# DECUS
## PROGRAM LIBRARY

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| DECUS NO. | 8-133 |
| TITLE | FIRST ORDER KINETICS |
| AUTHOR | Kenneth B. Wiberg |
| COMPANY | Department of Chemistry<br>Yale University<br>New Haven, Connecticut |
| DATE | June, 1968 |
| SOURCE LANGUAGE | |

# FIRST ORDER KINETICS

DECUS Program Library Write-up DECUS No. 8-133

This program is designed to calculate the rate constants and error parameters for first order rate processes. The program provides options for plotting the deviation between observed and calculated quantities on a CRT and for iterating to a "best" infinity value. The program may also be used in other cases in which one wishes to correlate the ln of one quantity with another, as in linear free energy relationships.

Specifications: The program uses most of memory for the main program, the subroutines and data storage. A storage map is:

| | |
|---|---|
| 7-15<br>63-1705 } | Main program |
| 2000-2177 | PLOT Subroutine (attached) |
| 3400-3666 | LSQ Subroutine (DECUS 8 |
| 4000-4057 | MESAGE Subroutine (DIGITAL-8-18-U mod. (see below) |
| 4075-4122 | DECPRT Subroutine (DIGITAL-8-22-U) |
| 4200-4311 | SICONV Subroutine (DIGITAL-8-28-U) |
| 4315-4366 | FIX and FLOAT Subroutines (Cf Floating Point System Manual) |
| 4400-4534 | MINMAX Subroutine (attached) |
| 4757-7577 | Floating Point Interpreter "C" (8-5C-S) |
| 2200-2377 | ABS array (holds absorbance values) |
| 2400-2577 | DIF array (holds devations between observed and calculated y's) |
| 2600-2777 | CALC array (holds calculated values of y's) |
| 3000-3177 | Y array (holds observed y values) |
| 3200-3377 | T array (holds values of time) |

The MESAGE subroutine was modified by replacing the

```
TLS
TSF
JMP. -1
```

printing sequence with

```
TSF
JMP. -1
TLS
```

which is compatible with the typeout routine in the floating point interpreter.

The program is written for a 4K PDP-8. If an oscilloscope display (Type 34D) is available, it may be used to examine the deviations between observed and calculated quantities. If it is not available, the program will still operate normally.

Description:

The program is loaded in the normal fashion using the binary loader. If the binary tape which is supplied is used, it will stop half way through (after loading the floating point interpreter). The CONTINUE key is then depressed in order to load the remainder of the program. The binary tape contains the main program and all needed subroutines.

The starting address is 200. When started, the computer will type:

```
FIRST ORDER KINETICS
DATA IN ABSORBANCE, M=1
DATA IN TRANSMITTANCE, M=2
DATA IN VOLUME, M=3
M=
```

The operator then types the proper number and return. Then appears

```
N IS THE NUMBER OF DATA POINTS
N=
```

The operator types the number of points. Then:

```
THE INFINITY VALUE=
```

The operator types the value of the measured quantity which is expected at infinite time. Then follows

```
NOW TYPE OBSERVED VALUES AND TIMES
```

The operator types the observed quantity and the corresponding time, and does this N times. As a check, when the last point has been accepted, there is typed:

```
ALL DATA HAVE BEEN ACCEPTED
```

If M=1 or 3, the rate constant is calculated by the subroutine LSQ (cf. DECUS 8 ) using

$$y_i = \ln (ABS_i - ABS_\infty) = m t_i + b$$

The rate constant and other quantities are typed as well as the calculated and observed y's and the deviation. (cf. the following output sheet, Fig 1) If M=2, there is typed

100 PC TRANSMITTANCE=

The operator types the value of the measured quantity when no light absorption occurs. Then follows:

O PC TRANSMITTANCE=

The dark current is then typed. If the former quantity is called MAX and the latter MIN, the absorbance values are given by

$$ABS_i = \frac{1}{2.303} \quad LN \quad \left(\frac{MAX-MIN}{TOBS-MIN}\right)$$

where TOBS is the observed value of transmittance at the given time. The remainder of the calculation proceeds as before.

After the data have been typed, there appears

IF PLOT IS DESIRED, RAISE KEY 1, PRESS CONTINUE

If the oscilloscope display is attached and one wished to examine the deviation as a function of time, switch register key 1 is raised and CONTINUE is depressed. The display will continue as long as key 1 remains up.

The plot is formed by first searching for the maximum and minimum values in the arrays using the subroutine MINMAX which is a modification of our standard version. Having the minimum and maximum values, the subroutine PLOT scales all values to be in the range 0-1777 and then plots the x and y axes, and the points in the DIF array. This is a particularly valuable option for it permits the user to quickly see if his data fit a first order process. One which fits well gives the type of scatter seen in Fig 2a, whereas one which does not (because it is not a first order reaction or because a poor infinity value was chosen) gives a curve of the type seen in Fig 2b.

When key 1 is dropped, there appears

ITER IS THE NUMBER OF ITERATIONS, ITER=

If the value -1 is given, the computer halts. Pressing CONTINUE restarts the program at the beginning. If the value 0 is given, the computer will print out the observed quantities (absorbance or volume) and the values obtained from the calculated y's. The computer then halts and may be restarted by depressing the CONTINUE key. If a positive integer is given, there will be typed:

MULTIPLY VINF BY

The operator types a value by which the infinity value is to be multiplied in the first iteration step. Then appears

VINF=

The operator types the infinity value to be used (usually the one given previously. If MODE=2, the infinity value must be given in absorbance rather than transmittance. The infinity absorbance may be obtained by first using ITER=0. After the data have been typed, depressing CONTINUE will again permit a plot to be observed and iterations to be carried out.

The computer will perform the desired number of iterations. Whenever the rms deviation is found to increase, the fractional change in the multiplier is halved, and the reciprocal is taken for the next iteration step. Thus, if the value typed above were 1.1 (giving a 10% increase in VINF in the first iteration), and the rms deviation were found to increase, the next step would use as a multiplier 1/1.05 or 0.952. This multiplier would continue to be used until the rms deviation no longer decreases. Then, the multiplier is again changed and will be 1.024.

This is not the ideal way in which to iterate to the "best" infinity value since the least squares criterion remains the minimization of the error in y, not in the observed quantity (absorbance or volume). However, a better calculation is not possible with the storage available in a 4K computer, and in our experience, the difference in result between the present calculation and the "correct" method is normally negligible.

The program permits the use of up to 42 data points. A larger number of points will lead to malfunction. If a double space is desired between lines of output data, the following locations may be changed:

| Location | Now | Change to |
|---|---|---|
| 55 | 0000 | 7777 |
| 1565 | 7200 (CLA) | 7240 (CLA CMA) |
| 1244 | 7200 (CLA) | 7240 (CLA CMA) |
| 1236 | 7200 (CLA) | 7240 (CLA CMA) |

```
FIRST ORDER KINETICS
DATA IN ABSORBANCE, M = 1
DATA IN TRANSMITTANCE, M = 2
DATA IN VOLUME, M = 3
M = 1
N IS THE NUMBER OF DATA POINTS
N = 12
THE INFINITY VALUE =0.135
NOW TYPE OBSERVED VALUES AND TIMES
0.700 0
0.665 10
0.626 20
0.598 30
0.568 40
0.510 60
0.463 80
0.425 100
0.373 140
0.304 180
0.245 240
0.200 320
ALL DATA HAVE BEEN ACCEPTED
THE RATE CONSTANT IS +0.6742559E-02
THE INTERCEPT IS -0.5654722E+00
THE RMS ERROR IS +0.2329548E-01
R = +0.9993565E+00
THE PERCENT ERROR IN K IS +0.6703959E+00
        T                Y              YCALC              DIF
+0.0000000E+00  -0.5709294E+00  -0.5654722E+00  +0.5457162E-02
+0.1000000E+02  -0.6348778E+00  -0.6328978E+00  +0.1979947E-02
+0.2000000E+02  -0.7113107E+00  -0.7003234E+00  +0.1098728E-01
+0.3000000E+02  -0.7700277E+00  -0.7677490E+00  +0.2278685E-02
+0.4000000E+02  -0.8370172E+00  -0.8351746E+00  +0.1842617E-02
+0.6000000E+02  -0.9808293E+00  -0.9700257E+00  +0.1080358E-01
+0.8000000E+02  -0.1114741E+01  -0.1104876E+01  +0.9864091E-02
+0.1000000E+03  -0.1237874E+01  -0.1239728E+01  -0.1853942E-02
+0.1400000E+03  -0.1435484E+01  -0.1509430E+01  -0.7394647E-01
+0.1800000E+03  -0.1777856E+01  -0.1779132E+01  -0.1276254E-02
+0.2400000E+03  -0.2207275E+01  -0.2183686E+01  +0.2358818E-01
+0.3200000E+03  -0.2733367E+01  -0.2723091E+01  +0.1027536E-01

IF PLOT IS DESIRED, RAISE KEY 1, PRESS CONTINUE
```

Fig. 1a Typical run using mode 1 (data in absorbance). The program continues after that shown by asking for the number of iterations. The quantities typed by the operator are underlined.

```
FIRST ORDER KINETICS
DATA IN ABSORBANCE, M = 1
DATA IN TRANSMITTANCE, M = 2
DATA IN VOLUME, M = 3
M = 2
N IS THE NUMBER OF DATA POINTS
N = 6
THE INFINITY VALUE =0.8328
NOW TYPE OBSERVED VALUES AND TIMES
.2995 0
.3366 20
.3704 40
.4090 60
.4758 100
.7310 320

ALL DATA HAVE BEEN ACCEPTED
100 PC TRANSMITTANCE = 1.1
0 PC TRANSMITTANCE = 0.1
THE RATE CONSTANT IS +0.6754450E-02
THE INTERCEPT IS -0.5707473E+00
THE RMS ERROR IS +0.4871432E-02
R = +0.9999778E+00
THE PERCENT ERROR IN K IS +0.1351247E+00
        T                Y              YCALC              DIF
+0.0000000E+00   -0.5708574E+00   -0.5707473E+00   +0.1100301E-03
+0.2000000E+02   -0.7113739E+00   -0.7058364E+00   +0.5537509E-02
+0.4000000E+02   -0.8370701E+00   -0.8409254E+00   -0.3855347E-02
+0.6000000E+02   -0.9807610E+00   -0.9760143E+00   +0.4746675E-02
+0.1000000E+03   -0.1237778E+01   -0.1246192E+01   -0.8413791E-02
+0.3200000E+03   -0.2734048E+01   -0.2732171E+01   +0.1876831E-02

IF PLOT IS DESIRED, RAISE KEY 1, PRESS CONTINUE

ITER IS THE NUMBER OF ITERATIONS, ITER = 0
THE RATE CONSTANT IS +0.6754450E-02
THE INTERCEPT IS -0.5707473E+00
THE RMS ERROR IS +0.4871432E-02
R = +0.9999778E+00
THE PERCENT ERROR IN K IS +0.1351247E+00
THE RMS ERROR BASED ON OBSERVED QUANT. IS +0.1794182E-02
THE INFINITY VALUE IS +0.1350141E+00
      TIME          ABSORBANCE          CALC              DIF
+0.0000000E+00   +0.7000547E+00   +0.7001166E+00   -0.6186962E-04
+0.2000000E+02   +0.6259832E+00   +0.6287096E+00   -0.2726435E-02
+0.4000000E+02   +0.5679912E+00   +0.5663254E+00   +0.1665830E-02
+0.6000000E+02   +0.5100395E+00   +0.5118238E+00   -0.1784324E-02
+0.1000000E+03   +0.4250417E+00   +0.4226120E+00   +0.2429723E-02
+0.3200000E+03   +0.1999698E+00   +0.2000919E+00   -0.1220405E-03
```

Fig. 1b Typical run using mode 2 (data in transmittance).

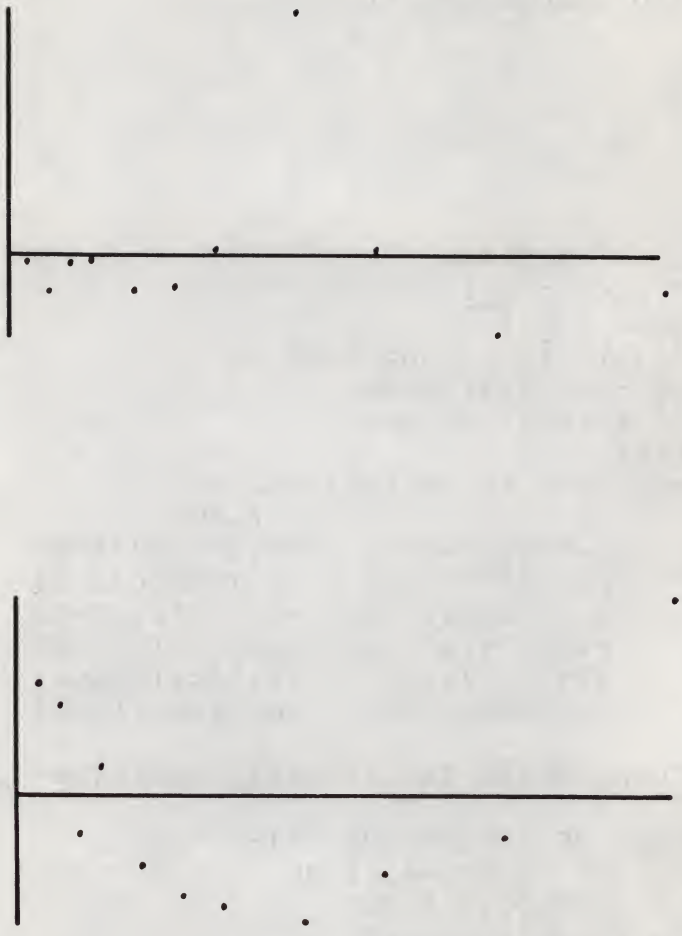

Fig. 2. Computer drawn plots of difference between observed and calculated quantities for a first order reaction. The upper plot corresponds to the data in Fig. 1 and shows a normal scatter. The lower plot is for data which are not well represented as a first order process.

```
                /FIRST ORDER KINETICS
                /PAGE 0
                CALL=4400
                FLPT=4407
                RETURN=5400
                FSQRT=2
                FEXP=6
                FLOG=7
                INPUT=13
                OUTPUT=14
                *7
0007  5600                  5600
0010  0000                  0
0011  0000    IT,           0                        /INDEX REGISTERS
0012  0000    IY,           0
0013  0000    ICALC,        0
0014  0000    IDIF,         0
0015  0000    IABS,         0
                *55
0055  0000                  0
                *67
0067  0000    CORR,         FLTG 0.0
0070  0000
0071  0000
                              /CORRECTION FACTOR
0072  0000    TEST,         FLTG 0.0
0073  0000
0074  0000
0075  0000    FACTOR,       FLTG 0.0
0076  0000
0077  0000
0100  0000    S,            FLTG 0.0
0101  0000
0102  0000
                              /SLOPE
0103  0000    B,            FLTG 0.0
0104  0000
0105  0000
                              /INTERCEPT
0106  0000    R,            0                        /CORRELATION COEFF.
0107  0000                  0
0110  0000                  0
0111  0000    ERROR,        FLTG 0.0
0112  0000
0113  0000
                              /ERROR
0114  0000    G,            FLTG 0.0
0115  0000
0116  0000
                              /FLOAT N
```

```
0117  0000  N,          0                       /NUMBER OF POINTS
0120  3200  LT,         3200                    /LOC(T)
0121  3000  LY,         3000                    /LOC(Y)
0122  2600  LCALC,      2600                    /LOC(CALC)
0123  2400  LDIF,       2400                    /LOC(DIF)
0124  2200  LABS,       2200                    /LOC(ABS)
0125  0000  M,          0                       /MODE
0126  0000  FIN,        FLTG 0.0
0127  0000
0130  0000
                            /FINAL VALUE
0131  4000  MESAGE,     4000
0132  4075  DECPRT,     4075
0133  4200  SICONV,     4200
0134  4315  FIX,        4315
0135  4355  FLOAT,      4355
0136  3400  LSQ,        3400
0137  2000  PLOT,       2000
0140  4400  MINMAX,     4400
0141  0000  ITER,       0
0142  0000  NEGN,       0
0143  7776  M2,         -2
0144  7777  CONST,      FLTG 0.434294
0145  3362
0146  6724
0147  0001  ONE,        1
0150  0000  ZERO,       FLTG 0.0
0151  0000
0152  0000
0153  0000  FLAG,       0
0154  0000  XLOC,       0                       /CONSTANTS FOR PLOT ROUTINE
0155  0000  YLOC,       0
0156  0000  XMIN,       FLTG 0.0
0157  0000
0160  0000
0161  0000  XRNG,       FLTG 0.0
0162  0000
0163  0000
0164  0000  YMIN,       FLTG 0.0
0165  0000
0166  0000
0167  0000  YRNG,       FLTG 0.0
0170  0000
0171  0000
0172  0000  XZERO,      FLTG 0.0
0173  0000
0174  0000
0175  0000  YZERO,      0
0176  0000              0
0177  0000              0
```

```
                /PAGE 1 OF FIRST ORDER KINETICS PROGRAM
                *200
0200  7200  START,     CLA
0201  3141              DCA ITER                /SET FOR NO ITERATIONS
0202  6032              KCC
0203  6046              TLS                     /PREPARE FOR OUTPUT
0204  4531              CALL MESAGE
0205  4543  TEXT /%#
0206  0611  FI
0207  2223  RS
0210  2440  T
0211  1722  OR
0212  0405  DE
0213  2240  R
0214  1311  KI
0215  1605  NE
0216  2411  TI
0217  0323  CS
0220  4543  %#
0221  0401  DA
0222  2401  TA
0223  4011   I
0224  1640  N
0225  0102  AB
0226  2317  SO
0227  2202  RB
0230  0116  AN
0231  0305  CE
0232  5440  ,
0233  1540  M
0234  7540  =
0235  6100  1/
0236  4531              CALL MESAGE
0237  4543  TEXT /%#
0240  0401  DA
0241  2401  TA
0242  4011   I
0243  1640  N
0244  2422  TR
0245  0116  AN
0246  2315  SM
0247  1124  IT
0250  2401  TA
0251  1603  NC
0252  0554  E,
0253  4015   M
0254  4075   =
0255  4062   2
0256  4543  %#
```

```
0257  0401  DA
0260  2401  TA
0261  4011   I
0262  1640  N
0263  2617  VO
0264  1425  LU
0265  1505  ME
0266  5440  ,
0267  1540  M
0270  7540  =
0271  6300  3/
0272  4531              CALL MESAGE
0273  4543  TEXT /%#
0274  1540  M
0275  7540  =
0276  0000  /
0277  4533              CALL SICONV
0300  3125              DCA M
0301  4531              CALL MESAGE
0302  4543  TEXT /%#
0303  1640  N
0304  1123  IS
0305  4024   T
0306  1005  HE
0307  4016   N
0310  2515  UM
0311  0205  BE
0312  2240  R
0313  1706  OF
0314  4004   D
0315  0124  AT
0316  0140  A
0317  2017  PO
0320  1116  IN
0321  2423  TS
0322  4543  %#
0323  1640  N
0324  7540  =
0325  0000  /
0326  4533              CALL SICONV
0327  3117              DCA N
0330  4531              CALL MESAGE
0331  4543  TEXT /%#
0332  2410  TH
0333  0540  E
0334  1116  IN
0335  0611  FI
0336  1611  NI
0337  2431  TY
```

```
0340  4026   V
0341  0114  AL
0342  2505  UE
0343  4075   =
0344  0000  /
0345  4407              FLPT
0346  0013              INPUT
0347  6126              FPUT FIN
0350  0000              FEXT
0351  4531              CALL MESAGE
0352  4543  TEXT /%#
0353  1617  NO
0354  2740  W
0355  2431  TY
0356  2005  PE
0357  4017   O
0360  0223  BS
0361  0522  ER
0362  2605  VE
0363  0440  D
0364  2601  VA
0365  1425  LU
0366  0523  ES
0367  4001   A
0370  1604  ND
0371  4024   T
0372  1115  IM
0373  0523  ES
0374  4543  %#
0375  0000  /
0376  5777              JMP I PG2
0377  0400  PG2,        400
```

```
                /PAGE 2 OF FIRST ORDER KINETICS PROGRAM
                        MIN=167
                        MAX=172
                        TEMP=175
                *400
0400  7200              CLA
0401  1117              TAD N                   /COMPLEMENT N
0402  7041              CIA
0403  3142              DCA NEGN
0404  1124              TAD LABS                /INITIALIZE REGISTERS
0405  3015              DCA IABS
0406  1120              TAD LT
0407  3011              DCA IT
0410  4407  READ,       FLPT
0411  0013              INPUT                   /READ ABS
0412  6415              FPUT I IABS             /AND STORE
0413  0013              INPUT                   /READ TIME
0414  6411              FPUT I IT               /AND STORE
0415  0000              FEXT
0416  2142              ISZ NEGN                /INCREMENT COUNTER
0417  5221              JMP .+2                 /CONTINUE LOOP
0420  5230              JMP NEXT                /CONTINUE PROGRAM
0421  2015              ISZ IABS
0422  2015              ISZ IABS
0423  2015              ISZ IABS
0424  2011              ISZ IT
0425  2011              ISZ IT
0426  2011              ISZ IT
0427  5210              JMP READ                /LOOP
0430  4531  NEXT,       CALL MESAGE
0431  4543  TEXT /%#
0432  0114  AL
0433  1440  L
0434  0401  DA
0435  2401  TA
0436  4010   H
0437  0126  AV
0440  0540  E
0441  0205  BE
0442  0516  EN
0443  4001   A
0444  0303  CC
0445  0520  EP
0446  2405  TE
0447  0400  D/
0450  7200              CLA
0451  1125              TAD M                   /TEST MODE
0452  1143              TAD M2
0453  7440              SZA                     /IS M = 2?
0454  5363              JMP YCALC               /NO: CALC Y'S
0455  7200              CLA
0456  1124              TAD LABS                /YES: CONV. TRANS TO ABS
```

```
0457  3015            DCA IABS
0460  4531            CALL MESAGE
0461  4543  TEXT /%#
0462  6160  10
0463  6040  0
0464  2003  PC
0465  4024   T
0466  2201  RA
0467  1623  NS
0470  1511  MI
0471  2424  TT
0472  0116  AN
0473  0305  CE
0474  4075   =
0475  4000   /
0476  4407            FLPT
0477  0013            INPUT                 /100% TRANS
0500  6172            FPUT MAX
0501  0000            FEXT
0502  4531            CALL MESAGE
0503  4543  TEXT /%#
0504  6040  0
0505  2003  PC
0506  4024   T
0507  2201  RA
0510  1623  NS
0511  1511  MI
0512  2424  TT
0513  0116  AN
0514  0305  CE
0515  4075   =
0516  4000   /
0517  4407            FLPT
0520  0013            INPUT                 /DARK CURRENT
0521  6167            FPUT MIN
0522  5172            FGET MAX
0523  2167            FSUB MIN
0524  6172            FPUT MAX
0525  0000            FEXT
0526  7200            CLA
0527  1117            TAD N
0530  7041            CIA
0531  3142            DCA NEGN
0532  4407  LOOP1,     FLPT
0533  5415            FGET I IABS           /TRANSMITTANCE
0534  2167            FSUB MIN              /-DARK CURRENT
0535  6175            FPUT TEMP
0536  5172            FGET MAX
0537  4175            FDIV TEMP
```

```
0540  0007            FLOG                /LN (T'/T)
0541  3144            FMPY CONST          /LOG = ABS
0542  6415            FPUT I IABS         /STORE ABS
0543  0000            FEXT
0544  2015            ISZ IABS
0545  2015            ISZ IABS
0546  2015            ISZ IABS
0547  2142            ISZ NEGN
0550  5332            JMP LOOP1           /CONTINUE LOOP
0551  4407            FLPT
0552  5126            FGET FIN            /TRANSFORM INFINITY VALUE
0553  2167            FSUB MIN
0554  6126            FPUT FIN
0555  5172            FGET MAX
0556  4126            FDIV FIN
0557  0007            FLOG
0560  3144            FMPY CONST
0561  6126            FPUT FIN
0562  0000            FEXT
0563  7200  YCALC,     CLA                 /SET UP REGISTERS
0564  1124            TAD LABS
0565  3015            DCA IABS            /FOR CALC OF Y
0566  1121            TAD LY
0567  3012            DCA IY
0570  1120            TAD LT
0571  3011            DCA IT
0572  1122            TAD LCALC
0573  3013            DCA ICALC
0574  1123            TAD LDIF
0575  3014            DCA IDIF
0576  5777            JMP I PG3
0577  0600  PG3,       600
```

```
                /PAGE 3 OF FIRST ORDER KINETICS PROGRAM
                FACTOR=75
                TEM2=156
                *600
0600  7200              CLA
0601  1117              TAD N
0602  7041              CIA
0603  3142              DCA NEGN
0604  4407              FLPT
0605  5150              FGET ZERO
0606  6111              FPUT ERROR
0607  6114              FPUT G
0610  5415              FGET I IABS
0611  2126              FSUB FIN
0612  6156              FPUT TEM2
0613  0000              FEXT
0614  7200              CLA
0615  1157              TAD TEM2+1          /DO VALUES INCREASE
0616  7510              SPA                 /OR DECREASE?
0617  5227              JMP NEG
0620  7200              CLA
0621  1147              TAD ONE
0622  4535  A1,         CALL FLOAT
0623  4407              FLPT
0624  6075              FPUT FACTOR         /SET FACTOR APPROPRIATELY
0625  0000              FEXT
0626  5233              JMP LOOP3
0627  7200  NEG,        CLA
0630  1147              TAD ONE
0631  7041              CIA
0632  5222              JMP A1
0633  4407  LOOP3,      FLPT
0634  5415              FGET I IABS
0635  5415              FGET I IABS
0636  2126              FSUB FIN
0637  3075              FMPY FACTOR
0640  0007              FLOG                /CALCLATE Y
0641  6412              FPUT I IY           /STORE Y
0642  0000              FEXT
0643  2012              ISZ IY
0644  2012              ISZ IY
0645  2012              ISZ IY
0646  2015              ISZ IABS
0647  2015              ISZ IABS
0650  2015              ISZ IABS
0651  2142              ISZ NEGN
0652  5233              JMP LOOP3
0653  4536              CALL LSQ
0654  4531              CALL MESAGE
0655  4543  TEXT /%#
0656  2410  TH
```

```
0657  0540  E
0660  2201  RA
0661  2405  TE
0662  4003   C
0663  1716  ON
0664  2324  ST
0665  0116  AN
0666  2440  T
0667  1123  IS
0670  4000   /
0671  4407              FLPT
0672  5150              FGET ZERO
0673  2100              FSUB S
0674  0014              OUTPUT
0675  0000              FEXT
0676  4531              CALL MESAGE
0677  4543  TEXT /%#
0700  2410  TH
0701  0540  E
0702  1116  IN
0703  2405  TE
0704  2203  RC
0705  0520  EP
0706  2440  T
0707  1123  IS
0710  4000   /
0711  4407              FLPT
0712  5103              FGET B
0713  0014              OUTPUT
0714  0000              FEXT
0715  4531              CALL MESAGE
0716  4543  TEXT /%#
0717  2410  TH
0720  0540  E
0721  2215  RM
0722  2340  S
0723  0522  ER
0724  2217  RO
0725  2240  R
0726  1123  IS
0727  4000   /
0730  4407              FLPT
0731  5111              FGET ERROR
0732  0014              OUTPUT
0733  0000              FEXT
0734  4531              CALL MESAGE
0735  4543  TEXT /%#
0736  2240  R
0737  7540  =
```

```
0740  0000  /
0741  4407              FLPT
0742  5106              FGET R
0743  0014              OUTPUT
0744  0000              FEXT
0745  4531              CALL MESAGE
0746  4543  TEXT /%#
0747  2410  TH
0750  0540  E
0751  2005  PE
0752  2203  RC
0753  0516  EN
0754  2440  T
0755  0522  ER
0756  2217  RO
0757  2240  R
0760  1116  IN
0761  4013   K.
0762  4011   I
0763  2340  S
0764  0000  /
0765  4407              FLPT
0766  5156              FGET TEM2
0767  0014              OUTPUT
0770  0000              FEXT
0771  5772              JMP I PG4
0772  1000  PG4,        1000
```

```
                /PAGE 4 OF FIRST ORDER KINETICS PROGRAM
                *1000
1000   7200             CLA
1001   1141             TAD ITER              /ADJUST INFINITY VALUE?
1002   7440             SZA
1003   5777             JMP ITRATE+1          /YES
1004   7200             CLA                   /NO, WRITE RESULTS
1005   1117             TAD N
1006   7041             CIA
1007   3142             DCA NEGN              /INDEX
1010   1120             TAD LT
1011   3011             DCA IT
1012   1121             TAD LY
1013   3012             DCA IY
1014   1122             TAD LCALC
1015   3013             DCA ICALC
1016   1123             TAD LDIF
1017   3014             DCA IDIF
1020   3055             DCA 55
1021   4531             CALL MESAGE
1022   4543   TEXT /%#
1023   4040
1024   4040
1025   4040
1026   4024    T
1027   4040
1030   4040
1031   4040
1032   4040
1033   4040
1034   4040
1035   4040
1036   4031    Y
1037   4040
1040   4040
1041   4040
1042   4040
1043   4040
1044   4040
1045   3103   YC
1046   0114   AL
1047   0340   C
1050   4040
1051   4040
1052   4040
1053   4040
1054   4040
1055   0411   DI
1056   0640   F
```

```
1057  4543  %#
1060  0000  /
1061  4407  LOOP4,     FLPT
1062  5411              FGET I IT
1063  0014              OUTPUT
1064  0000              FEXT
1065  4531              CALL MESAGE
1066  4040              TEXT /
1067  4000   /
1070  4407              FLPT
1071  5412              FGET I IY
1072  0014              OUTPUT
1073  0000              FEXT
1074  4531              CALL MESAGE
1075  4040              TEXT /
1076  4000   /
1077  4407              FLPT
1100  5413              FGET I ICALC
1101  0014              OUTPUT
1102  0000              FEXT
1103  4531              CALL MESAGE
1104  4040              TEXT /
1105  4000   /
1106  4407              FLPT
1107  5414              FGET I IDIF
1110  0014              OUTPUT
1111  0000              FEXT
1112  4531              CALL MESAGE
1113  4045              TEXT / %
1114  4300  #/
1115  2011              ISZ IT
1116  2011              ISZ IT
1117  2011              ISZ IT
1120  2012              ISZ IY
1121  2012              ISZ IY
1122  2012              ISZ IY
1123  2013              ISZ ICALC
1124  2013              ISZ ICALC
1125  2013              ISZ ICALC
1126  2014              ISZ IDIF
1127  2014              ISZ IDIF
1130  2014              ISZ IDIF
1131  2142              ISZ NEGN
1132  5261              JMP LOOP4
            /PLOT RESULTS ON CRT
1133  4531              CALL MESAGE
1134  4543  TEXT /%#
1135  1106  IF
1136  4020   P
```

```
1137   1417   LO
1140   2440   T
1141   1123   IS
1142   4004    D
1143   0523   ES
1144   1122   IR
1145   0504   ED
1146   5440   ,
1147   2201   RA
1150   1123   IS
1151   0540   E
1152   1305   KE
1153   3140   Y
1154   6154   1,
1155   4020    P
1156   2205   RE
1157   2323   SS
1160   4003    C
1161   1716   ON
1162   2411   TI
1163   1625   NU
1164   0540   E
1165   4543   %#
1166   0000   /
1167   7402          HLT
1170   4540          CALL MINMAX
1171   4537          CALL PLOT
1172   5773          JMP I PG5
1173   1200   PG5,   1200
```

```
                /PAGE 5 OF FIRST ORDER KINETICS PROGRAM
1177   1250     *1200
1200   4531     ITTEST,    CALL MESAGE
1201   4543     TEXT /%#
1202   1124     IT
1203   0522     ER
1204   4011      I
1205   2340     S
1206   2410     TH
1207   0540     E
1210   1625     NU
1211   1502     MB
1212   0522     ER
1213   4017      O
1214   0640     F
1215   1124     IT
1216   0522     ER
1217   0124     AT
1220   1117     IO
1221   1623     NS
1222   5440     ,
1223   1124     IT
1224   0522     ER
1225   4075      =
1226   4000      /
1227   4533              CALL SICONV
1230   3141              DCA ITER
1231   1121              TAD LY
1232   4535              CALL FLOAT
1233   4407              FLPT
1234   6072              FPUT TEST
1235   0000              FEXT
1236   7200              CLA
1237   3055              DCA 55                  /RESET FL. PT. OUTPUT
1240   1141              TAD ITER
1241   7500              SMA                     /IS ITER NEGATIVE?
1242   5247              JMP ITRATE              /NO: CONTINUE ITERATIONS
1243   7402              HLT                     /YES: HALT
1244   7200              CLA
1245   3055              DCA 55
1246   5774              JMP I RESTART           /RESTART PROGRAM
1247   4775     ITRATE,  CALL CHECK
1250   7200              CLA                     /GET DEV IN OBS QUANT
1251   1122              TAD LCALC               /AND RMS ERROR
1252   3013              DCA ICALC
1253   1123              TAD LDIF
1254   3014              DCA IDIF
1255   1124              TAD LABS
1256   3015              DCA IABS
```

```
1257  1117             TAD N
1260  7041             CIA
1261  3142             DCA NEGN                /INDEX
1262  4407             FLPT
1263  5150             FGET ZERO
1264  6111             FPUT ERROR
1265  0000             FEXT
1266  4407  LOOP5,     FLPT
1267  5413             FGET I ICALC
1270  0006             FEXP
1271  3075             FMPY FACTOR
1272  1126             FADD FIN
1273  6413             FPUT I ICALC
1274  5415             FGET I IABS
1275  2413             FSUB I ICALC
1276  6414             FPUT I IDIF
1277  3414             FMPY I IDIF
1300  1111             FADD ERROR
1301  6111             FPUT ERROR
1302  0000             FEXT
1303  2013             ISZ ICALC
1304  2013             ISZ ICALC
1305  2013             ISZ ICALC
1306  2014             ISZ IDIF
1307  2014             ISZ IDIF
1310  2014             ISZ IDIF
1311  2015             ISZ IABS
1312  2015             ISZ IABS
1313  2015             ISZ IABS
1314  2142             ISZ NEGN
1315  5266             JMP LOOP5
1316  4531             CALL MESAGE
1317  4543  TEXT /%#
1320  2410  TH
1321  0540  E
1322  2215  RM
1323  2340  S
1324  0522  ER
1325  2217  RO
1326  2240  R
1327  0201  BA
1330  2305  SE
1331  0440  D
1332  1716  ON
1333  4017   O
1334  0223  BS
1335  0522  ER
1336  2605  VE
1337  0440  D
```

```
1340  2125  OU
1341  0116  AN
1342  2456  T.
1343  4011   I
1344  2340  S
1345  0000  /
1346  4407              FLPT
1347  5111              FGET ERROR
1350  4114              FDIV G
1351  0002              FSQRT
1352  6111              FPUT ERROR
1353  0014              OUTPUT
1354  0000              FEXT
1355  4531              CALL MESAGE
1356  4543              TEXT /%#
1357  2410  TH
1360  0540  E
1361  1116  IN
1362  0611  FI
1363  1611  NI
1364  2431  TY
1365  4026   V
1366  0114  AL
1367  2505  UE
1370  4011   I
1371  2340  S
1372  0000  /
1373  5376              JMP .+3
1374  0200  RESTART,    200
1375  1637  CHECK,      CHK
1376  4407              FLPT
1377  5126              FGET FIN
```

```
                /PG 6 OF FIRST ORDER KINETICS PROGRAM
                *1400
1400   0014                 OUTPUT
1401   0000                 FEXT
1402   7200                 CLA
1403   1147                 TAD ONE
1404   7041                 CIA
1405   1141                 TAD ITER
1406   3141                 DCA ITER
1407   1141                 TAD ITER
1410   7440                 SZA
1411   5771                 JMP I PG7
1412   4531                 CALL MESAGE
1413   4543                 TEXT /%#
1414   4040
1415   4040
1416   4024   T
1417   1115   IM
1420   0540   E
1421   4040
1422   4040
1423   0000   /
1424   7200                 CLA
1425   1125                 TAD M
1426   1143                 TAD M2
1427   7550                 SPA SNA
1430   5243                 JMP ALTERN
1431   4531                 CALL MESAGE
1432   4040                 TEXT /
1433   4040
1434   4040
1435   2617   VO
1436   1425   LU
1437   1505   ME
1440   4040
1441   4000    /
1442   5254                 JMP LIST
1443   4531   ALTERN,       CALL MESAGE
1444   4040                 TEXT /
1445   4040
1446   0102   AB
1447   2317   SO
1450   2202   RB
1451   0116   AN
1452   0305   CE
1453   4000    /
1454   4531   LIST,         CALL MESAGE
1455   4040                 TEXT /
1456   4040
```

```
1457  4040
1460  4040
1461  0301  CA
1462  1403  LC
1463  4040
1464  4040
1465  4040
1466  4040
1467  4040
1470  4040
1471  0411  DI
1472  0640  F
1473  4543  %#
1474  0000  /
1475  7200        CLA
1476  1120        TAD LT
1477  3011        DCA IT
1500  1124        TAD LABS
1501  3015        DCA IABS
1502  1122        TAD LCALC
1503  3013        DCA ICALC
1504  1123        TAD LDIF
1505  3014        DCA IDIF
1506  1117        TAD N
1507  7041        CIA
1510  3142        DCA NEGN
1511  3055        DCA 55
1512  4407  LOOP6, FLPT                  /WRITE OUT RESULTS
1513  5411        FGET I IT
1514  0014        OUTPUT
1515  0000        FEXT
1516  4531        CALL MESAGE
1517  4040        TEXT /
1520  4000   /
1521  4407        FLPT
1522  5415        FGET I IABS
1523  0014        OUTPUT
1524  0000        FEXT
1525  4531        CALL MESAGE
1526  4040        TEXT /
1527  4000   /
1530  4407        FLPT
1531  5413        FGET I ICALC
1532  0014        OUTPUT
1533  0000        FEXT
1534  4531        CALL MESAGE
1535  4040        TEXT /
1536  4000   /
1537  4407        FLPT
```

```
1540  5414            FGET I IDIF
1541  0014            OUTPUT
1542  0000            FEXT
1543  4531            CALL MESAGE
1544  4045            TEXT / %
1545  4300  #/
1546  2011            ISZ IT
1547  2011            ISZ IT
1550  2011            ISZ IT
1551  2015            ISZ IABS
1552  2015            ISZ IABS
1553  2015            ISZ IABS
1554  2013            ISZ ICALC
1555  2013            ISZ ICALC
1556  2013            ISZ ICALC
1557  2014            ISZ IDIF
1560  2014            ISZ IDIF
1561  2014            ISZ IDIF
1562  2142            ISZ NEGN
1563  5312            JMP LOOP6
1564  7402            HLT
1565  7200            CLA
1566  3055            DCA 55
1567  5770            JMP I RESTRT
1570  1133  RESTRT,   1133
1571  1600  PG7,      1600
```

```
                /PAGE 7 OF FIRST ORDER KINETICS PROGRAM
                *1600
1600  4407  MODINF,   FLPT                    /MODIFY INFINITY VALUE
1601  5072           FGET TEST                /AND CONTINUE
1602  2111           FSUB ERROR
1603  6156           FPUT TEM2
1604  0000           FEXT
1605  7200           CLA
1606  1157           TAD TEM2+1
1607  7510           SPA                      /HAS RMS DEV DECREASED?
1610  5221           JMP CHGSGN               /NO: MOVE IN OPP. DIRECT.
1611  4407           FLPT                     /YES: CONTINUE
1612  5111           FGET ERROR
1613  6072           FPUT TEST
1614  5126           FGET FIN
1615  3067           FMPY CORR
1616  6126           FPUT FIN
1617  0000           FEXT
1620  5705           JMP I RUN
1621  7200  CHGSGN,   CLA
1622  4407           FLPT
1623  5302           FGET FL1
1624  4067           FDIV CORR
1625  2302           FSUB FL1
1626  3277           FMPY HALF
1627  1302           FADD FL1
1630  6067           FPUT CORR
1631  3126           FMPY FIN
1632  6126           FPUT FIN
1633  5111           FGET ERROR
1634  6072           FPUT TEST
1635  0000           FEXT
1636  5705           JMP I RUN
1637  0000  CHK,      0
1640  7450           SNA
1641  5275           JMP AX
1642  4531           CALL MESAGE
1643  4543  TEXT /%#
1644  1525  MU
1645  1424  LT
1646  1120  IP
1647  1431  LY
1650  4026   V
1651  0611  FI
1652  1640  N
1653  0231  BY
1654  4000   /
1655  4407           FLPT
1656  0013           INPUT
```

```
1657  6067              FPUT CORR
1660  0000              FEXT
1661  4531              CALL MESAGE
1662  4543  TEXT /%#
1663  2611  VI
1664  1606  NF
1665  4075   =
1666  4000   /
1667  4407              FLPT
1670  0013              INPUT
1671  6126              FPUT FIN
1672  0000              FEXT
1673  2141              ISZ ITER
1674  5637              RETURN CHK
1675  2141  AX,         ISZ ITER
1676  5705              JMP I RUN
1677  7777  HALF,       FLTG 0.5
1700  3777
1701  7774
1702  0000  FL1,        FLTG 1.0
1703  3777
1704  7774
1705  0563  RUN,        YCALC
```

```
ALTERN  1443
AX      1675
A1      0622
B       0103
CALL    4400
CHECK   1375
CHGSGN  1621
CHK     1637
CONST   0144
CORR    0067
DECPRT  0132
ERROR   0111
FACTOR  0075
FEXP    0006
FIN     0126
FIX     0134
FLAG    0153
FLOAT   0135
FLOG    0007
FLPT    4407
FL1     1702
FSQRT   0002
G       0114
HALF    1677
IABS    0015
ICALC   0013
IDIF    0014
INPUT   0013
IT      0011
ITER    0141
ITRATE  1247
ITTEST  1200
IY      0012
LABS    0124
LCALC   0122
LDIF    0123
LIST    1454
LOOP1   0532
LOOP3   0633
LOOP4   1061
LOOP5   1266
LOOP6   1512
LSQ     0136
```

```
LT       0120
LY       0121
M        0125
MAX      0172
MESAGE   0131
MIN      0167
MINMAX   0140
MODINF   1600
M2       0143
N        0117
NEG      0627
NEGN     0142
NEXT     0430
ONE      0147
OUTPUT   0014
PG2      0377
PG3      0577
PG4      0772
PG5      1173
PG7      1571
PLOT     0137
R        0106
READ     0410
RESTAR   1374
RESTRT   1570
RETURN   5400
RUN      1705
S        0100
SICONV   0133
START    0200
TEMP     0175
TEM2     0156
TEST     0072
XLOC     0154
XMIN     0156
XRNG     0161
XZERO    0172
YCALC    0563
YLOC     0155
YMIN     0164
YRNG     0167
YZERO    0175
ZERO     0150
```

```
                /SUBROUTINE FOR OBTAINING MINIMUM AND MAXIMUM
                /VALUES OF ARRAYS
                /SUBROUTINE MINMAX
                /SPECIAL VERSION FOR FIRST ORDER KINETICS PROGRAM
                RETURN=5400
                IX=11
                IY=12
                N=117
                TEMX=172
                TEMY=175
                TEMX1=161
                TEMY1=167
                XMIN=156
                XRNG=161
                YMIN=164
                YRNG=167
                FLPT=4407
                *4400
4400  0000  MINMAX,   0
4401  7300            CLA CLL
4402  7404            OSR
4403  0332            AND MASK
4404  7440            SZA
4405  5210            JMP .+3
4406  2200            ISZ MINMAX
4407  5600            RETURN MINMAX
4410  7201            CLA IAC
4411  3326            DCA FLAG        /FLAG = +1
4412  1333  START,    TAD XLOC        /SET INDEX VALUES
4413  3011            DCA IX
4414  1334            TAD YLOC
4415  3012            DCA IY
4416  1117            TAD N
4417  7041            CIA
4420  3327            DCA NEGN
4421  2327            ISZ NEGN
4422  4407            FLPT
4423  5411            FGET I IX   /FIRST VALUE OF X
4424  6172            FPUT TEMX   /SAVE IT
4425  5412            FGET I IY   /FIRST VALUE OF Y
4426  6175            FPUT TEMY   /SAVE IT
4427  0000            FEXT
4430  2011  LOOP,     ISZ IX      /GET MINIMUM VALUES
4431  2011            ISZ IX
4432  2011            ISZ IX
4433  2012            ISZ IY
4434  2012            ISZ IY
4435  2012            ISZ IY
4436  4407            FLPT
4437  5411            FGET I IX
4440  2172            FSUB TEMX
4441  6161            FPUT TEMX1
4442  5412            FGET I IY
4443  2175            FSUB TEMY
4444  6167            FPUT TEMY1
4445  0000            FEXT
```

```
4446  7200          CLA
4447  1162          TAD TEMX1+1
4450  7500  A1,     SMA
4451  5256          JMP NEXT
4452  4407          FLPT
4453  5411          FGET I IX
4454  6172          FPUT TEMX
4455  0000          FEXT
4456  7200  NEXT,   CLA
4457  1170          TAD TEMY1+1
4460  7500  A2,     SMA
4461  5266          JMP NEXT1
4462  4407          FLPT
4463  5412          FGET I IY
4464  6175          FPUT TEMY
4465  0000          FEXT
4466  2327  NEXT1,  ISZ NEGN
4467  5230          JMP LOOP
4470  7240          CLA CMA
4471  1326          TAD FLAG
4472  7440          SZA
4473  5311          JMP MAX
4474  4407          FLPT        /STORE MIN VALUES
4475  5172          FGET TEMX
4476  6156          FPUT XMIN
4477  5175          FGET TEMY
4500  6164          FPUT YMIN
4501  0000          FEXT
4502  2326          ISZ FLAG
4503  7200          CLA
4504  1330          TAD CHNG
4505  3250          DCA A1
4506  1330          TAD CHNG
4507  3260          DCA A2
4510  5212          JMP START   /NOW GET MAX VALUES
4511  7200  MAX,    CLA
4512  1331          TAD NORM
4513  3250          DCA A1
4514  1331          TAD NORM
4515  3260          DCA A2
4516  4407          FLPT        /STORE RANGES
4517  5172          FGET TEMX
4520  6161          FPUT XRNG     /XMIN ASSUMED TO BE ZERO HERE
4521  5175          FGET TEMY
4522  2164          FSUB YMIN
4523  6167          FPUT YRNG
4524  0000          FEXT
4525  5600          RETURN MINMAX
4526  0000  FLAG,    0
4527  0000  NEGN,    0
4530  7510  CHNG,    SPA
4531  7500  NORM,    SMA
4532  2000  MASK,    2000
4533  3200  XLOC,    3200
4534  2400  YLOC,    2400
```

```
                /PLOT DATA; XMIN IS ASSUMED TO BE ZERO
                /YRANGE IS ASSUMED TO INCLUDE ZERO
                *2000
2000  0000  PLOT,    0
2001  7200          CLA
2002  1777          TAD YLOC
2003  3012          DCA IY
2004  1776          TAD XLOC
2005  3011          DCA IX
2006  1363          TAD YFLOC
2007  3365          DCA JY
2010  1362          TAD XFLOC
2011  3364          DCA JX
2012  1117          TAD N
2013  7041          CIA
2014  3361          DCA INDEX
2015  4407  LOOPA,  FLPT              /FIX POINTS
2016  5411          FGET I IX
2017  2156          FSUB XMIN
2020  4161          FDIV XRNG
2021  3346          FMPY CONST
2022  0000          FEXT
2023  4757          CALL FIX
2024  3764          DCA I JX
2025  4407          FLPT
2026  5412          FGET I IY
2027  2164          FSUB YMIN
2030  4167          FDIV YRNG
2031  3346          FMPY CONST
2032  0000          FEXT
2033  4757          CALL FIX
2034  3765          DCA I JY
2035  2011          ISZ IX
2036  2011          ISZ IX
2037  2011          ISZ IX
2040  2012          ISZ IY
2041  2012          ISZ IY
2042  2012          ISZ IY
2043  2364          ISZ JX
2044  2365          ISZ JY
2045  2361          ISZ INDEX
2046  5215          JMP LOOPA
2047  4407          FLPT
2050  5351          FGET ZERO         /GET AXIS LOCATIONS
2051  2164          FSUB YMIN
2052  4167          FDIV YRNG
2053  3346          FMPY CONST
2054  0000          FEXT
2055  4757          CALL FIX
2056  3366          DCA YY
```

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2057  3355          DCA XVAL
2060  7200  STARTS, CLA           /DRAW AXES
2061  1366          TAD YY
2062  3356          DCA YVAL
2063  1354          TAD MAXV
2064  3360          DCA IND2
2065  1356          TAD YVAL        /X AXIS
2066  6063          DYL
2067  1355          TAD XVAL
2070  6057          DXS
2071  2355          ISZ XVAL
2072  2355          ISZ XVAL
2073  2360          ISZ IND2
2074  5267          JMP .-5
2075  7200          CLA
2076  1354          TAD MAXV        /Y AXIS
2077  3360          DCA IND2
2100  3355          DCA XVAL
2101  3356          DCA YVAL
2102  6053          DXL
2103  1356          TAD YVAL
2104  6067          DYS
2105  2356          ISZ YVAL
2106  2356          ISZ YVAL
2107  2360          ISZ IND2
2110  5303          JMP .-5         /AXES DRAWN
2111  7200          CLA
2112  1363          TAD YFLOC
2113  3365          DCA JY
2114  1362          TAD XFLOC
2115  3364          DCA JX
2116  1117          TAD N
2117  7041          CIA
2120  3360          DCA IND2
2121  7200  LOOPB,  CLA           /PLOT POINTS
2122  1764          TAD I JX
2123  6053          DXL
2124  7200          CLA
2125  1765          TAD I JY
2126  6067          DYS             /POINT PLOTTED
2127  7200          CLA
2130  1367          TAD M10
2131  3361          DCA INDEX
2132  2361          ISZ INDEX       /DELAY
2133  5332          JMP .-1
2134  2364          ISZ JX
2135  2365          ISZ JY
2136  2360          ISZ IND2
2137  5321          JMP LOOPB
2140  7200          CLA
```