

A FORTRAN Program
for
Plotting Atomic Absorption Data

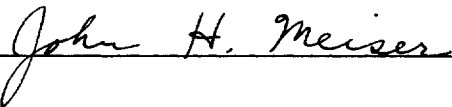
An Honors Thesis (ID 499)

by

Lucinda L. Glentzer

Thesis Director

Dr. John H. Meiser



Ball State University

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50011
Thesis
LD
2489
.Z4
1974
.G54

ACKNOWLEDGEMENTS

In the course of this research, I had the help of many individuals. Special thanks go to Dr. John H. Meiser of the Chemistry Department who not only sponsored this project, but has given me moral support from time to time. Dr. Meiser also provided initial funds for this research through his Ball State University Faculty Grant.

I wish to express my appreciation to the members of the staff of the Research Computing office at Ball State University for helping me to refine the computer program. I especially wish to thank Dr. Donald M. Smith of that office for taking his time to help me to understand the mathematics of the multiple regression process.

I am also grateful to Ball State University for the use of their computer facilities in the development of this program.

INTRODUCTION

The computer program contained herein was written to fulfill the thesis requirement of the Honors Program. The computer program is designed to convert readings taken from an atomic absorption spectrophotometer into concentrations over a wide range of variation in readings. This program was written specifically to transform the data developed in a current study of diffusion properties of metal ions made at Ball State University. However the program can readily be revised to a more general form.

THE EXPERIMENT

The research project for which the program was written is designed to measure metal ion concentration in diffusion studies. Experimentally a petri dish is filled with a 0.5% agar gel. Two reservoirs are then made in the agar with a distance of four centimeters between them. Solutions of metal ions are then placed into the reservoirs and allowed to diffuse for varying lengths of time. The ions are chosen so that precipitation of the counter-diffusing ions from the two reservoirs occurs at certain positions in the gel. This periodic precipitation appears as bands in the gel and is known as Liesegang phenomenon.

Analysis of the gel on a distance basis from one

reservoir or the other gives an indication of the position of the precipitated bands as well as the concentration of the species between the bands. Consequently, through analysis, the diffusion curves for both species are found. Although the present analysis of a diffusion sample involves removing two groups (sets A and B) of ten equally spaced sections between the two reservoirs, additional groups may be accommodated by the program. Currently, set A is taken close to one reservoir, then set B is removed parallel and offset from set A by one-half the distance between sections.

A typical investigation for an ion requires four parallel sets of sections from two separate samples to be analyzed after 24, 48, and 72 hour intervals. Since one gel formulation will produce 20 samples, this yields a total of 240 samples to be analyzed for each ion. Analytically, a set of standard solutions of the ion are tested and plotted (concentration versus absorption reading) to determine a calibration curve for each ion. Then each sample absorption reading must be converted to a concentration and plotted on a concentration versus distance graph.

The standard technique in converting atomic absorption readings involves a linear relationship between the readings and their respective concentrations. In the

samples used at Ball State University large variations in concentrations caused difficulty in maintaining the linear conditions. Since it is difficult to know the concentrations to be expected prior to sectioning the sample, it is almost impossible to choose starting concentrations that will yield a linear relationship in the samples to be analyzed. Different dilutions could be made on the same set of data, but this would be impractical. Consequently, the computer program has been written to provide for a wide range of concentrations so that unnecessary complications arising from dilution are not introduced.

METHOD

This program was written in FORTRAN IV programming language, and is compatible with the IBM FORTRAN G-level compiler. It has been run on Ball State University's IBM 360-50 computer and requires approximately 84,000 bytes of storage for execution.

The program uses data readings from standard samples of each ion to determine a calibration curve. In initial work, this curve was a straight line and its equation (a first degree polynomial) could be readily determined using the method of least-squares. This method proved to be highly accurate when the ion concentrations were in a

linear range (generally up to five parts per million). However, certain ions, for instance calcium, when diffused in higher concentrations (approximately 5 $\mu\text{g/ml}$) do not give calibration curves which are straight lines. Their curves may be second or third degree equations. Although the least-squares method could still be used, it involves the use of Cramer's Rule which is extremely time consuming when programmed for a computer. It was therefore decided that a multiple regression with independent variables x , x^2 , x^3 , and \sqrt{x} could be used to determine the equation of the molarity, where x is the reading taken from the atomic absorption spectrophotometer. The program was then rewritten using a multiple regression to determine the equation of the calibration curves.

In order to use a multiple regression, the molarity was used as the dependent variable, and the reading, its square root, its square, and its cube were used as independent variables. The multiple regression determines which of the variables are more highly correlated with the dependent variable.

The degree of correlation of two variables is measured by a coefficient of correlation. This program uses the Pearson product-moment correlation coefficient. It is given by the following formula:

$$r_{xy} = \frac{\sigma_{xy}}{\sigma_x \sigma_y}$$

where σ_{xy} is the covariance of x and y and σ_x , σ_y are the standard deviations of x and y, respectively. This formula was chosen since the covariance matrix was needed to determine the coefficients of the dependent variables chosen to enter the regression equation. The formula for the covariance of x and y is

$$\sigma_{xy} = (\sum XY - \sum X \sum Y / N) / N$$

The formula for the standard deviation of x is

$$\sigma_x = \sqrt{\sum (X - \bar{X})^2 / N}$$

In both of these formulas, each X and Y are paired observed values, N is the number of observations, and \bar{X} is the mean of the observed X's.

Since not all of the independent variables will enter the equation of the calibration curve, a "lowest acceptable correlation for entering" must be determined. This correlation value was determined using the t-statistic, a variation of the normal distribution (Gaussian or Bell curve). Therefore a z-score (normal distribution) was set to determine the correlation. The program used a constant z-score of 1.96. In comparing percentiles and z-scores, a z-score of 1.96 corresponds to 95% in a two-tailed test. This means that by choosing a z-score of 1.96, there is a probability of .95 that a particular independent variable does not correlate with the dependent variable by chance alone.

The covariance matrix is then condensed, retaining the

dependent variable and those independent variables which are more highly correlated (these have entered the regression equation). This matrix is then inverted. The diagonal elements of the inverted condensed covariance matrix are the beta weights of the variables and become the coefficients of their respective terms in the equation of the calibration curve.

This multiple regression subroutine was tested against BMD02R, a stepwise regression in the Biomedical Computer Program Series.¹ The results varied by less than 0.00001.

The data points were plotted on a graph using the CALCOMP plotter. This plotter was directed by a magnetic tape which was generated by the computer during execution of the program. On this same graph the calibration curve was drawn. By looking at this graph, one could estimate the accuracy of the calibration curve. It has proven to be fairly accurate if five or more data points are supplied. Fewer data points than this result in a less desirable fit.

Once the calibration curve was determined it was used to determine the molarity for each of the samples of two groups which were labeled groups A and B. The

¹The documentation for this program can be found in the BMD Biomedical Computer Programs.

Dixon, W.J., BMD Biomedical Computer Programs, University of California Press, Berkeley, 1971, pp. 233-258.

molarity of Group A was then plotted against its distance from the reservoir on a second graph. Group B was offset by .5 and plotted on that same graph. Then points from groups A and B were alternated and this combined group of A's and B's was plotted on a third graph.

I wrote the entire program with the exception of a small matrix inversion subroutine which was taken from an article written by Henry F. Kaiser.²

DOCUMENTATION

This program was written by Lucinda Glentzer at Ball State University in April 1973. It converts readings taken from an atomic absorption spectrophotometer into concentrations, over a wide range of variation in readings. These concentrations are then plotted against distance using the CALCOMP plotter.

²"A Fortran Program for Inverting a Positive Definite Matrix," Henry F. Kaiser and Kern W. Dickson. Educational and Psychological Measurement, 32, (1), 1972, pp. 179-180.

SET-UP

- A. GROUP CARD (I-field)
Col. Contents
3 Number of data groups for this run (≤ 5), LDO
- B. TITLE CARD (A-field)
Col. Contents
1-80 Title of data group, ID
- C. LENGTH CARD (I-field)
Col. Contents
2-3 Length of title on TITLE CARD, IOD
- D. CONSTANTS CARD (F-fields - decimals must be punched)
Col. Contents
1-10 Molarity of standard samples, CF(1)
11-20 $\mu\text{g/ml.}$ for standard samples, DF(2)
- E. STANDARD NUMBER CARD (I-field)
Col. Contents
1-3 Number of standard readings, N1
- F. STANDARD CARDS (E-fields)
N1 cards each containing
Col. Contents
1-10 Reading
11-20 $\mu\text{g/ml.}$
- G. SAMPLE NUMBER CARD (I-field)
Col. Contents
1-3 Number of Samples, N2
- H. SAMPLE (A) CARDS (E-fields)
N2 cards each containing
Col. Contents
1-10 Reading of a group A sample
- I. SAMPLE (B) CARDS (E-fields)
N2 cards, each containing
Col. Contents
1-10 Reading of a group B sample

Repeat B-I, LDO times.

SAMPLE SET-UP

```
//RC000000 JOB (3713,1017),116MEISER,MSGLEVEL=1,CLASS=D
// EXEC PLOTMISC,PROGRAM=ATABPLOT,TIME=99
//GO.STEPLIB DD DSN=RES,USERLIB,DISP=SHR
//SYSIN DD *
  1
178BA-B MG    MG  STANDARD
 23
0.02057    500.0
  6
    48.E00      1.E00
    98.E00      2.E00
   240.E00      5.E00
   484.E00     10.E00
   676.E00     15.E00
   882.E00     20.E00
 10
  525.E00
  398.E00
  367.E00
  275.E00
  267.E00
  193.E00
  176.E00
  105.E00
   97.E00
   60.E00
  457.E00
  439.E00
  338.E00
  305.E00
  244.E00
  227.E00
  151.E00
  123.E00
   83.E00
   65.E00
/*
//
```

Any questions concerning this program should be directed to Dr. John H. Meiser of the Chemistry Department at Ball State University.

PROGRAM

The following pages contain a copy of the computer program. It is followed by the computer print-out generated by the program for a set of sample data. The final pages are the graphs drawn by the CALCOMP plotter for this data.

```

//RCINDY1 JOB (3713,1017),008GLENTZER,MSGLEVEL=1,CLASS=D                JOB 374
// EXEC FORTPLCT
XXFORT EXEC PGM=IEYFORT                                                00000010
XXSYSPRINT DD SYSOUT=A                                                  00000020
XXSYSPLUNCH DD SYSOUT=B                                                00000030
XXSYSLIN DD DSNNAME=&LOADSET,DISP=(MOD,PASS),UNIT=SYSSQ,              X00000040
XX SPACE=(80,(200,100),RLSE),DCB=BLKSIZE=80                          00000050
//FORT.SYSIN DD *
IEF236I ALLCC. FOR RCINDY1 FORT
IEF237I 0E0 ALLOCATED TO SYSPRINT
IEF237I 0D0 ALLOCATED TO SYSPUNCH
IEF237I 134 ALLOCATED TO SYSLIN
IEF237I 0C0 ALLOCATED TO SYSIN
IEF142I - STEP WAS EXECUTED - COND CODE 0000
IEF285I SYS74122.T040301.RF000.RCINDY1.LOADSET PASSED
IEF285I VOL SER NOS= BSU555.
IEF373I STEP /FORT / START 74122.0506
IEF374I STEP /FORT / STOP 74122.0507 CPU OMIN 34.17SEC MAIN 86K LCS OK
XXLKED EXEC PGM=IEWL,PARM=(XREF,LET,LIST),COND=(4,LT,FORT)            00000060
XXSYSLIB DD DSNNAME=SYS1.FORTLIB,DISP=SHR                              00000070
XX DD DSNNAME=SYS1.PLOTLIB,DISP=SHR                                  00000080
XXSYSLMOD DD DSNNAME=&G0SET(MAIN),DISP=(NEW,PASS),UNIT=SYSDA,        X00000090
XX SPACE=(1024,(20,10,1)),DCB=BLKSIZE=1024                          00000100
XXSYSPRINT DD SYSOUT=A                                                00000110
XXSYSUT1 DD DSNNAME=&SYSUT1,UNIT=SYSDA,SPACE=(1024,(20,10),RLSE),    X00000120
XX DCB=BLKSIZE=1024                                                  00000130
XXSYSLIN DD DSNNAME=&LOADSET,DISP=(OLD,DELETE)                       00000140
XX DD DDNAME=SYSIN                                                    00000150
IEF236I ALLOC. FOR RCINDY1 LKED
IEF237I 231 ALLOCATED TO SYSLIB
IEF237I 130 ALLOCATED TO
IEF237I 134 ALLOCATED TO SYSLMOD
IEF237I 0E0 ALLOCATED TO SYSPRINT
IEF237I 135 ALLOCATED TO SYSUT1
IEF237I 134 ALLOCATED TO SYSLIN
IEF142I - STEP WAS EXECUTED - COND CODE 0000
IEF285I SYS1.FORTLIB KEPT
IEF285I VOL SER NOS= 051210.
IEF285I SYS1.PLOTLIB KEPT
IEF285I VOL SER NOS= INSTR1.
IEF285I SYS74122.T040301.RF000.RCINDY1.G0SET PASSED
IEF285I VOL SER NOS= BSU555.
IEF285I SYS74122.T040301.RF000.RCINDY1.SYSUT1 DELETED
IEF285I VOL SER NOS= BSU666.
IEF285I SYS74122.T040301.RF000.RCINDY1.LOADSET DELETED
IEF285I VOL SER NOS= BSU555.
IEF373I STEP /LKED / START 74122.0507
IEF374I STEP /LKED / STOP 74122.0507 CPU OMIN 07.39SEC MAIN 106K LCS OK
XXGO EXEC PGM=*.LKED.SYSLMOD,COND=((4,LT,FORT),(4,LT,LKED))          00000160
XXPLOTTAPE DD UNIT=DUAL,LABEL=(,NL),VOL=SER=PLOTTER,DISP=(NEW,KEEP), X00000170
XX DSNNAME=PLCT,DCB=DEN=2                                            00000180
XXFT05F001 DD DDNAME=SYSIN                                            00000190
XXFT06F001 DD SYSOUT=A                                                00000200
XXFT07F001 DD SYSCUT=B                                                00000210
//GO.SYSIN DD *
//
IEF236I ALLOC. FOR RCINDY1 GO
IEF237I 134 ALLOCATED TO PGM=*.DD
IEF237I 380 ALLOCATED TO PLOTTAPE
IEF237I 0C1 ALLOCATED TO FT05F001
IEF237I 0E0 ALLOCATED TO FT06F001

```

IEF237I 000 ALLOCATED TO FT07F001
IEF142I - STEP WAS EXECUTED - COND CODE 0000
IEF285I SYS74122.T040301.RF000.RCINDY1.GOSET PASSED
IEF285I VOL SER NOS= BSU555.
IEF285I PLOT KEPT
IEF285I VOL SER NOS= PLUTER.
IEF373I STEP /GO / START 74122.0507
IEF374I STEP /GO / STOP 74122.0509 CPU OMIN 09.49SEC MAIN 82K LCS OK
IEF285I SYS74122.T040301.RF000.RCINDY1.GOSET DELETED
IEF285I VOL SER NOS= BSU555.
IEF375I JOB /RCINDY1 / START 74122.0506
IEF376I JOB /RCINDY1 / STCP 74122.0509 CPU OMIN 51.05SEC

0001 DIMENSION Ibuff(4000),XY(6,32),XX(62),YY(32),YN(62),CF(2),ID(20),
*XS(6),XS2(6),XYS(6,6),SXY(6,6),RXY(5,5),SDX(5),IVA(5),B(5)
0002 CALL PLOTS(IBUFF,4000,6)
0003 CALL PLOT(0.0,-12.0,-3)
0004 READ(5,100) LDD
0005 DO 99 LIMIT=1,LDD
0006 READ(5,104) ID,IDD
0007 WRITE(6,106) ID
0008 READ(5,103)CF(1),CF(2),CL
0009 READ(5,100) N
0010 L=N+1
0011 J=N+2
0012 DO 21 I=1,N
0013 READ(5,101)XY(3,I),XY(6,I)
0014 XX(I)=XY(3,I)
0015 XY(2,I)=SQRT(XY(3,I))
0016 XY(1,I)=1.
0017 XY(4,I)=XY(3,I)**2
0018 XY(5,I)=XY(3,I)**3
0019 XY(6,I)=XY(6,I)*CF(1)/CF(2)
0020 15 YY(I)=XY(6,I)
0021 21 XY(6,I)=XY(6,I)*10000.
0022 CALL IFCURV(XY,N,XS,XS2,XYS,SXY,RXY,B,A,IVA,MCL)
0023 CALL SYMBOL(0.0,0.5,.28, ID,90.0,IDD)
0024 CALL PLOT(3.0,-12.0,-3)
0025 CALL CHNGY(MCL,IVA,B,A,YN,XX,N)
0026 CALL PLOT(0.0,3.5,-3)
0027 CALL SCALE(XX,5.0,N,+1)
0028 CALL SCALE(YY,5.0,N,+1)
0029 CALL AXIS(0.0,0.0,'READING',-7.5,0.0,0,XX(L),XX(J))
0030 CALL AXIS(0.0,0.0,'MOLES',+5.5,0.0,90.0,YY(L),YY(J))
0031 CALL LINE(XX,YY,N,1,-1,11)
0032 YN(L)=YY(L)
0033 YN(J)=YY(J)
0034 CALL FLINE(XX,YN,N,1,0,0)
0035 READ(5,100)N
0036 L=N+1
0037 J=N+2
0038 WRITE(6,107)
0039 DO 13 JKL=1,2
0040 DO 3 I=1,N
0041 READ(5,101)XY(JKL,I)
0042 3 XX(I)=XY(JKL,I)
0043 CALL CHNGY(MCL,IVA,B,A,YN,XX,N)
0044 IF(CL.EQ.0.0)GO TO 18
0045 DO 19 I=1,N
0046 19 YN(I)=YN(I)*CL
0047 18 WRITE(6,105)

```
0048      DO 31 I=1,N
0049      XY(JKL+2,I)=YN(I)
0050      31 WRITE(6,102)XX(I),YN(I)
0051      13 CONTINUE
0052      100 FORMAT(I3)
0053      101 FORMAT(2F10.0)
0054      102 FORMAT(10X,E12.5,2X,E12.5)
0055      103 FORMAT(3F10.1)
0056      104 FORMAT(20A4/I3)
0057      105 FORMAT(/)
0058      106 FORMAT('1',10X,20A4,/)
0059      107 FORMAT(12X,'READING',7X,'MOLARITY')
0060      108 FORMAT('1',11X,'DISTANCE',7X,'MOLARITY'//)
0061      CALL PLOT(8.5,-12.0,-3)
0062      CALL PLOT(0.0,1.75,-3)
0063      DO 9 I=1,N
0064      YY(I)=I
0065      9 CONTINUE
0066      CALL SCALE(YN,8.0,N,+1)
0067      CALL SCALE(YY,5.0,N,+1)
0068      CALL AXIS(0.0,0.0,'DISTANCE',-8.5,0.0,0.0,YY(L),YY(J))
0069      CALL AXIS(0.0,0.0,'MOLES',5.8,0.0,90.0,YN(L),YN(J))
0070      ICK=1
0071      DO 12 JK=1,2
0072      JKL=5-JK
0073      IF(JKL.EQ.4) GO TO 10
0074      DO 8 I=1,N
0075      8 YN(I)=XY(JKL,I)
0076      DO 4 I=1,N
0077      4 YY(I)=YY(I)-0.50
0078      10 CALL FLINE(YY,YN,-N,1,+1,ICK)
0079      ICK =11
0080      12 CONTINUE
0081      CALL PLOT(8.5,0.0,-3)
0082      JX=2*N
0083      DO 11 I=2,JX,2
0084      K=I/2
0085      JK=I-1
0086      XX(I)=K
0087      XX(JK)=XX(I)-0.5
0088      YN(I)=XY(4,K)
0089      YN(JK)=XY(3,K)
0090      11 CONTINUE
0091      L=2*N+1
0092      J=2*N+2
0093      CALL SCALE(XX,5.0,JX,+1)
0094      CALL SCALE(YN,8.0,JX,+1)
0095      CALL AXIS(0.0,0.0,'DISTANCE',-8.5,0.0,0.0,XX(L),XX(J))
```

```
0096      CALL AXIS(0.0,0.0,'MOLES',5,8.0,90.0,YN(L),YN(J))
0097      CALL FLINE(XX,YN,-JX,1,+1,11)
0098      CALL PLOT(8.0,-12.0,-3)
0099      WRITE(6,108)
0100      L=N*2
0101      DO 88 I=1,L
0102      88 WRITE(6,102)XX(I),YN(I)
0103      99 CONTINUE
0104      CALL PLOT(0.0,0.0,959)
0105      STOP
0106      END
```

FORTRAN IV G LEVEL 21

MAIN

DATE = 74122

05/06/12

PAGE 0004

OPTIONS IN EFFECT NOID,EBCDIC,SOURCE,NOLIST,NODECK,LOAD,NOMAP
OPTIONS IN EFFECT NAME = MAIN , LINECNT = 50
STATISTICS SOURCE STATEMENTS = 106,PROGRAM SIZE = 21216
STATISTICS NO DIAGNOSTICS GENERATED

00

13

```
0001      SUBROUTINE IFCURV(XY,N,XS,XS2,XYS,SXY,RXY,8,A,IVA,JKL)
0002      DIMENSION XY(6,32),XM(5),
          *XS(6),XS2(6),XYS(6,6),SXY(6,6),RXY(5,5),SDX(5),IVA(5),B(5)
0003      DO 97 I=1,6
0004          XS(I)=0.
0005          XS2(I)=0.
0006      DO 88 J=I,6
0007          XYS(I,J)=0.
0008      DO 98 K=1,N
0009      98 XYS(I,J)=XYS(I,J)+XY(I,K)*XY(J,K)
0010      88 XYS(J,I)=XYS(I,J)
0011      DO 97 J=1,N
0012          XS(I)=XS(I)+XY(I,J)
0013      97 XS2(I)=XS2(I)+XY(I,J)**2
0014          XN=N
0015      DO 99 I=1,5
0016          K=I+1
0017          SDX(I)=SQRT((XS2(K)-XS(K)**2/XN)/XN)
0018      DO 99 J=I,5
0019          L=J+1
0020      99 SXY(I,J)=(XYS(K,L)-XS(L)*XS(K)/XN)/XN
0021          WRITE(6,100)
0022      100 FORMAT(10X,'COVARIANCE MATRIX')
0023          WRITE(6,103)((SXY(I,J),J=I,5),I=1,5)
0024      101 FORMAT(5X,5F12.3/17X,4F12.3/29X,3F12.3/41X,2F12.3/53X,F12.3)
0025      DO 86 I=1,5
0026          DO 86 J=I,5
0027              RXY(I,J)=SXY(I,J)/(SDX(I)*SDX(J))
0028      86 RXY(J,I)=RXY(I,J)
0029          WRITE(6,102)
0030      102 FORMAT(//10X,'CORRELATION MATRIX')
0031          WRITE(6,101)((RXY(I,J),J=I,5),I=1,5)
0032      103 FORMAT(5X,5E12.5/17X,4E12.5/29X,3E12.5/41X,2E12.5/53X,E12.5)
0033          WRITE(6,201)
0034          CALL PARTAL(JKL,IVA,RXY,N,SXY)
0035      DO 92 I=2,JKL
0036      92 IVA(I)=IVA(I)+1
0037      DO 93 I=1,JKL
0038          DO 93 J=I,JKL
0039              RXY(I,J)=XYS(IVA(I),IVA(J))
0040      93 RXY(J,I)=RXY(I,J)
0041          CALL CCNS(RXY,XS,JKL)
0042      DO 85 I=1,JKL
0043      85 XS(I)=0.
0044          DO 84 I=1,JKL
0045              DO 84 J=1,JKL
0046      84 XS(I)=XS(I)+RXY(I,J)*XYS(L,IVA(J))
0047          DO 91 I=1,JKL
```

```
0048      91 B(I)=XS(I)
0049      DO 96 I=1,5
0050          XM(I)=I-1
0051      96 XS(I)=0.0
0052          XM(I)=.5
0053      DO 87 I=1,JKL
0054      87 XS(IVA(I))=B(I)
0055          WRITE(6,201)
0056          WRITE(6,202) XS(I)
0057          WRITE(6,203)(XM(I),XS(I+1),I=1,4)
0058          WRITE(6,201)
0059      201 FORMAT (///)
0060      202 FORMAT(10X,' THE CONSTANT TERM IS',E12.5)
0061      203 FORMAT(10X,' THE COEFFICIENT OF THE X**',F3.1,' TERM IS',E12.5)
0062      RETURN
0063      END
```

FORTRAN IV G LEVEL 21

IFCURV

DATE = 74122

05/06/12

PAGE 0003

OPTIONS IN EFFECT NOID,EBCDIC,SOURCE,NOLIST,NODECK,LOAD,NOMAP
OPTIONS IN EFFECT NAME = IFCURV , LINECNT = 50
STATISTICS SOURCE STATEMENTS = 63,PROGRAM SIZE = 3124
STATISTICS NO DIAGNOSTICS GENERATED

```
0001      SUBROUTINE PARTAL(I,IVA,RXY,N,XYS)
0002      DIMENSION IVA(5),RXY(5,5),XYS(5,5)
0003      DO 1 I=1,5
0004      1 IVA(I)=0
0005      KA=1
0006      IVA(1)=1
0007      DO 210 I=1,4
0008      JK=I+1
0009      DO 10 M=1,5
0010      DO 10 J=1,5
0011      10  XYS(M,J)=RXY(M,J)
0012      L=1
0013      DO 2 K=2,4
0014      2  IF(ABS(RXY(K,5)).GT.ABS(RXY(L,5))) L=K
0015      Z=1.96
0016      DF=N-1
0017      T=Z+(Z**3+Z)/(4.*(DF-1.))
0018      KA=KA+I
0019      X=N-KA
0020      R=T/SQRT(X+T**2)
0021      IF(ABS(RXY(L,5)).LT.R) RETURN
0022      IF(L.EQ.1) XLM=.5
0023      IF(L.GT.1) XLM=L-1
0024      WRITE(6,200) I,XLM
0025      200 FORMAT(10X,'VARIABLE',I2,' ENTERS AN X**',F3.0,' TERM')
0026      IVA(JK)=L
0027      DO 4 K=1,5
0028      IF(K.EQ.L) GO TO 100
0029      DO 3 J=1,5
0030      IF(J.EQ.L) GO TO 101
0031      RXY(K,J)=XYS(K,J)-XYS(K,L)*XYS(J,L)
0032      RXY(K,J)=RXY(K,J)/SQRT((1.-XYS(K,L)**2)*(1.-XYS(J,L)**2))
0033      GO TO 3
0034      101 RXY(K,J)=0.0
0035      3 CONTINUE
0036      GO TO 4
0037      100 DO 99 M=1,5
0038      99 RXY(K,M)=0.0
0039      4 CONTINUE
0040      210 CONTINUE
0041      I=I+1
0042      RETURN
0043      END
```

FORTRAN IV G LEVEL 21

PARTAL

DATE = 74122

05/06/12

PAGE 0002

OPTIONS IN EFFECT NOID,EBCDIC,SOURCE,NOLIST,NODECK,LOAD,NOMAP
OPTIONS IN EFFECT NAME = PARTAL , LINECNT = 50
STATISTICS SOURCE STATEMENTS = 43,PROGRAM SIZE = 1628
STATISTICS NO DIAGNOSTICS GENERATED

```
0001      SUBROUTINE DONS(A,T,N)
0002      DIMENSION A(5,N),T(N)
0003      NLESS1=N-1
0004      DO 100 K=1,N
0005          IF(A(1,1)-0.000001)101,101,102
0006      102 X=SQRT(A(1,1))
0007          DO 103 I=1,NLESS1
0008      103 T(I)=A(I+1,1)/X
0009          T(N)=1.0/X
0010          DO 104 J=1,NLESS1
0011      104 DO 104 I=1,NLESS1
0012      104 A(I,J)=A(I+1,J+1)-T(I)*T(J)
0013          DO 105 I=1,N
0014      105 A(I,N)=-T(I)*T(N)
0015          DO 100 J=1,NLESS1
0016      100 A(N,J)=A(J,N)
0017          DO 106 J=1,N
0018      106 DO 106 I=1,N
0019      106 A(I,J)=-A(I,J)
0020          GO TO 107
0021      101 WRITE(6,1000)
0022      1000 FORMAT(1X,'THE MATRIX IS SINGULAR, VERY NEARLY SINGULAR, OR INDEFI
          *NITE')
0023      107 RETURN
0024      END
```

FORTRAN IV G LEVEL 21

DONS

DATE = 74122

05/06/12

PAGE 0002

OPTIONS IN EFFECT NCID,EBCDIC,SOURCE,NOLIST,NODECK,LOAD,NOMAP
OPTIONS IN EFFECT NAME = DONS , LINECNT = 50
STATISTICS SOURCE STATEMENTS = 24,PROGRAM SIZE = 1268
STATISTICS NO DIAGNOSTICS GENERATED

```
0001      SUBROUTINE CHNGY(NUM,I,B,A,Y,X,N)
0002      DIMENSION I(NUM),B(NUM),Y(N),X(N)
0003      A=B(I)
0004      DO 1 L=1,N
0005      1 Y(L)=0.0
0006      DO 8 K=1,N
0007      DO 7 J=2,NUM
0008      KK=I(J)
0009      GO TO (9,2,3,4,5,9),KK
0010      2 Y(K)=Y(K)+SQRT(X(K))*B(J)
0011      GO TO 7
0012      3 Y(K)=Y(K)+X(K)*B(J)
0013      GO TO 7
0014      4 Y(K)=Y(K)+(X(K)**2)*B(J)
0015      GO TO 7
0016      5 Y(K)=Y(K)+(X(K)**3)*B(J)
0017      7 CONTINUE
0018      Y(K)=(Y(K)+A)/10000
0019      8 CONTINUE
0020      GO TO 99
0021      9 WRITE(6,100)
0022      100 FORMAT(1X,'WRONG DEPENDENT VARIABLE*')
0023      99 RETURN
0024      END
```

FORTRAN IV G LEVEL 21

CHNGY

DATE = 74122

05/06/12

PAGE 0002

OPTIONS IN EFFECT NOID,EBCDIC,SOURCE,NOLIST,NODECK,LOAD,NMAP
OPTIONS IN EFFECT NAME = CHNGY , LINECNT = 50
STATISTICS SOURCE STATEMENTS = 24,PROGRAM SIZE = 1120
STATISTICS NO DIAGNOSTICS GENERATED

STATISTICS NO DIAGNOSTICS THIS STEP -

NAME	ORIGIN	LENGTH	NAME	LOCATION	NAME	LOCATION	NAME	LOCATION	NAME	LOCATION
REFLX *	F720	1F8								
IHCSEXP *	F918	192								
			EXP	F918						

LOCATION REFERS TO SYMBOL IN CONTROL SECTION

DC	PLOTS	PLOTS
E4	IBCOM=	IHCCECMH
EC	SYMBOL	SYMBOL
F4	SCALE	SCALE
FC	LINE	LINE
104	SQRT	IHCSSQRT
53CC	PARTAL	PARTAL
5304	SQRT	IHCSSQRT
6004	SQRT	IHCSSQRT
6644	SQRT	IHCSSQRT
6FCC	NUMBER	NUMBER
6FD4	PLOTS	PLOTS
6FDC	SIN	IHCSSCN
6848	SQRT	IHCSSGRT
7808	REFLX	REFLX
7810	FIT4	FIT4
7818	AMAX1	IHC FMAXR
8E04	ADCON=	IHCFCVTH
8E08	ARITH=	IHC EFNTH
8E24	IHC UOPT	IHC UOPT
8E10	FCVLOUTP	IHCFCVTH
8E18	FCVCOUTP	IHCFCVTH
8E20	FCVZOUTP	IHCFCVTH
8DDC	IHC COMH2	IHC COMH2
8DB4	IHC COMH2	IHC COMH2
8DB8	IHC COMH2	IHC COMH2
808C	IHC COMH2	IHC COMH2
918D	IHC ECOMH	IHC ECOMH
8F68	IHCERRM	IHCERRM
930D	IHC ECOMH	IHC ECOMH
93FD	IHC ECOMH	IHC ECOMH
9688	SYMBOL	SYMBOL
9690	AMAX1	IHC FMAXR
A2FC	ALUG10	IHC SLOG
A904	IHCERRM	IHCERRM
AA2C	IHCERRM	IHCERRM
8050	IBCOM=	IHC ECOMH
8058	FIOCS REP	IHC EF IOS
C058	IHCERRM	IHCERRM
C5C0	INTSWTCH	IHC ECOMH
C564	IHC UOPT	IHC UOPT
C5C4	FIOCS=	IHC EF IOS
C878	IHCERRM	IHCERRM
D674	IBCOM=	IHC ECOMH
DEB0	ADCON=	IHCFCVTH
E1A0	IBCOM=	IHC ECOMH

LOCATION REFERS TO SYMBOL IN CONTROL SECTION

E0	PLOT	PLOTS
E8	IFCURV	IFCURV
F0	CHNGY	CHNGY
F8	AXIS	AXIS
100	FLINE	FLINE
53C8	IBCOM=	IHC ECOMH
53D0	DONS	DONS
6000	IBCOM=	IHC ECOMH
6640	IBCOM=	IHC ECOMH
6FC8	FRXPR=	IHC FRXPR
6FD0	SYMBOL	SYMBOL
6FD8	COS	IHCSSCN
6844	IBCOM=	IHC ECOMH
7804	WHERE	PLOTS
780C	PLOT	PLOTS
7814	SYMBOL	SYMBOL
8084	SEQDASD	IHC COMH2
8DFC	FIOCS=	IHC EF IOS
8E28	ADJSWTCH	IHC EFNTH
8E0C	FCV EOUTP	IHCFCVTH
8E14	FCV IOUTP	IHCFCVTH
8E1C	FCV AOUTP	IHCFCVTH
8DB0	IHCERR	IHCERRM
8DE0	IHCERRM	IHCERRM
8DB8	IHC COMH2	IHC COMH2
8DC0	IHC COMH2	IHC COMH2
91C0	IHC ECOMH	IHC ECOMH
8F64	IBCOM=	IHC ECOMH
93ED	IHC ECOMH	IHC ECOMH
9684	WHERE	PLOTS
968C	PLOT	PLOTS
A2F8	FRXPI=	IHC FRXPI
A8C8	IBCOM=	IHC ECOMH
AA28	IBCOM=	IHC ECOMH
804C	IHC UOPT	IHC UOPT
8054	IHC TRCH	IHC TRCH
C05C	IBCOM=	IHC ECOMH
C5BC	IBCOM=	IHC ECOMH
C568	INT6SWCH	IHCFCVTH
C5C8	ADCON=	IHCFCVTH
C634	IHCERRM	IHCERRM
D66J	IHC UATBL	IHC UATBL
DEAC	IBCOM=	IHC ECOMH
DEB4	FIOCS REP	IHC EF IOS
E1C8	IHCERRM	IHCERRM

LOCATION REFERS TO SYMBOL IN CONTROL SECTION

E568	SIN	IHCSSCN
E564	PLOT	PLOTS
ED44	IHCERRM	IHCERRM
EE98	PLOT	PLOTS
F4F0	IBCOM=	IHCCECMH
F4E8	ALOG	IHC SLOG
F70C	SYMBOL	SYMBOL
FA1C	IHCERRM	IHCERRM
ENTRY ADDRESS	00	
TOTAL LENGTH	FAB0	

LOCATION REFERS TO SYMBOL IN CONTROL SECTION

E56C	COS	IHCSSCN
ED00	IBCOM=	IHCCECMH
EE94	WHERE	PLOTS
EE9C	SQRT	IHCSSQRT
F4F4	IHCERRM	IHCERRM
F4EC	EXP	IHCSEXP
FA20	IBCOM=	IHCCECMH

1758A-8 PB PB STANDARD

COVARIANCE MATRIX

0.27511E 02 0.56071E 03 0.16955E 06 0.50781E 08 0.69269E 01
 0.11946E 05 0.38232E 07 0.11835E 10 0.14920E 03
 0.13253E 10 0.43180E 12 0.48573E 05
 0.14579E 15 0.15215E 08
 0.18702E 01

CORRELATION MATRIX

1.000	0.978	0.888	0.802	0.966
	1.000	0.961	0.897	0.998
		1.000	0.982	0.976
			1.000	0.921
				1.000

VARIABLE 1 ENTERS AN X** 1. TERM
 VARIABLE 2 ENTERS AN X** 2. TERM
 VARIABLE 3 ENTERS AN X** 1. TERM

THE CONSTANT TERM IS-0.26138E-01
 THE CCEFFICIENT OF THE X**0.5 TERM IS.16830E-01
 THE CCEFFICIENT OF THE X**1.0 TERM IS.85869E-02
 THE CCEFFICIENT OF THE X**2.0 TERM IS.97230E-05
 THE CCEFFICIENT OF THE X**3.0 TERM IS.0

READING MOLARITY

0.33300E 03	0.42186E-03
0.26600E 03	0.32204E-03
0.21200E 03	0.24763E-03
0.16700E 03	0.18965E-03
0.14400E 03	0.16140E-03
0.11500E 03	0.12764E-03
0.88000E 02	0.56269E-04
0.51000E 02	0.55728E-04
0.38000E 02	0.41795E-04
0.23000E 02	0.25722E-04

0.29700E 03	0.36719E-03
0.24300E 03	0.28970E-03
0.19700E 03	0.22790E-03
0.15100E 03	0.16990E-03
0.12600E 03	0.13991E-03
0.56000E 02	0.10527E-03
0.67000E 02	0.73059E-04
0.38000E 02	0.41795E-04
0.28000E 02	0.31098E-04

0.15000E 02 0.17004E-04

08
00

DISTANCE		POLARITY
0.50000E	00	0.42186E-03
0.10000E	01	0.36719E-03
0.15000E	01	0.32204E-03
0.20000E	01	0.28970E-03
0.25000E	01	0.24763E-03
0.30000E	01	0.22790E-03
0.35000E	01	0.18965E-03
0.40000E	01	0.16990E-03
0.45000E	01	0.16140E-03
0.50000E	01	0.13991E-03
0.55000E	01	0.12704E-03
0.60000E	01	0.10527E-03
0.65000E	01	0.96269E-04
0.70000E	01	0.73059E-04
0.75000E	01	0.55728E-04
0.80000E	01	0.41795E-04
0.85000E	01	0.41795E-04
0.90000E	01	0.31098E-04
0.95000E	01	0.25722E-04
0.10000E	02	0.17004E-04

