users recognise and abide by the legal requirements associated with these rights.

- Users may download and print one copy of any publication from the public portal for the purpose of private study or research.
- You may not further distribute the material or use it for any profit-making activity or commercial gain
- You may freely distribute the URL identifying the publication in the public portal

If you believe that this document breaches copyright please contact us providing details, and we will remove access to the work immediately and investigate your claim.

Danish Atomic Energy Commission
Research Establishment Risö

ELECTRONICS DEPARTMENT

On-line pulse radiolysis data handling program

by

K. Söe Højberg, Palle Pagsberg,
K.B. Hansen, Gunnar Jakobsen

August 1973

R-8-73

<p>Title and author(s)</p> <p>On-line pulse radiolysis data handling program</p> <p>by</p> <p>K. Søren Højberg, Paile Pagsberg, K.E. Hansen, Gunnar Jakobsen</p>	<p>Date August 1973</p>
<p>pages + tables + illustrations</p>	<p>Department or group</p> <p>Electronic</p>
<p>Abstract</p> <p>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 algorithms 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.</p>	<p>Group's own registration number(s)</p> <p>R-8-73</p>
<p>Available on request from the Library of the Danish Atomic Energy Commission (Atomenergikommissionens Bibliotek), Risø, Roskilde, Denmark. Telephone: (03) 35 51 01, ext. 334, telex: 5072.</p>	<p>Copies to</p>
	<p>Abstract to</p>

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.

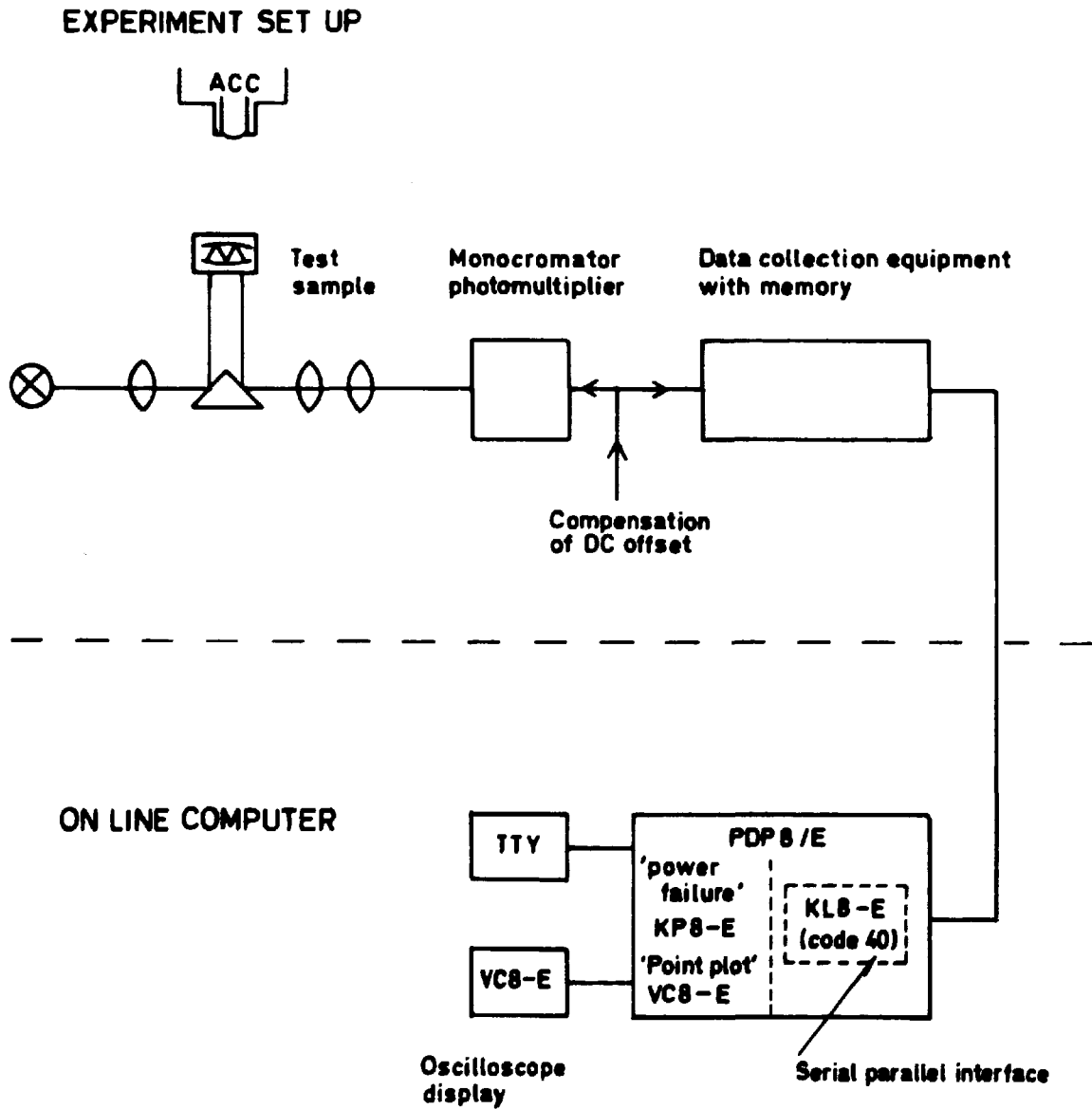


Figure 1. Hardware block diagram.

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 absorption in the sample (100% light) is

$$J_o = J - \frac{J'}{G} \quad (1)$$

The photomultiplier current is

$$J_s = J - \frac{J_M}{G} \quad (2)$$

The absorbance is

$$D = \log \frac{J_o}{J_s} \quad (3)$$

or

$$D = \log \frac{J - \frac{J'}{G}}{J - \frac{J_M}{G}} \quad (4)$$

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 button.

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 'absorption = 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 logarithm 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.

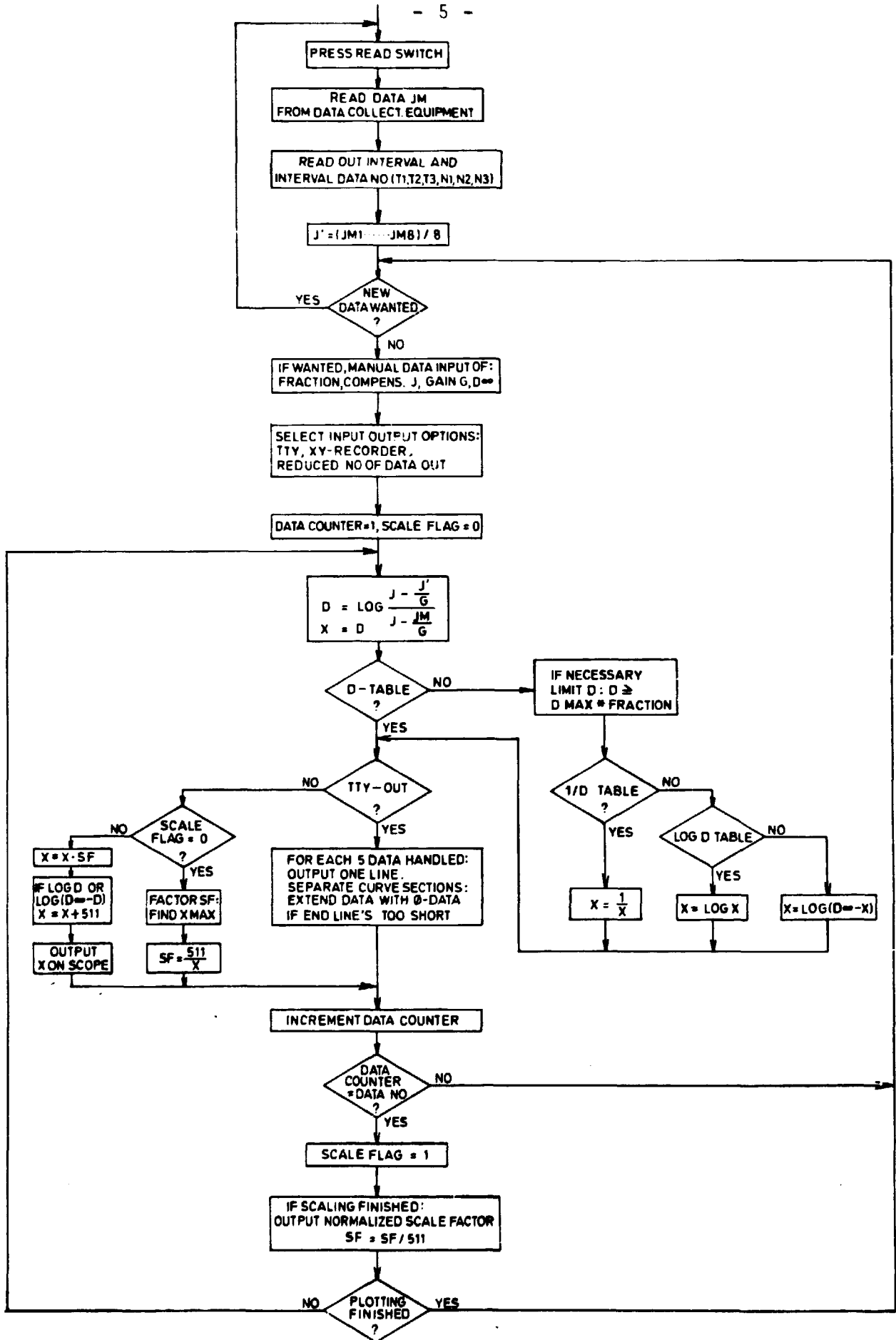


Figure 4. Flow diagram.

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).

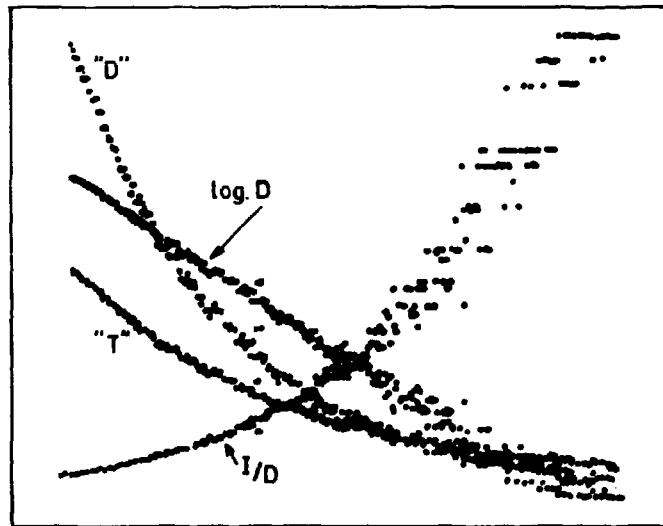


Figure 5. Display output example.

Ordinate 8 cm: 1 machine unit (number range = 511)

Abscissa 10 cm = 270 μ sec

T = original data (transmittance)

<p><u>/Communication (computer output</u> <u>underlined)</u></p> <p><u>PRESS READ</u> <u>SET SWITCHES</u> <u>N1, N2, N3</u> <u>70 101 101</u> <u>I1, I2, I3</u> <u>16 16 16</u></p> <p><u>N?</u> <u>1</u> 260. .05 255. <u>G?</u> <u>1</u> 2. <u>1=D,2=1/D,3=LOGD,4=LOGDU</u> <u>1</u> <u>SCF= .360E 01</u> <u>N?</u></p> <p><u>G?</u></p> <p><u>1=D,2=1/D,3=LOGD,4=LOGDU</u> <u>1</u></p>	<p>Comments</p> <p>/INPUT DATA FROM EXPERIMENT /INPUT/OUTPUT OPTION SELECTION (SCOPE) /NUMBER OF POINTS IN EACH /CURVE SEGMENT /SAMPLING INTERVALS = 1.E-6 sec = 1 usec</p> <p>/NEW CONSTANTS? /YES /DATA LIMIT VALUE (0...511) /FRACTION OF ABOVE LIMIT (see fig.1) /OFFSET 0...511 /GAIN CONSTANT? /YES</p> <p>{ /DISPLAY ON SCOPE.THEREFORE SCALING. /SCALE FACTOR = 0.036. /(0.036 D) IS DISPLAYED.SCOPE RANGE=1.</p> <p>/INPUT/OUTPUT OPTION SELECTION (TTY)</p> <p>/FIRST CURVE SEGMENT (N1,T1)</p> <table border="0"> <tr> <td>.277E 00</td> <td>.272E 00</td> <td>.266E 00</td> <td>.266E 00</td> <td>.264E 00</td> </tr> <tr> <td>.259E 00</td> <td>.253E 00</td> <td>.251E 00</td> <td>.253E 00</td> <td>.245E 00</td> </tr> <tr> <td>⋮</td> <td>⋮</td> <td>⋮</td> <td>⋮</td> <td>⋮</td> </tr> <tr> <td>.125E 00</td> <td>.119E 00</td> <td>.119E 00</td> <td>.115E 00</td> <td>.119E 00</td> </tr> <tr> <td>.111E 00</td> <td>.111E 00</td> <td>.106E 00</td> <td>.111E 00</td> <td>.115E 00</td> </tr> </table> <p>/SECOND CURVE SEGMENT (N2,T2)</p> <table border="0"> <tr> <td>.111E 00</td> <td>.110E 00</td> <td>.110E 00</td> <td>.110E 00</td> <td>.102E 00</td> </tr> <tr> <td>.102E 00</td> <td>.101E 00</td> <td>.102E 00</td> <td>.102E 00</td> <td>.101E 00</td> </tr> <tr> <td>⋮</td> <td>⋮</td> <td>⋮</td> <td>⋮</td> <td>⋮</td> </tr> <tr> <td>.336E-01</td> <td>.307E-01</td> <td>.307E-01</td> <td>.346E-01</td> <td>.356E-01</td> </tr> <tr> <td>.336E-01</td> <td>.000E 00</td> <td>.000E 00</td> <td>.000E 00</td> <td>.000E 00</td> </tr> </table> <p>/THIRD CURVE SEGMENT (N3,T3)</p> <table border="0"> <tr> <td>.307E-01</td> <td>.375E-01</td> <td>.298E-01</td> <td>.307E-01</td> <td>.298E-01</td> </tr> <tr> <td>.259E-01</td> <td>.336E-01</td> <td>.336E-01</td> <td>.336E-01</td> <td>.259E-01</td> </tr> <tr> <td>⋮</td> <td>⋮</td> <td>⋮</td> <td>⋮</td> <td>⋮</td> </tr> <tr> <td>.452E-02</td> <td>.109E-01</td> <td>.725E-02</td> <td>.361E-02</td> <td>-.107E-01</td> </tr> <tr> <td>.114E-02</td> <td>.000E 00</td> <td>.000E 00</td> <td>.000E 00</td> <td>.000E 00</td> </tr> </table>	.277E 00	.272E 00	.266E 00	.266E 00	.264E 00	.259E 00	.253E 00	.251E 00	.253E 00	.245E 00	⋮	⋮	⋮	⋮	⋮	.125E 00	.119E 00	.119E 00	.115E 00	.119E 00	.111E 00	.111E 00	.106E 00	.111E 00	.115E 00	.111E 00	.110E 00	.110E 00	.110E 00	.102E 00	.102E 00	.101E 00	.102E 00	.102E 00	.101E 00	⋮	⋮	⋮	⋮	⋮	.336E-01	.307E-01	.307E-01	.346E-01	.356E-01	.336E-01	.000E 00	.000E 00	.000E 00	.000E 00	.307E-01	.375E-01	.298E-01	.307E-01	.298E-01	.259E-01	.336E-01	.336E-01	.336E-01	.259E-01	⋮	⋮	⋮	⋮	⋮	.452E-02	.109E-01	.725E-02	.361E-02	-.107E-01	.114E-02	.000E 00	.000E 00	.000E 00	.000E 00
.277E 00	.272E 00	.266E 00	.266E 00	.264E 00																																																																								
.259E 00	.253E 00	.251E 00	.253E 00	.245E 00																																																																								
⋮	⋮	⋮	⋮	⋮																																																																								
.125E 00	.119E 00	.119E 00	.115E 00	.119E 00																																																																								
.111E 00	.111E 00	.106E 00	.111E 00	.115E 00																																																																								
.111E 00	.110E 00	.110E 00	.110E 00	.102E 00																																																																								
.102E 00	.101E 00	.102E 00	.102E 00	.101E 00																																																																								
⋮	⋮	⋮	⋮	⋮																																																																								
.336E-01	.307E-01	.307E-01	.346E-01	.356E-01																																																																								
.336E-01	.000E 00	.000E 00	.000E 00	.000E 00																																																																								
.307E-01	.375E-01	.298E-01	.307E-01	.298E-01																																																																								
.259E-01	.336E-01	.336E-01	.336E-01	.259E-01																																																																								
⋮	⋮	⋮	⋮	⋮																																																																								
.452E-02	.109E-01	.725E-02	.361E-02	-.107E-01																																																																								
.114E-02	.000E 00	.000E 00	.000E 00	.000E 00																																																																								

Table 1. Teletype. Communication and output example.