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**THREE-DIMENSIONAL RESPONSE
SURFACE PROGRAM IN
FORTRAN II FOR THE
IBM 1620 COMPUTER**

By

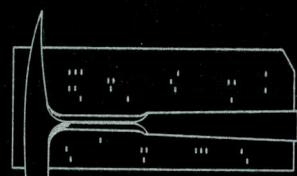
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Kansas Geological Survey



COMPUTER CONTRIBUTION 10

State Geological Survey

The University of Kansas, Lawrence

1967

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By

ROBERT J. SAMPSON and JOHN C. DAVIS

INTRODUCTION

Response surfaces are special forms of multiple regressions in which the independent variables are geographic coordinates. They are extensions of the process of fitting a regression line to data by the method of least squares. "Trend surfaces" are a variety of response surfaces commonly used in geologic analysis in which two independent geographic variables are used. The dependent variable may also be geographic (depth or elevation) or it may represent such characteristics as mineral or elemental content. Trend surfaces usually are depicted as undulating map surfaces in which elevation represents the dependent variable.

Response surfaces may be extended to three dimensions by the addition of another independent variable. Forms with three independent geographic variables may be pictured as a solid form with values of the dependent variable distributed through it. Harbaugh (1964) refers to this type of regression as a "hypersurface." It is possible to extend the concept to other dimensions, but the resulting regression cannot be portrayed in ordinary space, and consequently has little use. The relationships between multiple regression, trend surfaces, and hypersurfaces are illustrated in Figure 1.

Peikert (1963) and Harbaugh (1964) have written programs for larger computers which generate three-dimensional response surfaces. These programs have been used to analyze mineralogical changes within igneous bodies (Peikert, 1962, 1963, 1965; Whitten, 1963; Whitten and Boyer, 1964) oil gravity (Harbaugh, 1964) and oil-shale yield (Smith and Harbaugh, 1966). The program described here has been used on oil-gravity data and on mineral composition data from a black shale. The procedure is a useful means of summarizing almost any sort of spatially distributed compositional data.

PROGRAM DESCRIPTION

This program will generate polynomial response surfaces for three geographic coordinates up to the third degree. Data are not stored internally, so any number of data points may be utilized. The

complete program consists of three passes. On the first, data are accumulated and set into a series of simultaneous equations of the form

$$\begin{aligned}\Sigma W &= b_0 + b_1 \Sigma X + b_2 \Sigma Y + b_3 \Sigma Z + b_4 \Sigma X^2 + \dots + b_{19} \Sigma Z^3 \\ \Sigma XW &= b_0 \Sigma X + b_1 \Sigma X^2 + b_2 \Sigma XY + b_3 \Sigma XZ + b_4 \Sigma X^3 + \dots + b_{19} \Sigma XZ^3 \\ \Sigma YW &= b_0 \Sigma Y + b_1 \Sigma YX + b_2 \Sigma Y^2 + b_3 \Sigma YZ + b_4 \Sigma X^2Y + \dots + b_{19} \Sigma YZ^3 \\ &\vdots \\ \Sigma Z^3W &= b_0 \Sigma Z^3 + b_1 \Sigma XZ^3 + b_2 \Sigma YZ^3 + b_3 \Sigma Z^4 + b_4 \Sigma X^2Z^3 + \dots + b_{19} \Sigma Z^6\end{aligned}$$

where W is the dependent variable and X, Y, and Z are independent variables. In this program, X may be regarded as "east-west" or across-page, Y as "north-south" or down-page, and Z as depth. The origin of the coordinate system is arbitrarily chosen as the upper left rear corner of a cube (Fig. 2). This convention aides in orienting maps produced by the program. For plotting purposes, positive values of X are considered to be to the right of the origin, positive values of Y are forward of the origin, and positive values of Z are below the origin.

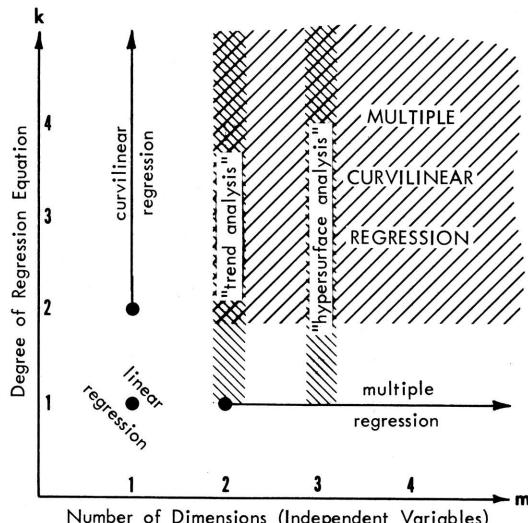


Figure 1.-Relationships between trend and hypersurface analysis, and general field of multiple regression.

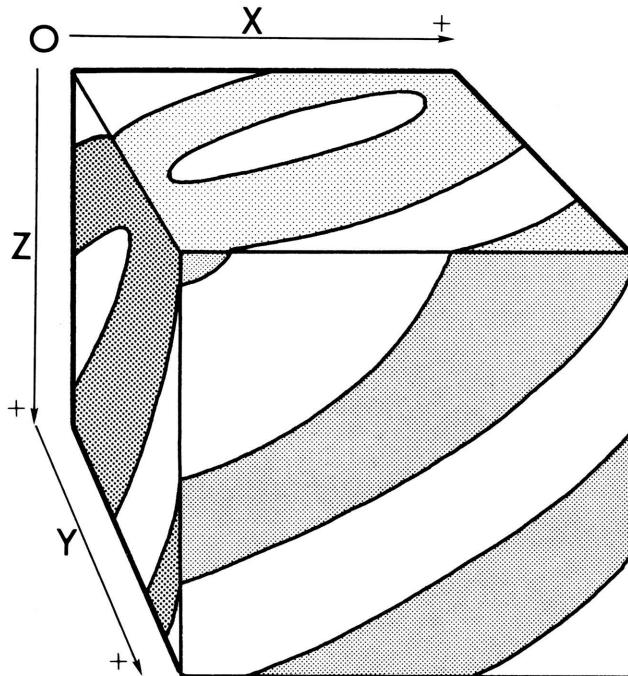


Figure 2.- Orientation of slice maps with respect to X, Y, and Z coordinates. X may conveniently be regarded as east-west, Y as north-south, and Z as depth, but this convention may be altered with no change in the program. All values increase positively away from the origin in the direction indicated.

Following solution of the simultaneous equations for the constants of the regression equation, input cards for the second and third passes are produced. On the second pass, expected values of W and residuals are produced for each data point and the goodness of fit and correlation coefficients are calculated for each regression. An F-value for testing the significance of the fit of each order, accompanied by appropriate degrees of freedom, are produced. F-values for evaluating the significance of the additional degrees also are produced for the second- and third-degree surfaces. Coefficients of the regression equation are punched.

The third pass produces 100 orthogonal control points on a "slice-map" at any selected constant values of X, Y, or Z for contouring values of W. These maps may be contoured and assembled into a solid representation of the distribution of W. Figure 3 shows a second-degree hypersurface, fitted to oil-gravity data from southeastern Kansas. This pass may be omitted if desired.

The program is designed for an IBM 1620 computer having 20K digits storage, and may be adapted to other similar-sized computers having automatic divide and indirect addressing features. A 1622 Card Read Punch or equivalent and an 80 or 120 column lister also are required. The lister should be wired to skip to a new page when a

minus (-) is read in the 80th column of a card. Output will then appear on sequentially numbered and titled pages.

The program requires PDQ FORTRAN Compiler C2 Without Reread Version 1 Modification 0, and Fixed Format Subroutines (IBM User's Group Program 2.0.031). The second pass uses relocatable subroutine SQRT. None are used in the first or third passes.

PASS ONE

After loading Pass One object deck and fixed format subroutines, the message LOAD DATA will be typed on the console typewriter. Cards are then entered into the computer in the following order.

Card 1 - This is a Title card containing any desired alphanumeric information in columns 1 through 72. Columns 73 through 80 are reserved for unassignable page numbers. This information will be reproduced at the top of each lister page.

Card 2 - This is the first of any number of Data cards. The first independent variable, X, is punched in columns 1 through 10. Columns 11 through 20 contain the second independent variable, Y. Columns 21 through 30 contain the third independent variable, Z. The dependent variable, W, is punched in columns 31 through 40. Data should contain decimal points.

The data are terminated by an End card containing the number 9.0E48 punched in columns 1 through 6. After the End card has been read at the end of the data string, 10 cards required for Pass Two and Pass Three will be punched. The message, STOP 100, will be typed on the console typewriter, signifying the end of Pass One. Another data set may be processed by pushing START, which will cause the computer to return to the beginning of Pass One.

PASS TWO

After loading the Pass Two object deck and subroutines, LOAD DATA will be typed on the console typewriter. The 10 cards produced by Pass One should then be loaded, followed by the Title card, Data cards, and End card. The machine will calculate and punch expected values and residuals for all three degrees, goodness of fit, and related values. If SENSE SWITCH 3 is on, 80-column output will be produced. If SENSE SWITCH 3 is off, 120-column output will be produced. The machine will type STOP 100 at the completion of computations. A new data set may then be processed.

PASS THREE

SENSE SWITCH 1 must be on. SENSE SWITCH 3 selects output format: on produces cards for 80-column listing; off produces cards for 120-

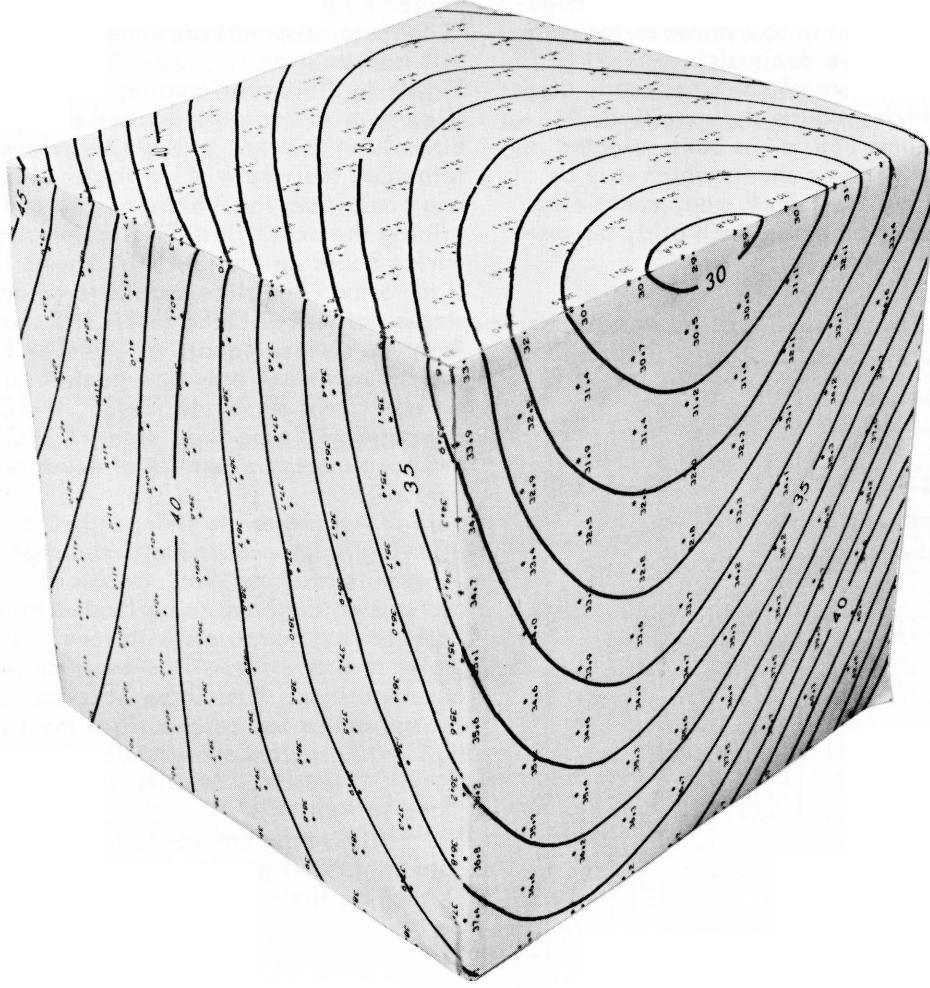


Figure 3.- Assembled and contoured slice-maps showing a second degree fit to API oil-gravity data in south-eastern Kansas. Original data from Harbaugh (1964).

column listing. After loading the Pass Three object deck and subroutines, the message LOAD DATA will be typed. The 10 cards produced by Pass One should then be loaded. The message ENTER PLOT CONTROL CARDS will be typed. The following series of cards should be entered.

Card 1 - Column 1 contains a number indicating the order of the desired equation. Column 2 is left blank; Column 3 contains the letter X, Y, or Z, denoting the independent variable to be held constant. Column 4 is blank. Columns 5 through 14 contain the desired value of the selected constant. This number must contain a decimal point. Columns 15 through 24 contain the value of a constant by which each value of W will be multiplied. This is useful when numbers of small value are being printed, and too few significant digits would be printed otherwise. The constant must not be zero, and must contain a decimal point. If no multiplication is desired, use 1.0.

Card 2 - Columns 1 and 2 are blank. Column 3 contains the letter X, Y, or Z, denoting the independent variable to be printed across the slice-map. Column 4 is blank. Columns 5 through 14 contain the value for the left edge of the slice-map. Columns 15 through 24 contain the size of increment steps across the slice-map (this value may be negative). The formula for the increment is:

$$\frac{(\text{Specified value for left margin} - \text{Desired value for right margin})}{9}$$

Left margin and increment values require decimal points.

Card 3 - Columns 1 and 2 are blank. Column 3 contains the letter X, Y, or Z, denoting the independent variable to be printed down the slice-map. Column 4 is blank. Columns 5 through 14 contain the value at the top edge of the slice-map, and columns 15 through 25 contain the size of increment

steps down the slice-map. This value may be negative and is obtained in the same manner as for card 2. These values must have decimals.

After the three control cards are read, cards will be punched which produce the specified slice-map. If the 80-column option has been selected, the map will consist of three sheets which may be spliced together into a 9 x 9 inch map, containing 100 data points spaced on a one-inch grid, accom-

panied by a title and brief explanation. Coordinates of the control points are listed along the upper and left map margins. An assembled map is shown in Figure 4. This configuration was chosen to obtain a slice-map with equally spaced data points using an 80-column printer. If the 120-column option is selected, the map will be produced on two sheets, one containing the 100 point grid and the other containing the map title. This option requires a special wiring board on the IBM 407, shown in Figure 5. If more than one slice-map is to be made from a single data set, SENSE SWITCH 2 should be off. Response surface equations will then be retained in the computer and only new control cards are needed for additional maps. If SENSE SWITCH 2 is on, the computer will type the statement STOP 100, pause, and then accept a new set of equations and control cards.

All passes are independent of one another, allowing batch processing of a number of problems. This saves machine time, as object decks and subroutines do not have to be loaded for each problem. Users having computers with tape or disc drives may prefer to convert Pass Two and Pass Three to procedures or subroutines. Pass Three also may be used for plotting control points for trend-surface maps produced by the IBM 1620 program published by Sampson and Davis (1966). Necessary modifications in this program are listed in Appendix B.

This program was tested using Harbaugh's (1964) data on API oil gravity from southeastern Kansas. Output for first- and second-degree equations is

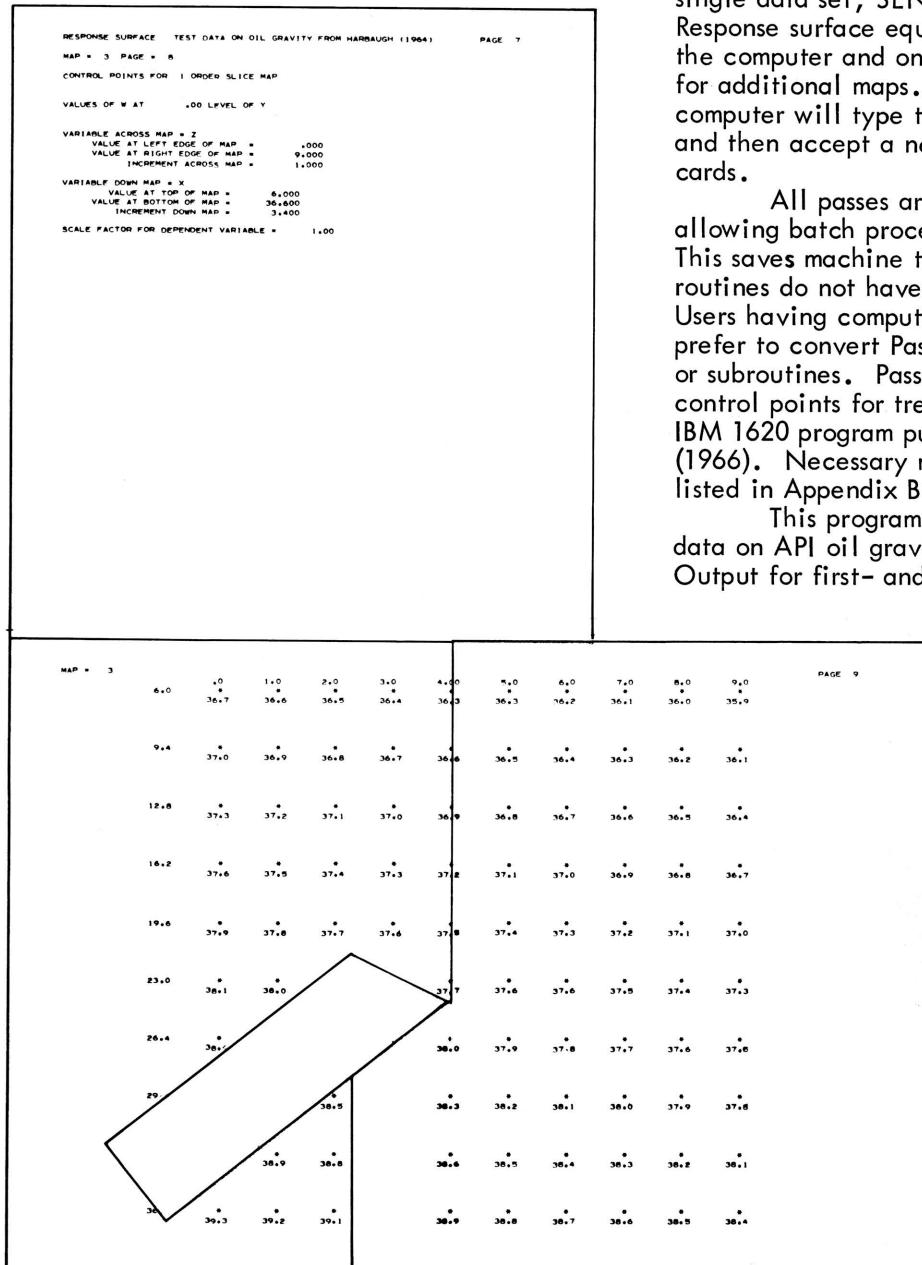


Figure 4. - Eighty-column slice-maps may be assembled by trimming the left margin of the third sheet of map output along the first row of asterisks. This sheet is then overlapped onto the second map sheet along the last row of asterisks.

essentially identical to his. The third-degree output differs because Harbaugh used an abbreviated equation, whereas this program uses the complete equation. Also, Harbaugh's method of calculating goodness of fit and related values produces erroneous results for the first-degree equation. This has been corrected in this program.

The program was written by Robert Sampson at the Idaho State University Computer Center as a part of ISU Geology Department Research Project 71. Machine time was donated by the ISU Computer Center, on equipment supplied in part by NSF Grant GP-2275.

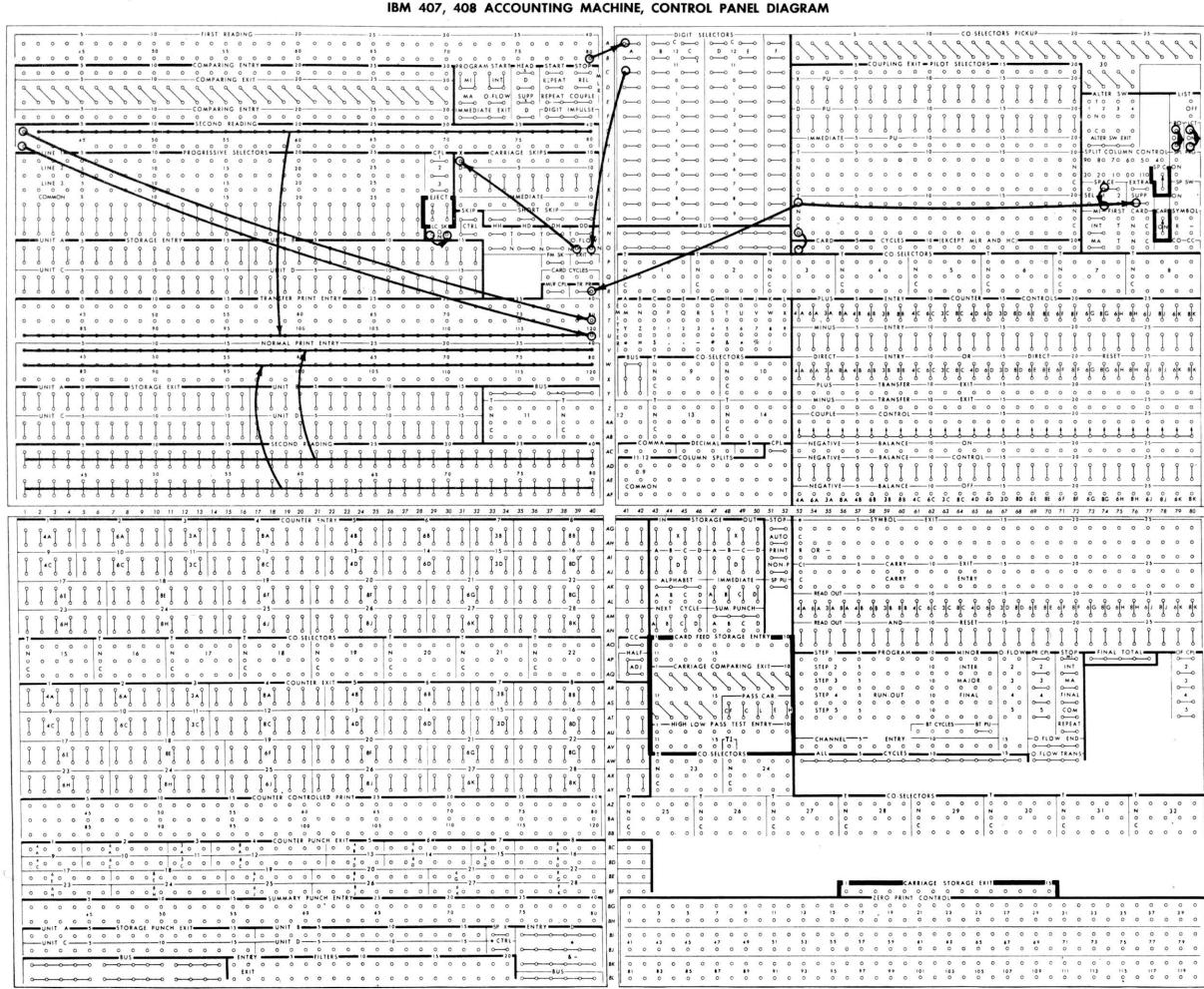


Figure 5.- Control panel modifications necessary to utilize the IBM 407 lister to print 120-column slice-maps. Standard wiring is used on the zero print control.

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- Peikert, E.W., 1962, Three-dimensional specific-gravity variation in the Glen Alpine Stock, Sierra Nevada, California: *Geol. Soc. America Bull.*, v. 73, no. 11, p. 1437-1442.
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- Smith, J.W., and Harbaugh, J.W., 1966, Stratigraphic and geographic variation of shale-oil specific gravity from Colorado's Green River Formation: *U.S. Bureau of Mines, Rept. Invest.* 6883, 11 p.
- Whitten, E.H.T., 1963, Application of quantitative methods in the geochemical study of granitic massifs: *Royal Soc. Canada Sp. Publ.* 6, p. 75-123.
- Whitten, E.H.T., and Boyer, R.E., 1964, Process-response models based on heavy-mineral content of the San Isabel Granite, Colorado: *Geol. Soc. America Bull.*, v. 75, no. 9, p. 841-862.

APPENDIX A.- Listing of FORTRAN II statements of three-dimensional response surface program and results from test data.

```
C      RESPONSE SURFACE ANALYSIS -- PART 1 -- JULY 1966
C      ROBERT SAMPSON -- PROGRAMMER
C      ISU COMPUTER CENTER PROJECT NO. 71
BEGIN TRACE
DIMENSION A(20,21),B(90),NUM(20),ITS(7)
1 DO 100 I=1,90
100 B(I)=0.0
DO 101 I=1,20
101 A(I,21)=0.0
PAGE=.57414745
IPAGE=0
INDEX=7
IS=1
ITS(1)=0
ITS(2)=1
ITS(3)=4
ITS(4)=10
ITS(5)=20
ITS(6)=35
ITS(7)=56
READ 1000
2 READ 1001,X,Y,Z,W
IB=0
IF (X-9.0E 48) 3,4,3
3 DO 200 IN=1,84
EXECUTE PROCEDURE 5000
SUM=(X**IX)*(Y**IY)*(Z**IZ)
B(IN)=B(IN)+SUM
IF (IN-20) 6,6,200
6 A(IN,21)=A(IN,21) + W*SUM
200 CONTINUE
GO TO 2
4 DO 102 I=1,20
EXECUTE PROCEDURE 5000
102 NUM(I)=IX*100 + IY*10 + IZ
DO 103 I=1,20
DO 104 J=1,20
IF=NUM(I) + NUM(J)
IS1 = IF/100
IS2 = IF/10 - IS1*10
IS = IF - IS1*99 - IS2*9 + 1
IB = 0
IN = ITS(IS)
9 IN = IN + 1
EXECUTE PROCEDURE 5000
IF (IF - (IX*100 + IY*10 + IZ)) 9,8,9
8 A(I,J) = B(IN)
A(J,I) = B(IN)
104 CONTINUE
103 CONTINUE
WBAR = A(1,21)/B(1)
AN = B(1)
DO 106 I=1,20
DO 107 J=1,20
IF (I - J) 50,107,50
50 F = -A(J,I)/A(I,I)
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DO 108 K=I,21
108 A(J,K) = A(J,K) + F*A(I,K)
107 CONTINUE
DO 300 M=1,3
IF (ITS(M+2) - I) 300,301,300
301 M2 = (M-1)*20
DO 302 M1=1,I
M3 = M2 + M1
B(M3) = A(M1,21)/A(M1,M1)
302 CONTINUE
GO TO 106
300 CONTINUE
106 CONTINUE
IPAGE=IPAGE+1
PUNCH 1000,PAGE,IPAGE
DO 128 I=1,64,8
123 PUNCH 1009,B(I),B(I+1),B(I+2),B(I+3),B(I+4),B(I+5),B(I+6),B(I+7)
PUNCH 1009,AN,WBAR
STOP 100
GO TO 1
BEGIN PROCEDURE 5000
IF (IB) 5101,5101,5100
5101 IB=1
DO 5102 IM=IS,INDEX
IX=IM-1
IY=0
IZ=0
5103 RETURN 5000
5100 IF (IY) 99,5104,5105
5104 IF (IX) 99,5102,5106
5106 IX=IX-1
IY=IZ+1
IZ=0
RETURN 5000
5105 IY=IY-1
IZ=IZ+1
RETURN 5000
5102 CONTINUE
END PROCEDURE 5000
1000 FORMAT (40H
132H
, A4,I3,1H-)
1001 FORMAT (4F10.3)
1002 FORMAT (E14.8)
1009 FORMAT (8D10)
FND TRACE
99 END

```

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C      RESPONSE SURFACE ANALYSIS PROGRAM -- PART 2 -- JULY, 1966
C      ROBERT SAMPSON -- PROGRAMMER
C      ISU COMPUTER CENTER PROJECT NO. 71
BEGIN TRACE
DIMENSION C(3,20),EV(3),R(3),D(3),M(3),SIGN(3),VAR(3),A(64)
1 READ 1000,PAGE
DO 100 I=1,64,8
100 READ 1001,A(I),A(I+1),A(I+2),A(I+3),A(I+4),A(I+5),A(I+6),A(I+7)
      READ 1001,AN,WBAR
      M(1)=3
      M(2)=9
      M(3)=19
      DO 101 I=1,3
      DO 102 J=1,20
102 C(I,J)=0.0
      IA=(I-1)*20
      K=M(I)+1
      DO 103 J=1,K
      L=J+IA
103 C(I,J)=A(L)
      EV(I)=0.0
101 CONTINUE
      TV=0.0
      LINE=70
      IPAGE=0
      READ 1000
2 READ 1002,X,Y,Z,W
      IF (X-9.0E 48) 3,4,3
3 IB=0
      DO 104 I=1,3
104 R(I)=0.0
      DO 105 I=1,20
      EXECUTE PROCEDURE 5000
      T=(X**IX)*(Y**IY)*(Z**IZ)
      DO 106 J=1,3
      IF (M(J)+1-I) 106,5,5
      5 R(J)=R(J)+C(J,I)*T
106 CONTINUE
105 CONTINUE
      DO 107 I=1,3
      D(I)=W-R(I)
107 EV(I)=EV(I)+(R(I)-WBAR)**2
      TV=TV+(W-WBAR)**2
      LINE=LINE+1
      IF (SENSE SWITCH 3) 6,7
6 IF (LINE=50) 37,37,8
8 LINE=1
      IPAGE=IPAGE+1
      PUNCH 1000,PAGE,IPAGF
      PUNCH 1003
      PUNCH 1004
37 PUNCH 1005,X,Y,Z,W,R(1),D(1),R(2),D(2),R(3),D(3)
      GO TO 2
7 IF (LINE=18) 9,9,10
10 LINE=1
      IPAGE=IPAGE+1
      PUNCH 1000,PAGE,IPAGF
      PUNCH 1006
9 PUNCH 1007,X,Y,Z,W,R(1),R(2),R(3),D(1),D(2),D(3)

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GO TO 2
4 N=AN
IPAGE=IPAGE+1
PUNCH 1000,PAGE,IPAGE
PUNCH 1008
MD=M(1)
DO 108 I=1,3
GF=EV(I)/TV
CC=SQRT(GF)
ND2=N-M(I)-1
AND2=ND2
AM=M(I)
AMS=TV-EV(I)
F=EV(I)*AND2/(AMS*AM)
IF (I-1) 11,12,11
12 PUNCH 1009,I,GF,CC,F,M(I),ND2
GO TO 108
11 MD=M(I)-MD
AM=MD
FADD=(EV(I)-EV(I-1))*AND2/(AMS*AM)
PUNCH 1009,I,GF,CC,F,M(I),ND2,FADD,MD,ND2
108 CONTINUE
PUNCH 1010
PUNCH 1011,C(1,1),C(2,1),C(3,1)
IB=0
EXECUTE PROCEDURE 5000
DO 109 I=2,20
EXECUTE PROCEDURE 5000
XI=IX
YI=IY
ZI=IZ
X=.677+XI*.0001
Y=.687+YI*.0001
Z=.697+ZI*.0001
IF (IZ) 13,13,14
13 Z=0.0
14 IF (IY) 15,15,16
15 Y=Z
Z=0.0
16 IF (IX) 17,17,18
17 X=Y
Y=Z
Z=0.0
18 DO 110 J=1,3
SIGN(J)=.10
IF (C(J,I)) 20,110,110
20 SIGN(J)=.20
C(J,I)=-C(J,I)
110 CONTINUE
IF (I-4) 21,21,22
21 PUNCH 1012,SIGN(1),C(1,I),X,Y,Z,SIGN(2),C(2,I),X,Y,Z,SIGN(3),
1C(3,I),X,Y,Z
GO TO 109
22 IF (I-10) 23,23,24
23 PUNCH 1013,SIGN(2),C(2,I),X,Y,Z,SIGN(3),C(3,I),X,Y,Z
GO TO 109
24 PUNCH 1014,SIGN(3),C(3,I),X,Y,Z
109 CONTINUE
STOP 100

```

```

GO TO 1
BEGIN PROCEDURE 5000
IF (IB) 5101,5101,5100
5101 IB=1
DO 5102 IM=1,4
IX=IM-1
IY=0
IZ=0
5103 RETURN 5000
5100 IF (IY) 99,5104,5105
5104 IF (IX) 99,5102,5106
5106 IX=IX-1
IY=IZ+1
IZ=0
RETURN 5000
5105 IY=IY-1
IZ=IZ+1
RETURN 5000
5102 CONTINUE
END PROCEDURE 5000
1000 FORMAT (40H
13H
1001 FORMAT (8D10)
1002 FORMAT (4F10.2)
1003 FORMAT (1,6X,7HX-COORD,3X,7HY-COORD,3X,7HZ-COORD,3X,7HW-COORD,6X,
16HLINEAR,6X,6HLINEAR,3X,9HQUADRATIC)
1004 FORMAT (3X,9HQUADRATIC,7X,5HCUBIC,7X,5HCUBIC,43X,1H2,/,48X,
17HSURFACE,4X,8HRESIDUAL,5X,7HSURFACE,/,4X,8HRESIDUAL,5X,7HSURFACE,
24X,8HRESIDUAL,43X,1H2,/)
1005 FORMAT (3X,4F10.3,3F12.3,/,3F12.3,43X,1H2)
1006 FORMAT (/,3X,7HX-COORD,3X,7HY-COORD,3X,7HZ-COORD,3X,7HW-COORD,8X,
16HLINEAR,3X,9HQUADRATIC,7X,5HCUBIC,/)
1007 FORMAT (4F10.3,/,33X,7HSURFACE,2X,3F12.3,/,33X,8HRESIDUAL,1X,
13F12.3)
1008 FORMAT (/,42H ORDER GOODNESS CORRELATION SIGNIFICANCE,
13H DEGREES OF SIGNIFICANCE DEGREES OF ,/,9X,
219HOF FIT COEFFICIENT,5X,6HOF FIT,6X,7HFREEDOM,2X,
314HOF ADDED TERMS,3X,7HFREEDOM,/)
1009 FORMAT (I6,2F11.7,F14.6,2I5,F15.6,I5,I6)
1010 FORMAT (/,9HEQUATIONS,/,8X,6HLINEAR,18X,9HQUADRATIC,17X,
15HCUBIC,/)
1011 FORMAT (3HW= ,F16.7,7X,3HW= ,F16.7,7X,3HW= ,F16.7)
1012 FORMAT (3X,A1,F15.7,1X,3A2,3X,A1,F15.7,1X,3A2,3X,A1,F15.7,1X,3A2)
1013 FORMAT (29X,A1,F15.7,1X,3A2,3X,A1,F15.7,1X,3A2)
1014 FORMAT (55X,A1,F15.7,1X,3A2)
END

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C      RESPONSE SURFACE ANALYSIS -- PART 3 -- JULY 1966
C      ROBERT SAMPSON -- PROGRAMMER
C      ISU COMPUTER CENTER PROJECT NO. 71
C      DIMENSION A(64),C(4,20),PLOT(10,10),DW(10),AC(10),M(4),VAR(3)
C      BEGIN TRACE
C      IMAP=0
C      IPAGE=0
C      SKIP=.20
C      IF (SENSE SWITCH 1) 200,201
200 M(1)=4
      M(2)=10
      M(3)=20
      GO TO 1
201 M(1)=3
      M(2)=6
      M(3)=10
      M(4)=15
1 READ 1000,PAGE
      IF (SENSE SWITCH 1) 202,203
203 PAGE=.57414745
      READ 1001,C(1,1),C(1,2),C(1,3)
      READ 1001,C(2,1),C(2,2),C(2,3),C(2,4),C(2,5),C(2,6)
      READ 1001,C(3,1),C(3,2),C(3,3),C(3,4),C(3,5),C(3,6),C(3,7),
      1C(3,8),C(3,9),C(3,10)
      READ 1001,C(4,1),C(4,2),C(4,3),C(4,4),C(4,5),C(4,6),C(4,7),
      1C(4,8),C(4,9),C(4,10),C(4,11),C(4,12),C(4,13),C(4,14),C(4,15)
      GO TO 2
202 DO 100 I=1,64,8
100 READ 1001,A(I),A(I+1),A(I+2),A(I+3),A(I+4),A(I+5),A(I+6),A(I+7)
      READ 1005
      DO 101 I=1,3
      DO 101 J=1,20
101 C(I,J)=0.0
      DO 102 I=1,4
102 C(1,I)=A(I)
      DO 103 I=1,10
103 C(2,I)=A(I+20)
      DO 104 I=1,20
104 C(3,I)=A(I+40)
2 PRINT 1002
      IPAGE=IPAGE+1
      READ 1003,IORD,ANC,CONST,SCALE
      READ 1004,ANACR,CONAC,AINCR
      READ 1004,ANDWN,CONDW,AINDW
      AC(1)=CONAC
      DO 105 I=2,10
105 AC(I)=AC(I-1)+AINCR
      IF (SENSE SWITCH 1) 204,205
204 ICON=(ANC-.66)*100.0
      VAR(ICON)=CONST
205 IACS=(ANACR-.66)*100.0
      IDWN=(ANDWN-.66)*100.0
      L=M(IORD)
      VAR(IDWN)=CONDW
      DO 106 I=1,10
      DW(I)=VAR(IDWN)
      VAR(IACS)=CONAC
      DO 107 J=1,10
      PLOT(I,J)=0.0

```

```

IB=0
DO 108 K=1,L
IF (SENSE SWITCH 1) 206,207
206 EXECUTE PROCEDURE 5000
T=(VAR(1)**IX)*(VAR(2)**IY)*(VAR(3)**IZ)*C(IORD,K)
GO TO 208
207 EXECUTE PROCEDURE 6000
T=(VAR(1)**IX)*(VAR(2)**IY)*C(IORD,K)
208 PLOT(I,J)=PLOT(I,J)+T
108 CONTINUE
    PLOT(I,J)=PLOT(I,J)*SCALE
    VAR(IACS)=VAR(IACS)+AINCR
107 CONTINUE
    VAR(IDWN)=VAR(IDWN)+AINDW
106 CONTINUE
    PUNCH 1000,PAGE,IPAGE,SKIP
    IPAGE=IPAGE+1
    IMAP=IMAP+1
    PUNCH 1006,IMAP,IPAGE,IORD
    IF (SENSE SWITCH 1) 210,211
210 PUNCH 1007,CONST,ANC
211 CCRL=CONAC+9.0*AINCR
    CCDW=CONDW+9.0*AINDW
    PUNCH 1017,ANACR,CONAC,CCRL,AINCR
    PUNCH 1018,ANDWN,CONDW,CCDW,AINDW
    PUNCH 1019,SCALE
    IF (SENSE SWITCH 3) 30,31
31 PUNCH 1020,IMAP,PAGE,IPAGE,AC(1),AC(2),AC(3),AC(4),AC(5),
    GO TO 32
30 PUNCH 1008,IMAP,PAGE,IPAGE,AC(1),AC(2),AC(3),AC(4),AC(5),
    1AC(6),AC(7),AC(8),AC(9),AC(10)
32 DO 110 I=1,10
    VN=0.0
    IF (I-5) 20,21,20
21 VN=ANDWN
20 IF (SENSE SWITCH 3) 36,37
37 PUNCH 1023,VN,DW(I),PLOT(I,1),PLOT(I,2),PLOT(I,3),PLOT(I,4),
    1PLOT(I,5)
    GO TO 38
36 PUNCH 1009,VN,DW(I),PLOT(I,1),PLOT(I,2),PLOT(I,3),PLOT(I,4),
    1PLOT(I,5),PLOT(I,6),PLOT(I,7),PLOT(I,8),PLOT(I,9),PLOT(I,10)
38 IF (I-10) 22,110,110
22 PUNCH 1010
110 CONTINUE
    IF (SENSE SWITCH 3) 34,35
35 IPAGE=IPAGE+1
    PUNCH 1021,IMAP,PAGE,IPAGE,AC(5),AC(6),AC(7),AC(8),AC(9),AC(10)
    DO 300 I=1,10
    PUNCH 1022,PLOT(I,5),PLOT(I,6),PLOT(I,7),PLOT(I,8),PLOT(I,9),
    1PLOT(I,10)
    IF (I-10) 40,300,300
40 PUNCH 1010
300 CONTINUE
34 IF (SENSE SWITCH 2) 5,2
5 STOP 100
    GO TO 1
    BEGIN PROCEDURE 5000
    IF (IB) 5101,5101,5100
5101 IB=1

```

```

DO 5102 IM=1,4
IX=IM-1
IY=0
IZ=0
5103 RETURN 5000
5100 IF (IY) 99,5104,5105
5104 IF (IX) 99,5102,5106
5106 IX=IX-1
IY=IZ+1
IZ=0
RETURN 5000
5105 IY=IY-1
IZ=IZ+1
RETURN 5000
5102 CONTINUE
END PROCEDURE 5000
BEGIN PROCEDURE 6000
IF (IB) 6101,6101,6100
6101 IB=1
DO 6102 IM=1,5
IX=IM-1
IY=0
RETURN 6000
6100 IF (IX) 99,6102,6103
6103 IX=IX-1
IY=IY+1
RETURN 6000
6102 CONTINUE
END PROCEDURE 6000
1000 FORMAT (40H
1 32H ,A4,I3,A1)
1001 FORMAT (8D10)
1002 FORMAT (24HENTER PLOT CONTROL CARDS )
1003 FORMAT (I1,1X,A1,1X,2F10.2)
1004 FORMAT (2X,A1,1X,2F10.2)
1005 FORMAT (1X)
1006 FORMAT (/,5HMAP =,I3,8H PAGE =,I3,//,18HCONTROL POINTS FOR ,I3,
116H ORDER SLICE MAP ,/)
1007 FORMAT (/,14HVALUES OF W AT ,F10.2,10H LEVEL OF ,A1//)
1008 FORMAT (6H MAP =,I3,63X,A4,I3,1H-/, ,18X,6F10.1//,
14F10.1,39X,1H2,/),
1009 FORMAT (5X,A1,3X,F10.1,8X,1H*,9X,1H*,9X,1H*,9X,1H*,9X,1H*,9X,1H*,
1/,8X,1H*,9X,1H*,9X,1H*,9X,1H*,40X,1H2//,19X,6F10.1//,4F10.1,39X,
21H2)
1010 FORMAT (///)
1017 FORMAT (22H VARIABLE ACROSS MAP = ,A1,/,5X,
128H VALUE AT LEFT EDGE OF MAP = ,F12.3,/,5X,
228H VALUE AT RIGHT EDGE OF MAP = ,F12.3,/,11X,
322H INCREMENT ACROSS MAP = ,F12.3,/)
1018 FORMAT (20H VARIABLE DOWN MAP = ,A1,/,8X,21H VALUE AT TOP OF MAP = ,
1F12.3,/,5X,24H VALUE AT BOTTOM OF MAP = ,F12.3,/,9X,
220H INCREMENT DOWN MAP = ,F12.3,/)
1019 FORMAT (37H SCALE FACTOR FOR DEPENDENT VARIABLE =,F10.2)
1020 FORMAT (6HMAP = ,I3,63X,A4,I3,1H-/,18X,5F10.1)
1021 FORMAT (6HMAP = ,I3,63X,A4,I3,1H-/,6F10.1)
1022 FORMAT (8X,1H*,9X,1H*,9X,1H*,9X,1H*,9X,1H*,9X,1H*,9X,1H*,9X,1H*,9X,1H*,19X,
1 5F10.1)
END TRACE
99 END

```

Output from Pass 1

RESPONSE SURFACE TEST DATA ON OIL GRAVITY FROM HARBAUGH (1964) PAGE 1-
 N236293684M982239858N03287695MM99727898NN614471364N614843783N522611998N435315700
 N430745700N452323300N738721759N633595645N659009686N561029349N556306060N612017573
 N520611105N515698117N517544743N532877583N237619266M990171956N09109471MN07094313M
 M734207337M932760699M93177950QM923649633M99650057KN020148100N613329906N596435170
 N596852306N611466751N6224323620030337579N921027865N947225128N827367103N830021438
 N285687893N14624334QN225602790N136985900N020123629N113700532N03626080PN128713783
 N111537061N115962531M83061691JM92070120RM899417337M97500204NM84366861RM91486493P
 M98928938JM99528690KM961596550M97002355JN9781609010026664330N911686943N895232838
 N324400000N236819262

80-column output from Pass 2 (incomplete)

RESPONSE SURFACE TEST DATA ON OIL GRAVITY FROM HARBAUGH (1964) PAGE 1

X-COORD	Y-COORD	Z-COORD	W-COORD	LINEAR	QUADRATIC	CUBIC
19.000	6.100	.700	39.400 SURFACE RESIDUAL	35.782 3.617	37.343 2.056	37.675 1.724
16.140	7.900	.300	37.400 SURFACE RESIDUAL	34.994 2.405	37.043 •356	38.827 -1.427
19.800	6.000	1.500	34.800 SURFACE RESIDUAL	35.803 -1.003	36.393 -1.593	36.175 -1.375
20.000	6.100	1.500	34.300 SURFACE RESIDUAL	35.787 -1.487	36.432 -2.132	36.239 -1.939
19.000	6.100	.700	39.400 SURFACE RESIDUAL	35.782 3.617	37.343 2.056	37.675 1.724
15.200	8.000	.900	35.000 SURFACE RESIDUAL	34.826 •173	35.673 -•673	36.521 -1.521

RESPONSE SURFACE TEST DATA ON OIL GRAVITY FROM HARBAUGH (1964) PAGE 15

ORDER	GOODNESS OF FIT	CORRELATION COEFFICIENT	SIGNIFICANCE OF FIT	DEGREES OF FREEDOM	SIGNIFICANCE OF ADDED TERMS	DEGREES OF FREEDOM
1	•1353954	•3679612	12.527852	3 240		
2	•2275214	•4769920	7.657891	9 234	4.651147	6 234
3	•3540070	•5949849	6.460685	19 224	3.373791	13 224

EQUATIONS

LINEAR			QUADRATIC			CUBIC		
W=	36.2936840		W=	37.6192660		W=	85.6878930	
+	•0822398 X1		+	•0901719 X1		-	4.6243348 X1	
-	•3287695 Y1		-	•9109471 Y1		-	25.6027960 Y1	
-	•0972789 Z1		-	•7094313 Z1		-	3.6985906 Z1	
			+	•0003420 X2		+	•2012362 X2	
			+	•0327606 X1Y1		+	1.3700532 X1Y1	
			-	•0317795 X1Z1		-	•3626080 X1Z1	
			+	•0236496 Y2		+	2.8713783 Y2	
			-	•0965005 Y1Z1		+	1.1537061 Y1Z1	
			+	•2014810 Z2		+	1.5962531 Z2	
						-	•0030616 X3	
						-	•0207012 X2Y1	
						+	•0099417 X2Z1	
						-	•0750020 X1Y2	
						-	•0043668 X1Y1Z1	
						-	•0148649 X1Z2	
						-	•0892893 Y3	
						-	•0952869 Y2Z1	
						-	•0615965 Y1Z2	
						-	•0700235 Z3,	

80-column output from Pass 3 (incomplete)

RESPONSE SURFACE TEST DATA ON OIL GRAVITY FROM HARBAUGH (1964)

PAGE 7

MAP = 3 PAGE = 8

CONTROL POINTS FOR 1 ORDER SLICE MAP

VALUES OF W AT .00 LEVEL OF Y

VARIABLE ACROSS MAP = Z

VALUE AT LEFT EDGE OF MAP =	.000
VALUE AT RIGHT EDGE OF MAP =	9.000
INCREMENT ACROSS MAP =	1.000

VARIABLE DOWN MAP = X

VALUE AT TOP OF MAP =	6.000
VALUE AT BOTTOM OF MAP =	36.600
INCREMENT DOWN MAP =	3.400

SCALE FACTOR FOR DEPENDENT VARIABLE = 1.00

MAP = 3

PAGE 8

	.0	1.0	2.0	3.0	4.0
6.0	*	*	*	*	*
	36.7	36.6	36.5	36.4	36.3

9.4	*	*	*	*	*
	37.0	36.9	36.8	36.7	36.6

12.8	*	*	*	*	*
	37.3	37.2	37.1	37.0	36.9

16.2	*	*	*	*	*
	37.6	37.5	37.4	37.3	37.2

X	19.6	*	*	*	*
		37.9	37.8	37.7	37.6

23.0	*	*	*	*	*
	38.1	38.0	37.9	37.8	37.7

120-column output from Pass 2 (incomplete)

RESPONSE SURFACE TEST DATA ON OIL GRAVITY FROM HARBAUGH (1964)				PAGE 1		PAGE 2	
X-COORD	Y-COORD	Z-COORD	W-COORD	LINEAR SURFACE	LINEAR RESIDUAL	QUADRATIC SURFACE	CUBIC SURFACE
19.000	6.100	.700	39.400	35.782	3.617	37.343	2.056
16.140	7.900	.300	37.400	34.994	2.405	37.043	.356
19.800	6.000	1.500	34.800	35.803	-1.003	36.393	-1.593
20.000	6.100	1.500	34.300	35.787	-1.487	36.432	-2.132
17.000	6.100	.700	39.400	35.782	3.617	37.343	2.056
15.200	8.000	.900	35.000	34.826	.173	35.673	-.673
17.860	7.800	.700	36.600	35.129	1.470	36.914	-.314
17.270	7.500	.500	38.700	35.199	3.500	37.079	1.620
16.500	7.400	.500	41.800	35.169	6.630	36.830	4.969
18.000	7.000	.100	41.400	35.462	5.937	38.069	3.330
25.010	4.300	1.700	38.500	36.771	1.728	37.451	1.048
25.000	4.300	2.000	30.900	36.741	-5.841	37.097	-6.197
24.030	4.500	1.600	37.200	36.634	.565	37.369	-.169
23.520	4.500	.900	39.600	36.660	2.939	38.237	1.362
23.750	5.000	.800	40.700	36.525	4.174	38.452	2.247
24.500	4.700	1.400	40.300	36.627	3.672	37.723	2.576
22.000	5.300	.500	41.000	36.311	4.688	38.515	2.484
21.100	5.500	1.700	33.600	36.047	-2.447	36.492	-2.892
22.500	5.400	.200	39.200	36.349	2.850	39.191	.008
23.000	5.500	.100	40.200	36.367	3.832	39.528	.671
19.100	6.200	2.300	30.300	35.602	-5.302	35.269	-4.969
7.850	6.400	3.300	30.800	34.514	-3.714	32.124	-1.324
19.490	6.400	3.000	26.600	35.500	-8.900	34.705	-8.105
12.270	6.400	3.400	35.700	34.867	.832	32.979	2.720
34.750	.100	8.500	39.500	38.291	1.208	40.246	-.746
37.600	.100	8.700	41.600	38.506	3.093	40.124	1.475
34.210	.300	8.300	33.900	38.201	-4.301	39.897	-5.997
33.980	.300	8.300	35.100	38.182	-3.082	39.929	-4.829
33.600	.200	7.900	38.800	38.222	.577	39.456	-.656
25.880	.200	7.800	37.300	37.597	-.297	40.329	-3.029
33.140	.200	7.800	37.100	38.194	-1.094	39.378	-2.278
33.340	.200	7.700	40.600	38.220	2.379	39.219	1.380
33.710	.700	7.900	39.100	38.067	1.032	39.167	-.067
28.420	.700	7.900	38.400	37.632	.767	39.785	-1.385
32.480	.900	8.700	40.200	37.822	2.377	40.408	-.208
32.000	.200	7.300	41.200	38.149	3.050	38.876	2.323
35.010	.100	6.500	36.500	38.507	-2.007	37.825	-1.325
27.600	.100	6.500	38.000	37.898	.101	38.505	-.505
35.000	.200	7.000	40.800	38.425	2.374	38.227	2.572
26.900	.600	6.700	39.700	37.656	2.043	38.458	1.241
32.000	.300	6.200	37.400	38.223	-.823	37.760	-.360
26.900	.300	5.900	38.400	37.339	1.060	38.325	.074
31.000	.400	5.500	36.800	38.176	-1.376	37.351	-.551
13.080	.200	5.100	36.300	37.218	-.918	37.892	-1.592
28.500	.800	5.000	37.800	37.888	-.088	37.075	.724
37.553							.246

RESPONSE SURFACE TEST DATA ON OIL GRAVITY FROM HARBAUGH (1964) PAGE 6

ORDER	GOODNESS OF FIT	CORRELATION COEFFICIENT	SIGNIFICANCE OF FIT	DEGREES OF FREEDOM	SIGNIFICANCE OF ADDED TERMS	DEGREES OF FREEDOM
1	.1353954	.3679612	12.527852	3 240		
2	.2275214	.4769920	7.657891	9 234	4.651147	6 234
3	.3540070	.5949849	6.460685	19 224	3.373791	13 224

EQUATIONS

LINEAR	QUADRATIC	CUBIC
W= 36.2936840	W= 37.6192660	W= 85.6878930
+ .0822398 X1	+ .0901719 X1	- 4.6243348 X1
- .3287695 Y1	- .9109471 Y1	- 25.6027960 Y1
- .0972789 Z1	- .7094313 Z1	- 3.6985906 Z1
+ .0003420 X2	+ .0003420 X2	- .2012362 X2
+ .0327606 X1Y1	+ .0327606 X1Y1	- 1.3700532 X1Y1
- .0317795 X1Z1	- .0317795 X1Z1	- .3626080 X1Z1
+ .0236496 Y2	+ .0236496 Y2	- 2.8713783 Y2
- .0965005 Y1Z1	- .0965005 Y1Z1	- 1.1537061 Y1Z1
+ .2014810 Z2	+ .2014810 Z2	- 1.5962531 Z2
-	-	- .0030616 X3
-	-	- .0207012 X2Y1
-	-	- .0099417 X2Z1
-	-	- .0750020 X1Y2
-	-	- .0043668 X1Y1Z1
-	-	- .0148649 X1Z2
-	-	- .0892893 Y3
-	-	- .0952869 Y2Z1
-	-	- .0615965 Y1Z2
-	-	- .0700235 Z3

120-column output from Pass 3 (incomplete)

RESPONSE SURFACE TEST DATA ON OIL GRAVITY FROM HARBAUGH (1964)

PAGE 43

MAP = 19 PAGE = 44

CONTROL POINTS FOR 1 ORDER SLICE MAP

VALUES OF W AT 6.00 LFVEL OF X

VARIABLE ACROSS MAP = Y

VALUE AT LEFT EDGE OF MAP = .000
VALUE AT RIGHT EDGE OF MAP = 9.000
INCREMENT ACROSS MAP = 1.000

VARIABLE DOWN MAP = Z

VALUE AT TOP OF MAP = .000
VALUE AT BOTTOM OF MAP = 9.000
INCREMENT DOWN MAP = 1.000

SCALE FACTOR FOR DEPENDENT VARIABLE = 1.00

PAGE 44										
MAP = 19	.0	1.0	2.0	3.0	4.0	5.0	6.0	7.0	8.0	9.0
	* 36.7	* 36.4	* 36.1	* 35.8	* 35.4	* 35.1	* 34.8	* 34.4	* 34.1	* 33.8
1.0	* 36.6	* 36.3	* 36.0	* 35.7	* 35.3	* 35.0	* 34.7	* 34.3	* 34.0	* 33.7
2.0	* 36.5	* 36.2	* 35.9	* 35.6	* 35.2	* 34.9	* 34.6	* 34.2	* 33.9	* 33.6
3.0	* 36.4	* 36.1	* 35.8	* 35.5	* 35.1	* 34.8	* 34.5	* 34.1	* 33.8	* 33.5
Z	4.0	* 36.3	* 36.0	* 35.7	* 35.4	* 35.0	* 34.7	* 34.4	* 34.0	* 33.7
	5.0	* 36.3	* 35.9	* 35.6	* 35.3	* 34.9	* 34.6	* 34.3	* 33.9	* 33.6
	6.0	* 36.2	* 35.8	* 35.5	* 35.2	* 34.8	* 34.5	* 34.2	* 33.9	* 33.5
	7.0	* 36.1	* 35.7	* 35.4	* 35.1	* 34.7	* 34.4	* 34.1	* 33.8	* 33.4
	8.0	* 36.0	* 35.6	* 35.3	* 35.0	* 34.6	* 34.3	* 34.0	* 33.7	* 33.3

APPENDIX B.- Modifications to "FORTRAN II Trend-surface Program With Unrestricted Input for the IBM 1620 Computer" (Sampson and Davis, 1966) to utilize Pass Three for producing slice-maps.

The final 11 cards of Pass One of the trend-surface program should be discarded. Cards listed below should be added at the end of Pass One.

```
C      MODIFICATION TO PRODUCE OUTPUT FOR INPUT TO MAP PROG-AM
      IF (SENSE SWITCH 2) 31,30
 30 PUNCH 1006,T(1),T(2),T(3),T(4),T(5),T(6),T(7),T(8),T(9),T(10),
     1T(11),T(12),T(13),T(14),T(15),T(16),T(17),T(18)
      PUNCH 1007,D(1,1),D(1,2),D(1,3)
      PUNCH 1007,D(2,1),D(2,2),D(2,3),D(2,4),D(2,5),D(2,6)
      PUNCH 1007,D(3,1),D(3,2),D(3,3),D(3,4),D(3,5),D(3,6),D(3,7),
     1D(3,8),D(3,9),D(3,10)
      PUNCH 1007,D(4,1),D(4,2),D(4,3),D(4,4),D(4,5),D(4,6),D(4,7),
     1D(4,8),D(4,9),D(4,10),D(4,11),D(4,12),D(4,13),D(4,14),D(4,15)
1007 FORMAT (8D10)
 31 PRINT 1005
      PAUSE
1000 FORMAT (3F10.3)
1001 FORMAT (5E16.8)
1002 FORMAT (E16.8/)
1003 FORMAT (18A4,5H PAGE,I2,1H-)
1004 FORMAT (/,18HCOEFFICIENT MATRIX,/)
1005 FORMAT (40HLOAD NEXT PASS BY PUSHING RESET AND LOAD)
1006 FORMAT (18A4)
      END TRACE
      END
```

Pass One of the trend-surface program will now produce 7 input cards to generate slice-maps when used in Pass Three (Appendix A). These cards are punched after the matrix is punched. If matrix output is suppressed, these cards are the only ones produced by trend-surface Pass One.

After loading the Pass Three response surface object deck and subroutines, the command LOAD DATA will be typed. SENSE SWITCH 1 should be off. The seven cards produced by trend-surface Pass One should be loaded. The computer will then type ENTER PLOT CONTROL CARDS. These cards have the following form:

Card 1 - This card contains a number between 1 and 4 punched in column 1 specifying the order of desired equation. Columns 5-14 are blank. Columns 15-24 contain a constant by which each value of Z will be multiplied. This number must contain a decimal point.

Card 2 - Columns 1 and 2 are blank. Column 3 contains X or Y, indicating the variable to be printed across the map. Column 4 is blank. Columns 5 through 14 contain the value of the left edge of the map. Columns 15 through 24 contain the value of the desired increment step. This value may be negative. Both of these numbers must contain decimals.

Card 3 - Columns 1 and 2 are blank. Column 3 contains X or Y, indicating the variable to be printed down the map. Column 4 is blank. Columns 5 through 14 contain the value at the top of the map, and columns 15 through 24 contain the value of the increment step. These numbers require decimals.

With the exceptions noted above, Pass Three operates in the same manner as described in the main body of this paper.

KANSAS GEOLOGICAL SURVEY COMPUTER PROGRAM
THE UNIVERSITY OF KANSAS, LAWRENCE

PROGRAM ABSTRACT

Title (If subroutine state in title):

Three-dimensional response surface program in FORTRAN II for the IBM 1620 computer

Computer: IBM 1620

Date: 1/18/67

Programming language: FORTRAN II

Author, organization: Robert J. Sampson, Idaho State University

John C. Davis, Kansas Geological Survey

Direct inquiries to: Authors, or

Name: Daniel F. Merriam

Address: Kansas Geological Survey, Univ. of Kansas

Lawrence, Kansas 66044

Purpose/description: Computes response surfaces (regressions) for a variable distributed in three-dimensional space by fitting polynomials up to the third degree. Also computes statistical measures and prints 100 control points for manual contouring of specified slice-maps.

Mathematical method: Regression coefficients are computed by pivotal condensation of a matrix of normal equations.

Restrictions, range: The program will accept any number of data points.

Storage requirements: 20K digits or equivalent

Equipment specifications: Memory 20K X 40K _____ 60K _____ K _____

Automatic divide: Yes X No _____ Indirect addressing Yes X No _____

Other special features required Requires PDQ FORTRAN C2 compiler and subroutines.

Additional remarks (include at author's discretion: fixed/float, relocatability; optional: running time, approximate number of times run successfully, programming hours)