

20

```

L.0055 AL=SS-RR*DCOS(THETA)
L.0056 F1=DEXP(IAL)
L.0057 F2=-RR*DSIN(THETA)
L.0058 A(I)=-F1*DSIN(F2)/TOR
L.0059 B(I)=F1*DCOS(F2)/TOR
L.0060 VO(I)=(B(I)*Q(I)-A(I)*P(I))*TOR
L.0061 7 UO(I)=(A(I)*Q(I)+B(I)*P(I))*TOR
L.0062 DO 100 J=2,NC0
L.0063 100 WRITE(9,101)P(I),Q(J),A(J),B(J),UO(J),VO(J)
L.0064 101 FORMAT(6E20.8)
L.0065 TEMP=0.
L.0066 9 CG=0.5*Q(1)
L.0067 C EVALUATION OF PROFILE
L.0068 C *****
L.0069 DO 6 I=2,NC0
L.0070 6 CG=CG+UO(I)*DSIN(WA(I)*T)+VO(I)*DCOS(WA(I)*T)
L.0071 CGF(NN)=CG
L.0072 TT(NN)=T
L.0073 IF(CG.GT.TEMP)TEMP=CG
L.0074 NN=NN+1
L.0075 IF(T.GT.TF)GO TO 99
L.0076 T=T+DELT2
L.0077 GO TO 9
L.0078 99 NN=NN-1
L.0079 Z=FAC/TEMP
L.0080 DO 102 K=1,NN
L.0081 102 CGF(K)=Z*CGF(K)
L.0082 DO 141 L=1,NN,16
L.0083 141 WRITE(6,140)(CGF(L+1),L=1,16)
L.0084 140 FORMAT(16F6.1)
L.0085 READ(9,1)DUMMY
L.0086 END
L.0087 /DATA

```

END OF PRINT * NO OF LINES PRINTED- 87

1
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6
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8

REGENERATION OF THE OUTPUT CURVE USING MODEL 1. (PARAMETERS = FUNCTION OF FREQUENCY)

$\alpha_0 =$	$.601$	$U0 =$	8.489	$M0 =$	64.282	$K0 =$	488.578
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START POINT NUMBER = 722 FINISH POINT NUMBER = 953 TIME AXIS INTERVAL = .144

CONCENTRATION PROFILE.

-2.1	-2.1	-2.2	-2.2	-2.1	-2.1	-2.0	-1.9	-1.8	-1.6	-1.5	-1.3	-1.1	-0.8	-0.5
25.0	26.4	27.6	28.7	29.9	31.0	32.1	33.3	34.4	35.5	36.6	37.6	38.7	39.7	40.7
42.7	43.6	44.5	45.3	46.2	47.0	47.7	48.4	49.1	49.7	50.3	50.8	51.3	51.7	52.1
52.8	53.0	53.2	53.4	53.5	53.5	53.4	53.4	53.3	53.2	53.0	52.8	52.5	52.1	51.4
50.9	50.4	49.9	49.3	48.7	48.1	47.4	46.7	46.0	45.2	44.4	43.6	42.8	42.0	40.3
39.4	38.5	37.6	36.7	35.8	34.9	34.0	33.1	32.2	31.3	30.4	29.5	28.6	27.8	26.1
25.3	24.4	23.7	22.9	22.1	21.4	20.7	20.0	19.3	18.6	18.0	17.4	16.8	16.2	15.7
14.6	14.2	13.7	13.2	12.8	12.4	12.0	11.7	11.3	11.0	10.7	10.4	10.1	9.8	9.3
9.1	8.9	8.7	8.5	8.3	8.1	7.9	7.7	7.6	7.4	7.2	7.1	6.9	6.8	6.6
6.3	6.2	6.0	5.9	5.7	5.6	5.4	5.2	5.1	4.9	4.8	4.6	4.4	4.3	4.1
3.7	3.6	3.4	3.3	3.0	2.8	2.7	2.5	2.3	2.2	1.9	1.8	1.6	1.4	1.2
3.9	3.8	3.6	3.5	3.3	3.2	3.0	2.9	2.7	2.6	2.3	2.2	2.0	1.8	1.6
1.0	1.1	1.1	1.2	1.2	1.3	1.3	1.3	1.3	1.3	1.5	1.6	1.7	1.8	1.9
-1.0	-1.1	-1.1	-1.2	-1.2	-1.3	-1.3	-1.3	-1.3	-1.3	-1.5	-1.6	-1.7	-1.8	-1.9
-2.1	-2.1	-2.2	-2.2	-2.1	-2.1	-2.0	-1.9	-1.8	-1.6	-1.5	-1.3	-1.1	-0.8	-0.5

```

L.C001 /FIC
L.C002 C REGENERATION OF THE OUTPUT CURVE FOR MODEL 3
L.C003 C *****
L.C004 DOUBLE PRECISION CGF(500),IT(500)
L.C005 DOUBLE PRECISION DA(50),UA(50),BMA(50),AKA(50),P(50),Q(50),B(50),VO(50),WA(50)
L.C006 DOUBLE PRECISION W,D,U,X,BM,AK,FF,SS,Z,Y,BE,UU,V,THETA,RR,AL,F1,F2
L.C007 2 FORMAT(5E20.8)
L.C008 3 FORMAT(4I5,2E20.8)
L.C009 4 FORMAT(13,2D20.8)
L.C010 1 FORMAT(4Y)
L.C011 10 FORMAT(//)
L.C012 11 FORMAT( REGENERATION OF THE OUTPUT CURVE USING MODEL 3 .//)
L.C013 12 FORMAT( DO=,F10.3,5X, UO=,F10.3,5X, MO=,F10.3 //)
L.C014 13 FORMAT( START POINT NUMBER =,14,5X, FINISH POINT NUMBER =,14,5X, TIME AXIS INTERVAL =,F5.3/)
L.C015 18 FORMAT(//, CONCENTRATION PROFILE, //)
L.C016 14 FORMAT(6D20.8)
L.C017 C READING OF DATA
L.C018 C *****
L.C019 READ(9,1)NCO
L.C020 READ(5,2)X,FG,FL,ACOL,TOR
L.C021 READ(5,3)J11,J12,JF1,JF2,DELT1,DELT2
L.C022 READ(5,1)AREA
L.C023 READ(5,14)P(1),Q(1),CA(1),UA(1),BMA(1),AKA(1),I=1,NCO
L.C024 READ(9,1)CA(1),UA(1),BMA(1)
L.C025 READ(9,1)FAC
L.C026 WRITE(6,1C)
L.C027 WRITE(6,11)
L.C028 WRITE(6,12)DA(1),UA(1),BMA(1)
L.C029 WRITE(6,13)J12,JF2,DELT2
L.C030 WRITE(6,18)
L.C031 NN=1
L.C032 FF=FL/FG
L.C033 PI=DATAN(1.)*4.
L.C034 T=DELT2*J12
L.C035 TF=DELT2*JF2
L.C036 DO 7 I=2,NCO
L.C037 CI=1-1
L.C038 D=DA(1)
L.C039 U=UA(1)
L.C040 BM=BMA(1)
L.C041 AK=AKA(1)
L.C042 AK=AK*ACOL/FL
L.C043 WA(1)=PI*CI/TOR
L.C044 W=WA(1)
L.C045 THETA=DATAN(4.*W*D*(BM*FF+1.)/(U*U))/2.
L.C046 SS=U*X/(2.*D)
L.C047 RR=DSORT(DSORT(U**4/(16.*D**4)+W*(BM*f+1.))**2*W/(D*D)))
L.C048 AL=SS-X*RR*DCOS(THETA)
L.C049 F1=DEXP(AL)
L.C050 F2=-RR*X*DSIN(THETA)
L.C051 A(1)=-F1*DSIN(F2)/TOR
L.C052 B(1)=F1*DCOS(F2)/TOR
L.C053 VO(1)=(B(1)*Q(1)-A(1)*P(1))*TOR
L.C054 7 UO(1)=(A(1)*Q(1)+B(1)*P(1))*TOR

```

```

L.0055 DO 100 J=2,NCG
L.0056 100 WRITE(9,101)PI(J),Q(J),A(J),B(J),UB(J),VO(J)
L.0057 101 FORMAT(6E20.8)
L.0058 TEMP=0.
L.0059 9 CG=C.5*Q(1)
L.0060 DO 6 I=2,NCG
L.0061 6 CG=CG+UB(I)*DSIN(WA(I)*T)+VO(I)*DCOS(WA(I)*T)
L.0062 CSF(NN)=CG
L.0063 TFINN)=T
L.0064 IF(CG.GT. TEMP)TEMP=CG
L.0065 NN=NN+1
L.0066 IF(T.GT.TF)GO TO 99
L.0067 T=T+DELTZ
L.0068 GO TO 9
L.0069 99 NN=NN-1
L.0070 Z=FAC/TEMP
L.0071 DO 102 K=1,NN
L.0072 102 CGF(K)=Z*CGF(K)
L.0073 DO 141 L=1,NN,16
L.0074 141 WRITE(6,140)(CGF(L+1),I=1,16)
L.0075 140 FORMAT(16F6.1)
L.0076 READ(9,1)DUMMY
L.0077 ENI
L.0078 /DATA

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END OF PRINT * NO OF LINES PRINTED- 73

BUTANE.

REGENERATION OF THE OUTPUT CURVE USING MODEL 3. (PARAMETERS = FUNCTION OF FREQUENCY)

U0= .988 U0= 8.489 M0= 64.304

START POINT NUMBER = 722 FINISH POINT NUMBER = 953 TIME AXIS INTERVAL = .144

CONCENTRATION PROFILE.

-3.6	-3.6	-3.6	-3.7	-3.6	-3.6	-3.6	-3.4	-3.2	-3.1	-2.9	-2.7	-2.5	-2.2
-1.9	-1.6	-1.2	-1.8	.0	.5	1.1	2.2	2.9	3.5	4.2	5.0	5.7	6.5
7.4	8.2	9.1	10.0	12.0	13.0	14.0	16.2	17.2	18.4	19.5	20.6	21.8	23.0
24.1	25.3	26.5	27.7	30.1	31.2	32.4	34.7	35.9	37.0	38.1	39.1	40.2	41.2
42.2	43.2	44.1	45.0	46.7	47.4	48.2	49.5	50.1	50.7	51.2	51.6	52.1	52.4
52.7	53.0	53.2	53.3	53.5	53.5	53.4	53.2	53.0	52.7	52.4	52.1	51.7	51.3
50.8	50.3	49.7	49.1	47.9	47.2	46.4	44.9	44.1	43.3	42.4	41.5	40.7	39.8
38.9	37.9	37.0	36.1	34.2	33.2	32.3	30.4	29.5	28.6	27.7	26.8	25.9	25.0
24.2	23.4	22.5	21.7	20.2	19.5	18.7	17.4	16.7	16.1	15.5	14.9	14.3	13.8
13.2	12.7	12.3	11.8	11.0	10.6	10.2	9.5	9.2	8.9	8.6	8.3	8.1	7.8
7.6	7.4	7.2	7.0	6.6	6.4	6.2	5.9	5.7	5.6	5.4	5.3	5.1	5.0
4.9	4.7	4.6	4.4	4.1	4.0	3.8	3.5	3.4	3.2	3.1	2.9	2.8	2.6
2.5	2.3	2.1	2.0	1.7	1.5	1.3	1.0	.9	.7	.6	.4	.3	.1
.0	.1	.2	.4	.6	.7	.8	-1.0	-1.1	-1.1	-1.2	-1.3	-1.3	-1.4
-1.4	-1.4	-1.5	-1.5	-1.5	-1.5	-1.5	0.0	0.0	0.0	0.0	0.0	0.0	0.0

REMOTE PRINT/DISPLAY FOR USER NO 20

```

L.0001 /FTC BCD
L.0002 IMPLICIT REAL*8(A-H,Q-Z)
L.0003 INTEGER OUTPUT
L.0004 COMMON TO(11,10),P(50),TA(10),E(10,10),A(10),T(10),UU(11),TX(11)
L.0005 COMMON UC,TL,ACTA,ACTB,M,L,ID,N,JJ-IN,IS,NN,INN
L.0006 C
L.0007 C

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DOCUMENTATION

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DEFINITION OF PROGRAM VARIABLES
N=NUMBER OF VARIABLES
M=DIMENSIONALITY OF THE SEARCH ,M $LESS THAN OR EQUAL TO N THE P
WILL SEARCH THROUGH THE FIRST M VARIABLES
TA(1)=1TH. COMPONENT OF THE STARTING POINT
TO(J,1)=THE 1TH. COMPONENT OF THE (J-1)END POINT. I.e. TO(3,1) MAR
THE END OF THE SEARCH ALONG THE SECOND VECTOR E(2,1)
E(J,1)=THE 1TH.COMPONENT OF THE JTH. SEARCH VECTOR
ID=THE CUMULATIVE NUMBER OF FUNCTIONAL EVALUATIONS
L=THE TOTAL NUMBER OF STAGES
AI(J)=THE STEP SIZE IN THE JTH. DIRECTION
TI(1)=THE WORKING VECTOR THAT CARRIES THE VALUES OF THE VARIABLES
P(50)=A ROW VECTOR OF SEARCH CONSTANTS AND PARAMETERS
UU(11)=A WORKING VARIABLE
THE USER MAY MAKE USEMOF THE FOLLOWING VARIABLE. THIS LIST MAY BE
ADDED TO OR SUBTRACTED FROM SO LONG AS THE COMMON IS KEPT THE
SAME IN ALL THE SUBROUTINES.
UD,TL,JJ,IN,NN,INN,TX(11),ACTA,ACTB.

```

FORMAT STATEMENTS

```

1001 FORMAT(3Y)
1002 FORMAT(10Y)
1003 FORMAT(10Y)
1004 FORMAT(10Y)
1005 FORMAT(10Y)
1006 FORMAT(1H,1X,' ROSENBROCK SEARCH WITH ',I3,' VARIABLES ',I3,I2,
1007 FORMAT(/,1X,' THE P-VECTOR IS ',/,5(F8.3,2X)))
1008 FORMAT(1X,1X,' THE INITIAL SEARCH MATRIX ',(/,10(F8.4,2X)))
1009 FORMAT(/,1X,' THE STEP SIZES ',/1X,10(F8.4,2X))
1010 FORMAT(/,1X,' THE INITIAL VALUES FOR EACH OF THE VARIABLES ',/5
1011 FORMAT(/,1X,' THIS IS THE END OF SEARCH ',I2,/,1X,' THE MINIMUM V
1012 FORMAT(/,1X,' THE TOTAL SEARCH ARE ',5(/,1X,' I(',I2,')=',E14.7,5X,' I(',I2,
1013 FORMAT(/,1X,' THIS IS THE END OF STAGE ',I3,/,1X,' THE TOTAL
1014 FORMAT(/,1X,' THE COORDINATES OF THE END PO
1015 FORMAT(/,1X,' THE OBJECTIVE FUNCTION IS',E14.7,/,1X,' THE NEW SEARCH MATRIX')
1016 FORMAT(/,1X,' THE TOTAL NUMBER OF STAGES IS ',I3,' AND THIS HAS E
1017 FORMAT(/,1X,' THE SEARCH ROUTINE HAS CONVERGED WITH IN THE DESI
1018 FORMAT(5(1X,E14.7,5X))

```

	DEFINITION OF THE LOGICAL INPUT/OUTPUT UNITS
0.0050	
0.0051	
0.0052	

```

L.0053 C
L.0054 INPUT=5
L.0055 OUTPUT=1
L.0056 UO=0.00
L.0057 C
L.0058 C
L.0059 C
L.0060 C
L.0061 C
L.0062 C
L.0063 C
L.0064 C
L.0065 C
L.0066 C
L.0067 C
L.0068 C
L.0069 C
L.0070 C
L.0071 C
L.0072 C
L.0073 C
L.0074 C
L.0075 C
L.0076 C
L.0077 C
L.0078 C
L.0079 C
L.0080 C
L.0081 C
L.0082 C
L.0083 C
L.0084 C
L.0085 C
L.0086 C
L.0087 C
L.0088 C
L.0089 C
L.0090 C
L.0091 C
L.0092 C
L.0093 C
L.0094 C
L.0095 C
L.0096 C
L.0097 C
L.0098 C
L.0099 C
L.0100 C
L.0101 C
L.0102 C
L.0103 C
L.0104 C
L.0105 C
L.0106 C
L.0107 C
L.0108 C
L.0109 C
L.0110 C
L.0111 C

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DATA DEFINITION

THE FOLLOWING VARIABLES MUST BE DEFINED ON INPUT

N
M, LESS THAN OR EQUAL TO N
P(1), A(J)/P(1)=MINIMUM STEP SIZE
P(2)=10.
P(3)=MINIMUM DESIRED VALUE OF THE OBJECTIVE FUNCTION
P(4)=MAXIMUM ALLOWABLE CHANGE IN EACH VARIABLE FOR CONVERGENCE
P(5) MAY NOT BE USED
P(6)=MAXIMUM NUMBER OF STAGES DESIRED
P(7)=STEP SIZE REDUCTION AT THE END OF EACH STAGE
P(8-29), FREE FOR USERS BENEFIT
P(31-40)=MAXIMUM VALUE FOR EACH OF THE VARIABLES
P(41-50)=MINIMUM VALUES FOR EACH OF THE VARIABLES
E(N,N)=SEARCH MATRIX
USER CAN USE 1 0 0
0 1 0
0 0 1

A(J)=STEP SIZE (0.1)
TA(I)=THE COORDINATE OF A FEASIBLE STARTING POINT

DATA INPUT

```

READ(INPUT,1001)N,M,JJ
READ(INPUT,1002)(P(1),-1,50)
READ(INPUT,1003)((E(I,J),J=1,10),I=1,10)
READ(INPUT,1004)(A(I),I=1,10)
READ(INPUT,1005)(TA(I),I=1,10)
WRITE(OUTPUT,1006)N,M,JJ
WRITE(OUTPUT,1007)(P(1),I=1,50)
WRITE(OUTPUT,1008)((E(I,J),J=1,10),I=1,10)
WRITE(OUTPUT,1009)(A(I),I=1,10)
WRITE(OUTPUT,1010)(TA(I),I=1,10)
DO 115 I=1,N
  T(I)=TA(I)
  TO(M+1,I)=T(I)
  CALL U(P(5))
  ID=0
  L=0
  WRITE(OUTPUT,1012)L,IO,P(5),(TO(M+1,I),I=1,N)
  L=1
  ID=1
MINIMIZATION CYCLE
  CALL COSER
  WRITE(OUTPUT,1012)L,IO,P(5),(TO(M+1,I),I=1,N)
  CONVERGENCE TFSTS
  IF(P(5)-P(3))100,100,101
  DO 102 I=1,N
    TA(I)=TO(M+1,I)

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115

110

101

102

```

0.0112 DO 103 I=1,N
0.0113 IF(DABS(TO(M+1,I))-TO(1,I))-P(4))103,103,104
0.0114 CONTINUE
0.0115 103 CONTINUE
0.0116 GOTO 112
0.0117 C
0.0118 C
0.0119 C
0.0120 104 CALL CQPIP(N,E,TO)
0.0121 L=L+1
0.0122 DO 201 I=1,N
0.0123 A(I)=A(I)*P(7)
0.0124 C
0.0125 C
0.0126 C
0.0127 DO 105 J=1,N
0.0128 DO 105 I=1,N
0.0129 IF(DABS(E(I,J))-1.00)105,105,106
0.0130 CONTINUE
0.0131 GOTO 107
0.0132 DO 108 I=1,N
0.0133 DO 108 J=1,N
0.0134 E(I,J)=0.00
0.0135 DO 109 I=1,N
0.0136 E(I,I)=1.00
0.0137 107 WRITE(OUTPUT,1013)
0.0138 DO 114 J=1,N
0.0139 114 WRITE(OUTPUT,1016)(E(J,I),I=1,N)
0.0140 IF(L-P(5))110,110,111
0.0141 111 WRITE(OUTPUT,1014)
0.0142 GOTO 113
0.0143 112 WRITE(OUTPUT,1015)
0.0144 113 STOP
0.0145 END
0.0146 /FTC BCD
0.0147 SUBROUTINE CQSER
0.0148 IMPLICIT REAL*8(A-H,O-Z)
0.0149 C
0.0150 C
0.0151 C
0.0152 REAL*8 AJ(21)
0.0153 REAL*8 TI(10)
0.0154 DIMENSION AA(10),AT(10),BT(10),TMIN(10),TMAX(10)
0.0155 COMMON TO(11,10),P(50),TA(10),E(10,10),A(10),T(10),UU(11),TX(11)
0.0156 COMMON UC,TL,ACTA,ACTB,M,L,LD,N,JJ,IN,IS,NN,INN
0.0157 DO 191 I=1,N
0.0158 AA(I)=A(I)/P(1)
0.0159 AT(I)=A(I)
0.0160 BT(I)=A(I)/P(2)
0.0161 TO(1,I)=TA(I)
0.0162 LL=30+I
0.0163 LM=LL+10
0.0164 TMAX(I)=P(LL)
0.0165 TMIN(I)=P(LM)
0.0166 TI(I)=TI(I)
0.0167 T(I)=TA(I)
0.0168 DO 350 J=1,M
0.0169 P(5)=AA(I,J)
0.0170 IF (DABS(AT(J))-DABS( (5))) 340,1801,1801

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```

L.0171 1801 CONTINUE
L.0172 CALL U(ANS)
L.0173 UU(1)=ANS
L.0174 ID=ID+1
L.0175 K=1
L.0176 LLL=0
L.0177 AJ(1)=1.00
L.0178 AJ(2)=1.00
L.0179 DO 961 I=1,M
L.0180 T1(I)=T(I)
L.0181 CALL GRAD(T,J,IG)
L.0182 ID=ID+2
L.0183 DO 962 I=1,M
L.0184 T(I)=T1(I)
L.0185 GO TO(200,190,190,200,212),IG
L.0186 190 AT(J)=-AT(J)
L.0187 BT(J)=-BT(J)
L.0188 200 CONTINUE
L.0189 CA=AT(J)
L.0190 IDG=0
L.0191 210 DO 221 I=1,N
L.0192 T(I)=TO(J,I)+CA*E(J,I)
L.0193 IF( T(I)-TMAX(I))2101,2102,2102
L.0194 T(I)=TMAX(I)-.00100
L.0195 GO TO 220
L.0196 2101 IF( T(I)-TMIN(I))2104,2104,221
L.0197 2104 T(I)=TMIN(I)+.00100
L.0198 220 CONTINUE
L.0199 221 CONTINUE
L.0200 LLL=LLL+1
L.0201 CALL U(ANS)
L.0202 U11=ANS
L.0203 ID=ID+1
L.0204 IF(U11-UU(J))270,2701,2701
L.0205 2701 GO TO(250,5205,260),K
L.0206 5205 IF(LLL-2)320,320,5206
L.0207 5206 CA=CA-AT(J)*AJ(LLL-1)+AT(J)
L.0208 LLL=0
L.0209 AJ(1)=1.00
L.0210 AJ(2)=1.00
L.0211 GO TO 210
L.0212 250 K=3
L.0213 U11P=U11
L.0214 CA=CA-BT(J)
L.0215 GO TO 210
L.0216 260 CA=CA-BT(J)
L.0217 IF(U11-U11P)211,212,212
L.0218 211 U11P=U11
L.0219 IDG=IDG+1
L.0220 IF(IDG-1)210,212,212
L.0221 212 CA=.0000100*A(J)
L.0222 GO TO 320
L.0223 270 GO TO (280,290,300),K
L.0224 280 K=2
L.0225 290 UU(J)=U11
L.0226 IF(LLL-20)5203,5204,5204
L.0227 5204 AJ(1)=AJ(LLL-2)
L.0228 AJ(2)=AJ(LLL-1)
L.0229 LLL=3

```

```

L.0230      GOTO 5002
L.0231      5203 IF(LLL-2)5001,5001,5002
L.0232      5001 CA=CA+AT(J)
L.0233      GOTO 210
L.0234      5002 AJ(LLL)=AJ(LLL-1)+AJ(LLL-2)
L.0235      CA=CA+AT(J)*AJ(LLL)
L.0236      GOTO 210
L.0237      300 DO 310 I=1,N
L.0238      310 TO(J+1,I)= T(I)
L.0239      UU(J)=U(I)
L.0240      UU(J+1)=UU(J)
L.0241      GO TO 350
L.0242      320 CA=CA-AT(J)
L.0243      321 DO 330 I=1,N
L.0244      T(I)=TO(J,I)+CA*E(J,I)
L.0245      IF( T(I)-TMIN(I))5100,5100,5101
L.0246      5100 T(I)=TMIN(I)+.00100
L.0247      GOTO 330
L.0248      5101 IF( T(I)-TMAX(I))330,5102,5102
L.0249      5102 T(I)=TMAX(I)-.00100
L.0250      330 TO(J+1,I)= T(I)
L.0251      UU(J+1)=UU(J)
L.0252      GO TO 350
L.0253      340 CA=0.00
L.0254      DO 5004 I=1,N
L.0255      5004 TO(J+1,I)=TO(J,I)
L.0256      U(J+1)=UU(J)
L.0257      350 CONTINUE
L.0258      PA = UU(M+1)
L.0259      GO 2000 I=1,N
L.0260      2000 I)=TO(N+1,I)
L.0261      CALL U(ANS)
L.0262      RETURN
L.0263      END
L.0264      /FTC BCD
L.0265      SUBROUTINE GRAD(A,J,IG)
L.0266      IMPLICIT REAL*8(A-H,O-Z)
L.0267      REAL*8 A(10)
L.0268      DIMENSION A(10),X(10),AB(10),AO(10)
L.0269      COMMON TO(11,10),PI(50),TA(10),E(10,10),Z(10),T(10),UU(11),TX(11)
L.0270      COMMON UC,TL,ACTA,ACTB,M,L,IO,N,JJ,IN,IS,NN,INN
L.0271      DO 182 I=1,N
L.0272      182 X(I)=E(J,I)*Z (J)
L.0273      DO 31 I=1,M
L.0274      31 AO(I)=A(I)
L.0275      AB(I)=AO(I)
L.0276      DO 101 I=1,M
L.0277      101 T(I)=AB(I)
L.0278      CALL U(ANS)
L.0279      V=ANS
L.0280      V1=V
L.0281      DO 32 I=1,M
L.0282      32 AB(I)=AO(I)+X(I)*.0010
L.0283      DO 102 I=1,M
L.0284      102 T(I)=AB(I)
L.0285      CALL U(ANS)
L.0286      V=ANS
L.0287      V2=V
L.0288      IF(V2-V1)33,34,35

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L.0289 C      THE FIRST DERIVATIVE IS NEGATIVE
L.0290      IG=1
L.0291      RETURN
L.0292 C      THE FIRST DERIVATIVE IS POSITIVE
L.0293      IG=2
L.0294      RETURN
L.0295      DO 36 I=1,M
L.0296      AB(I)=AO(I)-X(I)*.00100
L.0297      DO 103 I=1,M
L.0298      T(I)=AB(I)
L.0299      CALL U(ANS)
L.0300      ID=ID+1
L.0301      V=ANS
L.0302      VO=V
L.0303      IF(V1-VO)37,38,39
L.0304 C      THE SECOND DERIVATIVE IS NEGATIVE
L.0305      IG=3
L.0306      RETURN
L.0307 C      THE SECOND DERIVATIVE IS POSITIVE
L.0308      IG=4
L.0309      RETURN
L.0310      N2=1
L.0311      DO 1 I=1,M
L.0312      AB(I)=AO(I)-.00100*X(I)*(-1.00)**(N2+1)*2.00** (N2)
L.0313      DO 104 I=1,M
L.0314      T(I)=AB(I)
L.0315      CALL U(ANS)
L.0316      ID=ID+1
L.0317      V=ANS
L.0318      VO=V
L.0319      IF(V1-VO)31,3,39
L.0320      N2=N2+1
L.0321      IF(N2-5)2,40,40
L.0322 C      BOTH THE FIRST AND SECOND DERIVATIVES ARE ZERO
L.0323      IG=5
L.0324      RETURN
L.0325      END
L.0326 /FTC      BCD
L.0327      SUBROUTINE CQIP(N,E,TO)
L.0328      IMPLICIT REAL*8(A-H,O-Z)
L.0329      REAL*8 E(10,10),TO(11,10)
L.0330 C      * THIS IS ROSENBROCK'S METHOD OF FORMING AN N DIMENSIONAL ORTHOGONA
L.0331 C      SET E(J,I), THE INITIAL VECTOR E(1,1) IS THE UNIT VECTOR IN THE
L.0332 C      DIRECTION TO(1,1) TO TO(J+1,1).
L.0333 C      *
L.0334 C      C(16,10),TO(11,10),A(10,10),B(10,10),MODB(10),E(10,10)
L.0335      REAL*8 MOD,F(10,10)
L.0336      DO 1 J=1,N
L.0337      DO 1 I=1,N
L.0338      C(J,I)=TO(J+1,1)-TO(J,I)
L.0339      DO 16 J=1,N
L.0340      DO 16 I=1,N
L.0341      SUM=0.00
L.0342      DO 2 K=J,N
L.0343      SUM=SUM+C(K,I)
L.0344      *
L.0345 C      THE SET OF VECTORS A(J,I) REPRESENTS THE VECTORS TO(1,1) TO
L.0346 C      TO(J+1,1), TO(2,1) TO TO(J+1,2),...,TO(J,1) TO TO(J+1,1)
L.0347 C

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L.0348 C 16 *
L.0349 A(J,I) =SUM
L.0350 DO 3 I=1,N
L.0351 B(I,I)=A(I,I)
L.0352 MOD=0.00
L.0353 DO 4 I=1,N
L.0354 MGR=MOD+(B(I,I))**2
L.0355 C *
L.0356 MODB(J) IS THE SQUARE ROOT OF THE SUM OF SQUARES I.E. THE NOR-
L.0357 MALISING FACTOR
L.0358 C *
L.0359 MODB(1)=DSQRT(MOD)
L.0360 IF(MODB(1).LE.0.00) GOTO 13
L.0361 DO 5 I=1,N
L.0362 E(I,I)=B(I,I)/MODB(1)
L.0363 SUM=0.00
L.0364 DO 6 I=1,N
L.0365 SUM4=SUM+A(2,I)*E(1,I)
L.0366 DO 8 I=1,N
L.0367 B(2,I)=A(2,I)-SUM*E(1,I)
L.0368 SUM=0.00
L.0369 DO 9 I=1,N
L.0370 SUM=SUM+B(2,I)**2
L.0371 MODB(2)=DSQRT(SUM)
L.0372 IF(MODB(2).LE.0.00) GOTO 13
L.0373 DO 10 I=1,N
L.0374 C *
L.0375 E(2,I) IS THE UNIT VECTOR IN THE DIRECTION TO(1,I) TO TO(J+1,I)
L.0376 C *
L.0377 E(2,I) IS THE UNIT VECTOR ORTHOGONAL TO E(1,I)
L.0378 C *
L.0379 E(2,I)=B(2,I)/MODB(2)
L.0380 C *
L.0381 IF N IS LESS THAN 3 THE SUBROUTINE OPTS OUT
L.0382 C *
L.0383 IF(N-3)7,11,11
L.0384 DO 14 K=3,N
L.0385 DO 15 I=1,K
L.0386 SUM=0.00
L.0387 DO 12 J=2,K
L.0388 SUM=0.00
L.0389 DO 18 L=1,N
L.0390 SUM=SUM +A(K,L)*E(J-1,L)
L.0391 SOM=SUM+SUM*E(J-1,I)
L.0392 F(K,I) = SOM
L.0393 DO 21 I=1,N
L.0394 B(K,I)=A(K,I)-F(K,I)
L.0395 MOD=0.00
L.0396 DO 17 I=1,N
L.0397 MOD=MOD+B(K,I)**2
L.0398 MODB(K)=DSQRT(MOD)
L.0399 IF(MODB(K).LE.0.00) GOTO 13
L.0400 C *
L.0401 A SET OF UNIT VECTORS E(J,I) (J=3,...) IS FORMED MUTUALLY
L.0402 C *
L.0403 ORTHOGONAL AND ORTHOGONAL TO E(1 AND 2,I)
L.0404 DO 14 I=1,N
L.0405 E(K,I)=B(K,I)/MODB(K)
L.0406 GOTO 7
L.0407 DO 22 J=1,N

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L.0407 DO 22 I=1,N
L.0408 E(I,J)=0.00
L.0409 DO 23 I=1,N
L.0410 23 E(I,I)=1.00
L.0411 7 CONTINUE
L.0412 RETURN
L.0413 END

END OF PF NT * NO OF LINES PRINTED- 413

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L.0001 /FTC
L.0002 SUBROUTINE U(ANS)
L.0003 IMPLICIT REAL*8(A-H,O-Z)
L.0004 REAL*8 ANS
L.0005 COMMON TO(11,10),P(50),TA(10),E(10,10),A(10),T(10),UU(11),TX(11)
L.0006 COMMON UG,TL,ACTA,ACTB,M,L,ID,N,JJ,IN,IS,NN,INN
L.0007 REAL*8 WA(50),AD(50),BD(50),AC(50),BC(50)
L.0008 900 FORMAT(Y)
L.0009 901 FORMAT(5E20.8)
L.0010 902 FORMAT(40X,2E20.8)
L.0011 IF(UG.GT.0.)GO TO 910
L.0012 READ(9,900)NCO
L.0013 NCO=NCO+1
L.0014 PI=4.*DATAN(1.)
L.0015 READ(5,901)XX,FG,FL,ACOL,TOR
L.0016 FF=FL/FG
L.0017 READ(5,902)(AD(I),BD(I),I=1,NCO)
L.0018 910 UU=UU+1.
L.0019 DO=1(1)
L.0020 U=T(2)
L.0021 BM=T(3)
L.0022 AK=T(4)
L.0023 AK=AK*ACOL/FL
L.0024 C EVOLUTION OF THE FOURIER COEFFICIENTS
L.0025 C *****
L.0026 DO 970 I=2,NCO
L.0027 C1=I-1
L.0028 WA(I)=PI*C1/TOR
L.0029 W=WA(I)
L.0030 SS=U*XX/(2.*DO)
L.0031 Z=SS*SS
L.0032 Y=1.D+00/DSQRT((BM*W/AK)**2+1.)
L.0033 BE=-DATAN(BM*W/AK)
L.0034 UUU=Z-XX*XX*AK/DD*(Y*DCOS(BE)-1.)*FF
L.0035 V=XX*XX/DD*(W-AK*Y*DSIN(BE)*FF)
L.0036 THETA=DATAN(V/UUU)/2.
L.0037 RR=DSQRT(DSQRT(UUU*UUU+V*V))
L.0038 AL=55-RR*DCOS(THETA)
L.0039 F1=DEXP(AL)
L.0040 F2=-RR*DSIN(THETA)
L.0041 AC(I)=-F1*DSIN(F2)/TOR
L.0042 970 BC(I)=F1*DCOS(F2)/TOR
L.0043 SSQ=0.
L.0044 AC(1)=0.
L.0045 BC(1)=0.5/TOR
L.0046 DO 971 I=1,NCO
L.0047 971 SSQ=SSQ+(AC(I)-AD(I))**2+(BC(I)-BD(I))**2
L.0048 ANS=SSQ
L.0049 RETURN
L.0050 END

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L.0001 , ROSENBROCK SEARCH WITH 4 VARIABLES 4 1

L.0002 THE P-VECTOR IS

L.0003	10.000	0.000	0.001	0.000
L.0004	50.000	1.000	0.000	0.000
L.0005	0.000	0.000	0.000	0.000
L.0006	0.000	0.000	0.000	0.000
L.0007	0.000	0.000	0.000	0.000
L.0008	0.000	0.000	0.000	0.000
L.0009	0.000	0.000	0.000	0.000
L.0010	0.000	0.000	0.000	0.000
L.0011	0.000	0.000	0.000	0.000
L.0012	0.000	0.000	0.000	0.000
L.0013	0.000	0.000	0.000	0.000
L.0014	0.000	0.000	0.000	0.000
L.0015	1.000	10.000	65.000	1000.000
L.0016	0.000	0.000	0.000	0.000
L.0017	0.000	0.000	0.000	0.000
L.0018	0.500	8.000	64.000	400.000
L.0019	0.000	0.000	0.000	0.000
L.0020	0.000	0.000	0.000	0.000
L.0021	0.000	0.000	0.000	0.000
L.0022	0.000	0.000	0.000	0.000
L.0023	0.000	0.000	0.000	0.000
L.0024	0.000	0.000	0.000	0.000

THE INITIAL SEARCH MATRIX

L.0025	1.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
L.0026	0.0000	1.0000	0.0000	0.0000	0.0000	0.0000	0.0000
L.0027	0.0000	0.0000	1.0000	0.0000	0.0000	0.0000	0.0000
L.0028	0.0000	0.0000	0.0000	1.0000	0.0000	0.0000	0.0000
L.0029	0.0000	0.0000	0.0000	0.0000	1.0000	0.0000	0.0000
L.0030	0.0000	0.0000	0.0000	0.0000	0.0000	1.0000	0.0000
L.0031	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	1.0000
L.0032	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
L.0033	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
L.0034	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
L.0035	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
L.0036	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
L.0037	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
L.0038	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
L.0039	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
L.0040	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
L.0041	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
L.0042	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
L.0043	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
L.0044	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
L.0045	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
L.0046	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
L.0047	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
L.0048	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
L.0049	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
L.0050	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
L.0051	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
L.0052	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
L.0053	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
L.0054	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000

THE STEP SIZES

THE INITIAL VALUES FOR EACH OF THE VARIABLES

T(1)=	0.698	T(2)=	8.489
T(3)=	64.304	T(4)=	522.478
T(5)=	0.000	T(6)=	0.000
T(7)=	0.000	T(8)=	0.000

T(5' 0.000 T(10)= 0.000

THIS IS THE END OF STAGE 0
THE TOTAL NUMBER OF FUNCTIONAL EVALUATIONS IS 0
THE VALUE OF THE OBJECTIVE FUNCTION IS .5340823D-05
THE COORDINATES OF THE END POINT ARE
.6978891D+00 .8488784D+01 .6430408D+02 .5224785D+03

THIS IS THE END OF STAGE 1
THE TOTAL NUMBER OF FUNCTIONAL EVALUATIONS IS 48
THE VALUE OF THE OBJECTIVE FUNCTION IS .5052007D-05
THE COORDINATES OF THE END POINT ARE
.5978891D+00 .8488785D+01 .6425408D+02 .4847785D+03

THE NEW SEARCH MATRIX
- .2652508D-02 .2652508D-07 - .1326254D-02 - .9999956D+00
.5999965D+00 .7035825D-10 - .3517912D-05 - .2652506D-02
.1975226D-06 -1.0000000D+00 - .3903128D-10 - .3197442D-07
- .8115646D-12 .4108754D-05 .9999991D+00 - .1326259D-02

THIS IS THE END OF STAGE 2
THE TOTAL NUMBER OF FUNCTIONAL EVALUATIONS IS 100
THE VALUE OF THE OBJECTIVE FUNCTION IS .5038686D-05
THE COORDINATES OF THE END POINT ARE
.6024779D+00 .8488784D+01 .6430137D+02 .4902784D+03

THE NEW SEARCH MATRIX
.8343094D-03 .1784565D-06 .8598740D-02 .9999627D+00
- .2425478D+00 - .2026673D-04 .9701053D+00 - .8139627D-02
.9701391D+00 - .5066803D-05 .2425320D+00 - .2894974D-02
.4336809D-11 1.0000000D+00 .2089127D-04 - .1182106D-08

THIS IS THE END OF STAGE 3
THE TOTAL NUMBER OF FUNCTIONAL EVALUATIONS IS 157
THE VALUE OF THE OBJECTIVE FUNCTION IS .5028925D-05
THE COORDINATES OF THE END POINT ARE
.6006432D+00 .8488784D+01 .6428246D+02 .4880785D+03

THE NEW SEARCH MATRIX
1.0000000D-05 .0000000D-75 .0000000D-75 .0000000D-75
.0000000D-75 1.0000000D+00 .0000000D-75 .0000000D-75
.0000000D-75 .0000000D-75 .0000000D-75 .0000000D+00
.0000000D-75 .0000000D-75 .0000000D-75 .0000000D-75

L.0114 THIS IS THE END OF STAGE 4
 L.0115 THE TOTAL NUMBER OF FUNCTIONAL EVALUATIONS IS 209
 L.0116 THE VALUE OF THE OBJECTIVE FUNCTION IS .5028913D-05
 L.0117 THE COORDINATES OF THE END POINT ARE
 L.0118 .6006432D+00 .8488785D+01 .6428246D+02 .4885785D+03
 L.0119
 L.0120 THE NEW SEARCH MATRIX
 L.0121 -.5551115D-16 .2000000D-05 .0000000D-75 1.0000000D+00
 L.0122 1.0000000D+00 .7629395D-05 .0000000D-75 .0000000D-75
 L.0123 .2775558D-10 -1.0000000D+00 .0000000D-75 .0000000D-75
 L.0124 .2775558D-10 -1.0000000D+00 .0000000D-75 .0000000D-75
 L.0125
 L.0126
 L.0127
 L.0128
 L.0129 THIS IS THE END OF STAGE 5
 L.0130 THE TOTAL NUMBER OF FUNCTIONAL EVALUATIONS IS 258
 L.0131 THE VALUE OF THE OBJECTIVE FUNCTION IS .5028913D-05
 L.0132 THE COORDINATES OF THE END POINT ARE
 L.0133 .6006432D+00 .8488783D+01 .6428246D+02 .4885785D+03
 L.0134
 L.0135 THE SEARCH ROUTINE HAS CONVERGED WITH IN THE DESIRED LIMITS

END OF PRINT * NO OF LINES PRINTED- 135

THE P-VECTOR IS

L.0004 *000.000 10.000 0.000 .001 0.000
 L.0006 50.000 1.000 0.000 0.000 0.000
 L.0008 0.000 0.000 0.000 0.000 0.000
 L.0010 0.000 0.000 0.000 0.000 0.000
 L.0012 0.000 0.000 0.000 0.000 0.000
 L.0014 0.000 0.000 0.000 0.000 0.000
 L.0016 1.000 10.000 65.000 1000.000 0.000
 L.0018 0.000 0.000 0.000 0.000 0.000
 L.0020 .500 8.000 64.000 400.000 0.000
 L.0022 0.000 0.000 0.000 0.000 0.000
 L.0024 THE INITIAL SEARCH MATRIX

THE INITIAL SEARCH MATRIX

L.0025 1.0000 0.0000 0.0000 0.0000 0.0000
 L.0027 0.0000 1.0000 0.0000 0.0000 0.0000
 L.0029 0.0000 0.0000 1.0000 0.0000 0.0000
 L.0031 0.0000 0.0000 0.0000 1.0000 0.0000
 L.0033 0.0000 0.0000 0.0000 0.0000 1.0000
 L.0035 0.0000 0.0000 0.0000 0.0000 0.0000
 L.0037 0.0000 0.0000 0.0000 0.0000 0.0000
 L.0039 0.0000 0.0000 0.0000 0.0000 0.0000
 L.0041 0.0000 0.0000 0.0000 0.0000 0.0000
 L.0043 0.0000 0.0000 0.0000 0.0000 0.0000
 L.0045 0.0000 0.0000 0.0000 0.0000 0.0000
 L.0047 0.0000 0.0000 0.0000 0.0000 0.0000
 L.0049 0.0000 0.0000 0.0000 0.0000 0.0000
 L.0051 0.0000 0.0000 0.0000 0.0000 0.0000
 L.0053 0.0000 0.0000 0.0000 0.0000 0.0000
 L.0055 0.0000 0.0000 0.0000 0.0000 0.0000
 L.0057 0.0000 0.0000 0.0000 0.0000 0.0000
 L.0059 0.0000 0.0000 0.0000 0.0000 0.0000
 L.0061 0.0000 0.0000 0.0000 0.0000 0.0000

THE STEP SIZES

.1000 .1000 .1000 .1000 .1000

THE INITIAL VALUES FOR EACH OF THE VARIABLES

T(1)= .698 T(2)= 8.489
 T(3)= 64.304 T(4)= 522.478
 T(5)= 0.000 T(6)= 0.000
 T(7)= 0.000 T(8)= 0.000
 T(9)= 0.000 T(10)= 0.000

L.0062 THE VALUE OF THE OBJECTIVE FUNCTION IS .1379424D-04
L.0063 THE COORDINATES OF THE END POINT ARE
L.0064 .6978891D+00
L.0065 .6430408D+02
L.0066
L.0067
L.0068
L.0069
L.0070
L.0071
L.0072
L.0073
L.0074
L.0075
L.0076
L.0077
L.0078
L.0079
L.0080
L.0081
L.0082
L.0083
L.0084
L.0085
L.0086
L.0087
L.0088
L.0089
L.0090
L.0091
L.0092
L.0093
L.0094
L.0095
L.0096
L.0097
L.0098
L.0099
L.0100
L.0101
L.0102
L.0103

THIS IS THE END OF STAGE 1
THE TOTAL NUMBER OF FUNCTIONAL EVALUATIONS IS 39
THE VALUE OF THE OBJECTIVE FUNCTION IS .4776596D-05
THE COORDINATES OF THE END POINT ARE
.9978891D+00 .8488785D+01 .6430408D+02

THE NEW SEARCH MATRIX
1.0000000D+00 .3333333D-05 .3333333D-05
-.4714045D-05 .7071068D+00 .7071068D+00
.2284785D-20 -.7071068D+00 .7071068D+00

THIS IS THE END OF STAGE 2
THE TOTAL NUMBER OF FUNCTIONAL EVALUATIONS IS 81
THE VALUE OF THE OBJECTIVE FUNCTION IS .4774412D-05
THE COORDINATES OF THE END POINT ARE
.9878891D+00 .8488786D+01 .6430408D+02

THE NEW SEARCH MATRIX
-1.0000000D+00 .6737734D-04 .6737734D-04
.9523595D-04 .7071068D+00 .7071068D+00
-.1995133D-12 -.7071068D+00 .7071068D+00

THIS IS THE END OF STAGE 3
THE TOTAL NUMBER OF FUNCTIONAL EVALUATIONS IS 116
THE VALUE OF THE OBJECTIVE FUNCTION IS .4774412D-05
THE COORDINATES OF THE END POINT ARE
.9878891D+00 .8488786D+01 .6430408D+02

THE SEARCH ROUTINE HAS CONVERGED WITH IN THE DESIRED LIMITS

REMOTE PRINT/DISPLAY FOR USER NO 20

FILE NAME MG59T DEPT OF CHEM ENG

DATE= 69-339 TIME= 18-04-28 VI-1

L.0001 /FTC

L.0002 C REGENERATION OF THE OUTPUT CURVE FOR MODEL 1
 L.0003 C *****
 L.0004 DOUBLE PRECISION CGF(500),TT(500)
 L.0005 DOUBLE PRECISION DA(50),UA(50),BMA(50),AKA(50),A(50),Q(50),P(50),VO(50),WA(50)
 L.0006 DOUBLE PRECISION W,D,U,X,BM,AK,FF,SS,Z,Y,BE,UU,V,THETA,RR,AL,F1,F2
 L.0007 2 FORMAT(5E20.8)
 L.0008 3 FORMAT(4I5,2E20.8)
 L.0009 4 FORMAT(13,2D20.8)
 L.0010 1 FORMAT(4Y)
 L.0011 10 FORMAT(//)
 L.0012 11 FORMAT(' REGENERATION OF THE OUTPUT CURVE USING MODEL 1. ' //)
 L.0013 12 FORMAT(' DO= ',F10.3,5X, ' UO= ',F10.3,5X, ' MO= ',F10.3,5X, ' KO= ',F10.3 //)
 L.0014 13 FORMAT(' START POINT NUMBER = ',I4,5X, ' FINISH POINT NUMBER = ',I4,5X, ' TIME AXIS INTERVAL = ',F5.3 //)
 L.0015 18 FORMAT(' CONCENTRATION PROFILE. ' //)
 L.0016 14 FORMAT(6D20.8)
 L.0017 C READING OF DATA
 L.0018 C *****
 L.0019 READ(9,1)NCO
 L.0020 READ(5,2)X,FG,FL,ACOL,TOR
 L.0021 READ(5,3)J11,J12,JF1,JF2,DELT1,DELT2
 L.0022 READ(5,4)AREA
 L.0023 READ(5,14)(P(I),Q(I),DA(I),UA(I),BMA(I),AKA(I),I=1,NCO)
 L.0024 READ(9,1)DA(1),UA(1),BMA(1),AKA(1)
 L.0025 READ(9,1)FAC
 L.0026 WRITE(6,10)
 L.0027 WRITE(6,11)
 L.0028 WRITE(6,12)DA(1),UA(1),BMA(1),AKA(1)
 L.0029 WRITE(6,13)J12,JF2,DELT2
 L.0030 WRITE(6,18)
 L.0031 NN=1
 L.0032 FF=FL/FG
 L.0033 PI=DATAN(1.)*4.
 L.0034 T=DELT2*J12
 L.0035 TF=DELT2*JF2
 L.0036 EVALUATION OF THE FOURIER COEFFICIENTS
 L.0037 C *****
 L.0038 DO 7 I=2,NCO
 L.0039 C1=I-1
 L.0040 D=DA(1)
 L.0041 U=UA(1)
 L.0042 BM=BMA(1)
 L.0043 AK=AKA(1)
 L.0044 AK=AK*ACOL/FL
 L.0045 WA(1)=PI*C1/TOR
 L.0046 W=WA(1)
 L.0047 SS=U*X/(2.*D)
 L.0048 Z= SS*SS
 L.0049 Y=1.D+00/DSQRT((BM*W/AK)**2+1.)
 L.0050 BE=-DATAN(BM*W/AK)
 L.0051 UU=Z-X*X*AK/D*(Y*DCOS(BE)-1.)*FF
 L.0052 V=X*X/D*(W-AK*Y*DSIN(BE)*FF)
 L.0053 THETA=DATAN(V/UU)/2.
 L.0054 RR=DSQRT(DSQRT(UU*UU+V*V))

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L.0055 AL=SS-RR*AL*HETA)
L.0056 F1=DEXP(AL)
L.0057 F2=-RR*DSIN(THETA)
L.0058 A(I)=-F1*DSIN(THETA)
L.0059 B(I)=F1*DCOS(F2)/TOR
L.0060 VO(I)=(B(I)*Q(I)-A(I)*P(I))*TOR
L.0061 7 UO(I)=(A(I)*Q(I)+B(I)*P(I))*TOR
L.0062 DO 100 J=2,NCQ
L.0063 100 WRITE(9,101)P(J),Q(J),A(J),B(J),UO(J),VO(J)
L.0064 101 FORMAT(6E20.8)
L.0065 TEMP=0.
L.0066 9 CG=0.5*Q(1)
L.0067 C EVALUATION OF PROFILE
L.0068 C *****
L.0069 DO 6 I=2,NCQ
L.0070 6 CG=CG+UO(I)*DSIN(WA(I)*T)+VO(I)*DCOS(WA(I)*T)
L.0071 CGF(NN)=CG
L.0072 TT(NN)=T
L.0073 IF(CG.GT.TEMP)TEMP=CG
L.0074 NN=NN+1
L.0075 IF(T.GT.TF)GO TO 99
L.0076 T=T+DELT2
L.0077 GO TO 9
L.0078 99 NN=NN-1
L.0079 Z=FAC/TEMP
L.0080 DO 102 K=1,NN
L.0081 102 CGF(K)=Z*CGF(K)
L.0082 DO 141 L=1,NN,16
L.0083 141 WRITE(6,140)(CGF(L+I),I=1,16)
L.0084 140 FORMAT(16F6.1)
L.0085 READ(9,1)DUMMY
L.0086 END
L.0087 /DATA

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