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**EVALUATION OF REACTION KINETICS FOR
GAS-POWDER SYSTEMS**

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SUBJECT DESCRIPTORS

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EVALUATION OF REACTION KINETICS FOR GAS-POWDER SYSTEMS

Jerry L. Stakebake and G. Edward Bixby

Abstract. Kinetic models for the reaction between a gas and powder are presented and discussed. Rates from the "progressive conversion" model are dependent on the amount of material present. This model is described by an equation that yields both the rate constant and the reaction order. The "phase boundary" model produces rates for topochemical reactions which are dependent on the powder surface area. Applications of these models to uranium powder hydriding are discussed. Computer programs for analyzing data also are included.

INTRODUCTION

Experimental programs are underway to evaluate the reaction between gases and various powders. The primary interest in these programs is the rate of reaction between the gas and the solid powder. Evaluation of reaction kinetics involves consideration of two fundamental processes: (1) the chemical reaction itself and (2) transport of the gas to the reaction zone. Both of these processes may involve several individual steps that may be rate controlling for the entire reaction. This report evaluates some of the basic fundamentals of powder reaction kinetics; it also illustrates their application to the hydriding of uranium powder.

KINETIC MODELS

Chemical reactions result from atomic and molecular collisions. If the reactants are mixed on an atomic level, the reaction kinetics can be described mathematically with equations involving only time and concentration. This results in what will be termed the "progressive conversion" model.

Often, however, gases and solids are not mixed on the atomic level and the gas must diffuse or penetrate to the phase boundary before reacting.

If the gas diffuses very slowly into the solid, the reaction takes place at a gas-solid interface, which results in a "phase boundary" model.

Both the "progressive conversion" and "phase boundary" models may include several different steps in the reaction. The following steps are possible:

1. Diffusion of the gaseous reactant to the solid surface.
2. Adsorption of the gaseous reactant.
3. Diffusion of the gas either into the bulk or to the solid reactant-gas interface.
4. Reaction of the gas with the solid.
5. Diffusion of any gaseous product to the solid surface.
6. Desorption of the gaseous reaction product.

At times some of these steps do not exist. The resistance of each step to the progress of the reaction varies. The step with the highest resistance is said to be rate controlling.

Progressive Conversion Model

The basic assumption of this model is that the reacting gas diffuses rapidly through the solid particle so that the reaction takes place uniformly throughout the particle. This type of behavior is illustrated in Figure 1 for the hydriding of a metal particle. The reaction rate is then dependent only on the concentration of the metal available—providing that the availability of the reacting gas is not limited by either the adsorption or diffusion steps.

Evaluation of the "progressive conversion" model involves expressions that relate reactant concentration to time.¹ If M_0 is the initial concentration of

FIGURE 1. Progressive Conversion Model

the solid and M_t is the amount reacted at time t , then the amount left unreacted is $M_0 - M_t$. The rate of disappearance of the solid is

$$\frac{-d(M_0 - M_t)}{dt} = \frac{dM_t}{dt} = K(M_0 - M_t)^n \quad (1) \quad \text{or}$$

where K = rate constant and n = order of reaction.

If this is integrated with the boundary condition that $M_t = 0$ when $t = 0$, and $n \neq 1$, then

$$K = \frac{1}{t(n-1)} \left[\frac{1}{(M_0 - M_t)^{n-1}} - \frac{1}{M_0^{n-1}} \right] \quad (2)$$

Since the parameter being measured is W_t , the amount of gas being reacted at time t , and W_m is the maximum amount of gas reacted, then

$$M_t = \frac{W_t}{W_m} M_0 \quad (3)$$

The general solution to Equation 2 becomes

$$K = \frac{1}{t(n-1)} \left[\frac{1}{\left(M_0 - \frac{W_t M_0}{W_m} \right)^{n-1}} - \frac{1}{M_0^{n-1}} \right] \quad (4)$$

Rearranging Equation 4 results in

$$\left(M_0 - \frac{W_t M_0}{W_m} \right)^{n-1} = K(n-1)t + M_0^{1-n}$$

$$M_0^{1-n} \left(1 - \frac{W_t}{W_m} \right)^{1-n} = K(n-1)t + M_0^{1-n}$$

$$\left(1 - \frac{W_t}{W_m} \right) = \left[K(n-1)M_0^{n-1}t + 1 \right]^{1/(1-n)}$$

By further rearranging, the working equation becomes

$$W_t = W_m \left[1 - \left(1 + K(n-1)M_0^{n-1}t \right)^{1/(1-n)} \right] \quad (5)$$

when $t < M_0^{1-n}/K(1-n)$ and $n = 1$.

Where $t \geq M_0^{1-n}/K(1-n)$ and $0 < n < 1$, then $W_t = W_m$.

For Equation 5,

n = order of the reaction.

W_t = weight gain at time t , in milligrams per gram.

M_0 = milligrams of atoms of solid material at $t = 0$.

W_m = weight gain at $t = \infty$, in milligrams per gram.

K = rate constant.

In the special case where $n = 1$ for a 1st-order reaction, Equation 4 becomes

$$K = \frac{1}{t} \ln \frac{M_0}{M_0 - M_t} \quad (6)$$

FIGURE 2. Phase Boundary Model

By substitution of Equation 3 into Equation 6

$$W_t = W_m(1 - e^{-Kt}) \quad (7)$$

Phase Boundary Model

The reaction predicted by this model occurs at the gas-solid interface and is illustrated in Figure 2. In this case the reaction front moves toward the center of the solid particle. During the reaction, the total particle size may increase, decrease, or remain the same depending on the molar volume of the reaction product. The core, however, remains unreacted. The product layer may be porous with no protective qualities or it may be dense and thus present a diffusion barrier between the solid and gas.

This model can be evaluated by assuming the reaction produces a product layer of thickness, y , which reduces the initial radius, r_0 , of each spherical particle. (See Figure 2.) The volume of unreacted material at time t becomes

$$V_t = \frac{4}{3} \pi (r_0 - y)^3 \quad (8)$$

If α is the fraction of the solid material reacted at time t , the volume of material unreacted becomes

$$V = \frac{4}{3} \pi r_0^3 (1 - \alpha) \quad (9)$$

By equating Equations 8 and 9, the thickness of the product layer becomes

$$y = r_0 [1 - (1 - \alpha)^{1/3}] \quad (10)$$

If the reaction produces a product having a molar volume greater than that of the solid reactant, a protective, non-porous layer is formed and the reaction becomes diffusion controlled. This results in a parabolic rate expression for the growth of the product layer, which is given by

$$y^2 = k_p t \quad (11)$$

where k_p is the parabolic rate constant.

Combining Equation 11 with Equation 10 produces the Jander² equation

$$y^2 = r_0^2 [1 - (1 - \alpha)^{1/3}]^2 = k_p t \quad (12)$$

or

$$[1 - (1 - \alpha)^{1/3}]^2 = \frac{k_p t}{r_0^2} = k_j t \quad (13)$$

where k_j is the observed Jander rate constant.

If the product layer is porous, the phase boundary reaction results in a linear growth of the product layer. Thus

$$\frac{dy}{dt} = k \text{ or } y = kt \quad (14)$$

where k is the linear rate constant.

Combining Equations 10 and 14 yields

$$y = r_0 [1 - (1 - \alpha)^{1/3}] = kt \quad (15)$$

or

$$1 - (1 - \alpha)^{1/3} = \frac{k_L t}{r_0} = k_L t \quad (16)$$

where k_L is the experimentally determined phase boundary rate. Equation 16 has been used by Muromura and Ouchi³ to evaluate the nitrogenation of plutonium hydride.

Alternative Derivation of the Phase Boundary Model

When the gas-solid reaction is phase-boundary controlled, the reaction rate is proportional to the surface area of the unreacted material. Thus

$$\frac{dV_t}{dt} = k_A S_t \quad (17)$$

where V_t is the volume at time t , S_t is the surface area, and k_A is the surface area dependent rate constant. The unreacted fraction is $(1 - \alpha)$ where α is the fraction reacted, that is,

$$(1 - \alpha) = \frac{V_t}{V_0} = \frac{r_t^3}{r_0^3} \quad (18)$$

or

$$r_t^2 = r_0^2 (1 - \alpha)^{2/3} \quad (19)$$

where V_0 = initial volume and r_t = radius at time t .

The rate of change of the unreacted fraction becomes

$$\frac{-d(1 - \alpha)}{dt} = \frac{d(V_t/V_0)}{dt} = \frac{V_0 \frac{dV_t}{dt}}{V_0^2} = \frac{k_A S_t}{V_0} \quad (20)$$

then

$$\frac{d\alpha}{dt} = \frac{k_A S_t}{V_0} = \frac{k_A 4\pi r_t^2}{\frac{4}{3}\pi r_0^3} = \frac{3k_A r_t^2}{r_0^3} \quad (21)$$

Substitution of Equation 19 into Equation 21 results in

$$\frac{d\alpha}{dt} = \frac{3k_A r_0^2 (1 - \alpha)^{2/3}}{r_0^3} = \frac{3k_A (1 - \alpha)^{2/3}}{r_0} \quad (22)$$

Equation 22 shows that the maximum reaction order for a topochemical reaction is 2/3.

Integration of Equation 22, assuming that $\alpha = 0$ when $t = 0$, results in the expression

$$1 - (1 - \alpha)^{1/3} = \frac{k_A t}{r_0} \quad (23)$$

If $k_A/r_0 = k_L$ = the linear phase boundary rate constant, then Equation 23 equals Equation 16.

COMPUTER ANALYSIS

Analysis of data, using the different reaction models, was done by computer or calculator. A time-shared computer was used for the "progressive conversion" model. A copy of the Fortran program for Equations 5 and 7 are included as Appendix A. Copies of the program on paper tape in addition to instructions may be obtained from the authors.

Data analysis according to the "phase boundary" model was performed on a Hewlett Packard Model 9825A calculator. The programs used for the Jander equation and the general phase-boundary reaction equation are included in Appendixes B and C respectively. Questions regarding data processing should be directed to the authors.

APPLICATIONS

To illustrate the application of the kinetic models to real reaction systems, data from the hydriding of uranium powder will be evaluated. Uranium powder samples were prepared by a series of hydriding and dehydriding cycles. Conditions for the hydriding runs being reported were 100 °C and either 13.3 kPa or 26.6 kPa hydrogen pressure. Figure 3 shows a hydriding run at 100 °C and 13.3 kPa hydrogen that was analyzed using the "progressive conversion" model and Equation 5. This model describes the process very well and shows the reaction to be 2/3-order. The correlation coefficient obtained using Equation 5 was 0.9983.

Since the order of the run in Figure 3 was 2/3, it might be expected that a topochemical reaction is

FIGURE 3. Application of the General Rate Equation (Equation 5) to Uranium Hydriding at 100 °C in 13.3 kPa Hydrogen. The maximum gas reacted was 12.2 mg/g, rate constant was 2.387, and 0.65 was the order of reaction.

FIGURE 4. Application of Equation 16 to the 1st-Order Reaction of Run 10 in 26.6 kPa Hydrogen at 97 °C and the 2/3-Order Reaction of Run 2 in 13.3 kPa of Hydrogen at 100 °C. The solid lines are the predicted fit. In Run 2, the phase boundary rate was 0.652 min^{-1} ; it was 0.827 min^{-1} in Run 10.

FIGURE 5. Evaluation of Hydriding Data Obtained at 97 °C in 26.6 kPa Hydrogen Using Equations 5 and 7 for a 1st-Order Reaction

taking place. In this case, the experimental data might better be fit by the “phase boundary model.” Figure 4, Run 2, shows the fit of Equation 16 to these data. The fit appears good for about 95% of the reaction. The correlation coefficient obtained in this case was 0.9989. It should be noted that Equation 16 does not accurately fit the data from the first and last part of the run.

Figure 5 shows an experimental run at 97 °C in 26.6 kPa hydrogen. The experimental data were analyzed using Equation 5, which showed the reaction to be 1st-order, and Equation 7. The correlation coefficient obtained using both of

these equations was 0.9984. Since this experimental run was shown to be 1st-order, the “progressive conversion” model may offer a better representation than the “phase boundary” model. Figure 4, Run 10, shows the evaluation using Equation 16 for the “phase boundary” model. Although the model appears to fit well overall, there was some deviation at the beginning and end of the run. The correlation coefficient was 0.9968.

Use of the Jander equation (Equation 13) to explain the hydriding of uranium powder is not valid, as can be seen in Figure 6. This indicates that gas transport is not the rate-limiting step in this reaction.

FIGURE 6. Application of the Jander Equation to the Analysis of Uranium Powder Hydriding in 26.6 kPa Hydrogen at 91 °C

CONCLUSION

Two models are presented for the reaction of gases with powders. The "progressive conversion" model is dependent on the amount or concentration of the solid powder. The "phase boundary" model is related to the constant growth of the product layer and to the surface area of the unreacted powder. If the product layer becomes a barrier to the reacting gas, then the rate is controlled by the diffusion process, and the Jander equation applies.

In the special application of these models to the hydriding of uranium powder, both the "progressive

conversion" and "phase boundary" models appear to be equally applicable. This is undoubtedly true because of the small particle size being used.

REFERENCES

1. K. J. Laidler. *Chemical Kinetics*. McGraw-Hill Book Co., New York. 1965.
2. S. F. Hulbert. *J. Brit. Ceram. Soc.*, Vol. 6, p. 11. (1969).
3. T. Muromura and K. Ouchi. *J. Inorg. Nucl. Chem.*, Vol. 36, p. 2525. (1974).

APPENDIX A

Computer Program for Equations 5 and 7

```

00010 PROGRAM GEBNL(INPUT=65/80,OUTPUT=65,TAPE1=65,TAPE7=65,TAPE5=INPUT)
00020 DIMENSION SS(99),BK(5),Z(4,99),BDEL(4),NZ(4)
00030 COMMON PAR(800,5),XTRAN(5,800)
00040 DIMENSION SAVE(5,5),XSAVE(5,5)
00050 DIMENSION XPROD(6,6),DEL(800),T(5)
00060 COMMON/GENTNL/X(800,5),YXP(800),J,N,Z,ITER,BDEL,NOPT,
00070+NOPT2,NZ,NNL,INL,NP,XPY(5),YTH(800),NOUT
00080 45 FORMAT(/' ITERATION #      SUMS OF SQUARES      ',
00090+'NL PARAMETER          DELTA'//)
00100 46 FORMAT(4X,I2,6X,1PE15.8,5X,1PE12.5,2X,1PE10.3)
00110 INTEGER B
00120 51 FORMAT(/IX'THE T STATISTICS AND 68 C.L. DELTAS ARE'//)
00130 52 FORMAT(/IX'THE STANDARD ERROR IS      '1PE15.8)
00140 49 FORMAT(/IX'THE CORRELATION COEFFICIENT IS      ',F6.4)
00150 53 FORMAT(/IX'THE SUM OF THE SQUARED ERRORS IS      '1PE15.8)
00160 54 FORMAT(/IX'  I      MEASURED VALUE      PREDICTED VALUE      ERROR'//)
00170 55 FORMAT(/15X' REGRESSION ANALYSIS'//)
00180 59 FORMAT(/IX'THE REGRESSION EQUATION PARAMETERS ARE'//)
00190 70 FORMAT(1X,2HA(,I2,2H)=,1PE15.8)
00200 71 FORMAT(1X,2HT(,I2,2H)=,1PE9.2,2X,4HDEL(,I2,2H)=,2X,
00210+1PE10.3)
00220 80 FORMAT(14,2X,1PE15.8,3X,1PE15.8,3X,1PE10.3)
00230 87 FORMAT(/' MATRIX IS SINGULAR OR EPS IS TOO LARGE')
00240 88 FORMAT(/' INVERSE WAS NOT OBTAINED')
00250 89 FORMAT(/' INSUFFICIENT NUMBER OF DATA POINTS',
00260+' FOR THIS ORDER FIT')
00270 44 FORMAT(/' #          SS          NL1          NL2',
00280+'          NL3          NL4'/22X,'DEL1',9X,
00290+'DEL2',9X,'DEL3',9X,'DEL4'//)
00300 43 FORMAT(1X,I2,5(2X,1PE11.4))
00310 42 FORMAT(' NL(',I1,')=',1PE12.5)
00320 41 FORMAT(/' THE NON-LINEAR PARAMETERS ARE'//)
00330 40 FORMAT(18X,4(1PE11.4,2X))
00340 REWIND 1
00350 PRINT 55
00360 ITER=1
00370 ILAST=0
00380 NEXPT=2
00390 16 CALL GENTNL(PAR)
00400 DO 400 I=1,N
00410 DO 400 K=1,J
00420 400 XTRAN(K,I)=X(I,K)
00430 DO 510 I=1,J
00440 DO 510 K=1,J
00450 XPROD(I,K)=0
00460 DO 510 M=1,N
00470 510 XPROD(I,K)=XPROD(I,K)+XTRAN(I,M)*X(M,K)
00480 DO 519 I=1,J
00490 DO 519 M=1,J
00500 519 SAVE(I,M)=XPROD(I,M)
00510 B=J

```

APPENDIX A (continued)

```

00520 DO 700 I=1,J
00530 XPY(I)=0.
00540 DO 700 M=1,N
00550 700 XPY(I)=XTRAN(I,M)*YXP(M)+XPY(I)
00560 DO 520 I=1,J
00570 BK(I)=XPROD(I,I)
00580 XPROD(I,J+1)=XPY(I)
00590 JJ=J+1
00600 DO 520 K=1,JJ
00610 520 XPROD(I,K)=XPROD(I,K)/BK(I)
00620 EPS=1E-30
00630 INDIC=0.
00640 CALL INVK(XPY,XPROD,EPS,SIMUL,INDIC,J)
00650 IF(SIMUL.EQ.0) GO TO 1200
00660 DO 600 I=1,J
00670 DO 600 K=1,J
00680 600 XPROD(K,I)=XPROD(K,I)/BK(I)
00690 DO 760 I=1,J
00700 DO 760 K=1,J
00710 XSAVE(I,K)=0.0
00720 DO 760 L=1,J
00730 760 XSAVE(I,K)=XSAVE(I,K)+XPROD(I,L)*SAVE(L,K)
00740 DO 761 I=1,J
00750 761 XSAVE(I,I)=XSAVE(I,I)-1.0
00760 DO 850 I=1,N
00770 YTH(I)=0
00780 DO 850 K=1,J
00790 850 YTH(I)=YTH(I)+X(I,K)*XPY(K)
00800 SUM=0
00810 SUM1=0.
00820 SUM2=0.
00830 DO 900 I=1,N
00840 SUM1=SUM1+YXP(I)*YXP(I)
00850 SUM2=SUM2+YXP(I)
00860 DEL(I)=YXP(I)-YTH(I)
00870 900 SUM=DEL(I)**2+SUM
00880 RCOF=ABS(1-SUM/(SUM1-SUM2*SUM2/N))
00890 RCOF=SQRT(RCOF)
00900 SS(ITER)=SUM
00910 IF(NOPT.EQ.2.AND.ILAST.NE.2)GO TO 951
00920 E=SUM/(N-J-NNL)
00930 IF(E) 1003,1003,901
00940 901 SE=SQRT(E)
00950 DO 950 I=1,J
00960 F=XPROD(I,I)
00970 IF(F) 1002,949,949
00980 949 SF=SQRT(F)
00990 BK(I)=SE*SF
01000 950 T(I)=XPY(I)/(SE*SF)
01010 951 IF(NOPT.LE.1) GO TO 1101
01020 IF(NOUT.EQ.0) GO TO 99
01030 IF(ITER.NE.1) GO TO 10002

```


APPENDIX A (continued)

```

01040 IF(NOPT2.EQ.1) PRINT 44
01050 IF(NOPT2.EQ.2) PRINT 45
01060 10002 IF(NOPT2.EQ.1) PRINT 43,ITER,SUM,(Z(I,ITER),I=1,NNL)
01070 IF(NOPT2.EQ.1) PRINT 40,(BDEL(I),I=1,NNL)
01080 IF(NOPT2.EQ.2) PRINT 46,(ITER,SUM,Z(INL,ITER),BDEL(1))
01090 99 CALL SEARCH(ITER,ILAST,Z,SS,NEXPT,BDEL,J,XPY,NOPT2,
01100+NZ,NNL,INL,NOUT)
01110 IF(ILAST.NE.1) GO TO 16
01120 IF(ITER.NE.1.AND.ITER.NE.99) PRINT 33,ITER
01130 33 FORMAT(/' CONVERGENCE OBTAINED AT ITERATION # ',I2)
01140 1101 PRINT 59
01150 PRINT 70,(I,XPY(I),I=1,J)
01160 IF(NOPT.EQ.2) PRINT 41
01170 IF(NOPT.EQ.2) PRINT 42,(I,Z(I,ITER),I=1,NNL)
01180 1100 CONTINUE
01190 PRINT 53, SUM
01200 PRINT 52, SE
01210 PRINT 49,RCOF
01220 PRINT 51
01230 PRINT 71,(I,T(I),I,BK(I),I=1,J)
01240 PRINT 1560
01250 1560 FORMAT(/IX,'OUTPUT DATA POINTS?')
01260 READ(5,*) OUT
01270 IF(OUT.EQ.0) GO TO 1369
01280 PRINT 54
01290 PRINT 80,(I,YXP(I),YTH(I),DEL(I),I=1,N)
01300 1250 FORMAT(' TYPE THE ID NO., MIN, MAX AND NO. PTS. FOR ',
0 1310+' THE CONTINUOUS VARIABLE ')
01320 1241 FORMAT(' TYPE THE NO. AND NO. OF VALUES FOR ',
01330+' A DISCRETELY CHANGING VARIABLE ')
01340 1251 FORMAT(' TYPE THE VALUES FOR THE REMAINING PARAMETERS ')
01350 1369 PRINT 1660
01360 1660 FORMAT(/IX,'DO YOU WANT A PLOT FILE?')
01370 READ(5,*) IPLOT
01380 IF(IPLOT.EQ.0) GO TO 1300
01390 REWIND 7
01400 NOLD=N
01410 PRINT 1250
01420 READ(5,*) IP,PMIN,PMAX,N
01430 DO 1281 I=1,NOLD
01440 1281 WRITE(7,*) PAR(I,IP),YXP(I),YTH(I)
01450 IF(NP.EQ.1) GO TO 1259
01460 IIDIS=0
01470 PRINT 1241
01480 READ(5,*) IP2,IDIS
01490 IF(IDIS.EQ.0) IP2=NP+1
01500 IF(IDIS.LT.1) IDIS=1
01510 IF(IDIS.EQ.1) GO TO 1242
01520 IIDIS=1
01530 PRINT 1810
01540 1810 FORMAT(' TYPE THE DISCRETE VALUES')
01550 READ(5,*) (T(I),I=1,IDIS)

```

APPENDIX A (continued)

```

01560 1242 IREAD=NP-IIDIS-1
01570 IF(IREAD.EQ.0) GO TO 1259
01580 PRINT 1251
01590 READ(5,*)(SS(I),I=1,IREAD)
01600 1259 DDEL=(PMAX-PMIN)/(N-1)
01610 IF(NP.NE.1) GO TO 1258
01620 IIDIS=1
01630 IP2=2
01640 DO 1257 I=1,NOLD
01650 1257 DEL(I)=PAR(I,1)
01660 1258 CONTINUE
01670 DO 1253 I=1,N
01680 PAR(I,IP)=PMIN+(I-1)*DDEL
01690 DO 1253 IJ=1,NP
01700 JJ=IJ
01710 IF(JJ.GE.IP) JJ=JJ+1
01720 IF(JJ.GE.IP2) JJ=JJ+1
01730 IF(JJ.EQ.IP) JJ=JJ+1
01740 1253 PAR(I,JJ)=SS(IJ)
01750 DO 1271 IHUG=1,IIDIS
01760 DO 1270 I=1,N
01770 1270 PAR(I,IP2)=T(IHUG)
01780 IF(NOPT.EQ.2) NOPT=1
01790 CALL GENTEP(PAR)
01800 DO 1271 I=1,N
01810 XTRAN(IHUG,I)=0.0
01820 DO 1271 K=1,J
01830 1271 XTRAN(IHUG,I)=XTRAN(IHUG,I)+X(I,K)*XPY(K)
01840 DO 1280 I=1,N
01850 DO 1279 IHUG=1,IIDIS
01860 1279 BK(IHUG)=XTRAN(IHUG,I)
01870 1280 WRITE(7,*) PAR(I,IP),(BK(IHUG),IHUG=1,IIDIS)
01880 GO TO 1300
01890 1200 PRINT 87
01900 GO TO 1300
01910 1002 PRINT 88
01920 GO TO 1300
01930 1003 PRINT 89
01940 GO TO 1300
01950 1300 REWIND 1
01960 IF(IPLOT.NE.0)REWIND 7
01970 STOP
01980 END
01990 SUBROUTINE SEARCH(ITER,ILAST,Z,SS,NEXPT,BDEL,J,XPY,NOPT2,
02000+NZ,NNL,INL,NOUT)
02010 DIMENSION A(6,6),X(6),Z(4,99),SS(99),XPY(5),BDEL(4),NZ(4)
02020 9 FORMAT(' NO MINIMUM WAS PREDICTED')
02030 10 FORMAT(' THE PREDICTED MINIMUM IS '1PE12.5)
02040 11 FORMAT('/' SEARCH HALTED AT ITERATION # ',I2)
02050 12 FORMAT(' MODEL DOES NOT FIT RESPONSE SURFACE')
02060 ILAST=ILAST-1
02070 IF(ITER.EQ.99) GO TO 800

```

APPENDIX A (continued)

```

02080 IF(ILAST.EQ.1) GO TO 920
02090 GO TO(5,6),NOPT2
02100 5 NC=0
02110 DO 8 I=1,NNL
02120 K=J-(NNL-I)
02130 BDEL(I)=XPY(K)/XPY(NZ(I))
02140 DENOM=Z(I,ITER)
02150 IF(Z(I,ITER).EQ.0) DENOM=1E-20
02160 DENOM2=DENOM
02170 IF(DENOM.EQ.1.E-20) DENOM2=BDEL(I)
02180 IF(ABS(BDEL(I)/DENOM).GT..1)BDEL(I)=.1*BDEL(I)*
02190+ABS(DENOM2/BDEL(I))
02200 Z(I,ITER+1)=Z(I,ITER)+BDEL(I)
02210 ADEL=ABS(BDEL(I)/Z(I,ITER+1))
02220 8 IF(ADEL.LT.1.E-05) NC=NC+1
02230 ITER=ITER+1
02240 IF(NC.GE.NNL) GO TO 7
02250 RETURN
02260 7 ILAST=2
02270 J=J-NNL
02280 RETURN
02290 6 IF(ITER.EQ.1.AND.BDEL(1).EQ.0) GO TO 800
02300 IF(NEXPT.EQ.4) GO TO 710
02310 IF(NEXPT) 400,50,100
02320 100 IF(NEXPT.EQ.2) FUN=1
02330 IF(NEXPT.EQ.1) FUN=-2
02340 Z(INL,ITER+1)=Z(INL,ITER)+FUN*BDEL(1)
02350 NEXPT=NEXPT-1
02360 GO TO 900
02370 50 NCP=ITER-3
02380 DO 80 I=1,3
02390 A(I,4)=SS(NCP+I)
02400 A(I,1)=1.
02410 A(I,2)=Z(INL,NCP+I)
02420 80 A(I,3)=Z(INL,NCP+I)**2
02430 INDIC=1
02440 EPS=1.E-20
02450 CALL INVK(X,A,EPS,SIMUL,INDIC,3)
02460 IF(X(3).LT.1.E-10) GO TO 750
02470 AMIN=-X(2)/(2.*X(3))
02480 90 IF(NOUT.NE.0)PRINT 10,AMIN
02490 DELM=Z(INL,NCP+1)-AMIN
02500 ADELM=ABS(DELM)
02510 ADEL=ABS(BDEL(1))
02520 IF(2*ADEL-ADELM) 200,300,300
02530 200 BDEL(1)=- (DELM/ADELM)*ADEL
02540 Z(INL,ITER+1)=Z(INL,NCP+1)+2*BDEL(1)
02550 GO TO 890
02560 300 Z(INL,ITER+1)=AMIN
02570 ADELM=ADELM/ABS(AMIN)
02580 ADEL=ADEL/ABS(AMIN)
02590 IF(ADELM.LT.5E-04.AND.ADEL.LT.1E-03) ILAST=2

```

APPENDIX A (continued)

```

02600 BDEL(1)=-SIGN(1.,DELM)*(ABS(BDEL(1))+ABS(DELM))/4.
02610 IF(NEXPT.EQ.3) BDEL(1)=BDEL(1)/2.
02620 GO TO 890
02630 400 IF(SS(ITER).GT.SS(NCP+1).AND.ITER.EQ.NCP+4) GO TO 700
02640 IF(SS(ITER)-SS(ITER-1)) 410,410,420
02650 410 Z(INL,ITER+1)=Z(INL,ITER)+BDEL(1)
02660 GO TO 900
02670 420 NEXPT=0.
02680 Z(INL,ITER+1)=Z(INL,ITER-1)-BDEL(1)
02690 GO TO 900
02700 750 IF(NOUT.NE.0)PRINT 9
02710 IF(SS(NCP+1).LT.SS(NCP+2).AND.SS(NCP+1).LT.SS(ITER))
02720+GO TO 690
02730 EBDON=X(2)+2.*X(3)*Z(INL,NCP+1)
02740 BDEL(1)=-ABS(BDEL(1))*(X(2)+2.*X(3)*Z(INL,NCP+1))/ABS(EBDON)
02750 Z(INL,ITER+1)=Z(INL,NCP+1)+2.*BDEL(1)
02760 GO TO 890
02770 690 Z(INL,ITER+1)=Z(INL,ITER)
02780 BDEL(1)=2.*BDEL(1)
02790 NEXPT=2
02800 GO TO 900
02810 700 IF(NOUT.NE.0)PRINT 12
02820 BDEL(1)=Z(INL,NCP+2)-Z(INL,NCP+1)
02830 FUN=-1
02840 NITER=0
02850 NEXPT=4
02860 710 CONTINUE
02870 NITER=NITER+1
02880 FUN=-1*FUN
02890 Z(INL,ITER+1)=Z(INL,NCP+1)+FUN*BDEL(1)*1.1892
02900 IF(NITER.LE.2) GO TO 900
02910 NEXPT=3
02920 NCOUNT=1
02930 Z(INL,NCP+4)=Z(INL,ITER)
02940 SS(NCP+4)=SS(ITER)
02950 DO 720 I=1,5
02960 A(I,1)=1
02970 A(I,2)=Z(INL,NCP+1)
02980 A(I,3)=Z(INL,NCP+1)*Z(INL,NCP+1)
02990 A(I,4)=A(I,2)*A(I,3)
03000 A(I,5)=A(I,3)*A(I,3)
03010 720 A(I,6)=SS(NCP+1)
03020 INDIC=1
03030 EPS=1E-10
03040 CALL INVK(X,A,EPS,SIMUL,INDIC,5)
03050 AMIN=Z(INL,NCP+1)
03060 719 S=0
03070 CHS=0
03080 DO 722 I=2,5
03090 722 S=S+X(I)*(I-1)*AMIN**(I-2)
03100 DO 723 I=3,5
03110 723 CHS=CHS+X(I)*(I-1)*(I-2)*AMIN**(I-3)

```


APPENDIX A (continued)

```
03120 AK=S-CHS*AMIN
03130 XNEW=-AK/CHS
03140 DELTA=ABS((XNEW-AMIN)/XNEW)
03150 IF(DELTA.LT.1E-05) GO TO 726
03160 IF(NCOUNT.GE.20) GO TO 724
03170 NCOUNT=NCOUNT+1
03180 AMIN=XNEW
03190 GO TO 719
03200 724 IF(NOUT.NE.0) PRINT 725
03210 725 FORMAT(' NEWTONS METHOD FAILED TO CONVERGE')
03220 726 AMIN=XNEW
03230 GO TO 90
03240 800 PRINT 11,ITER
03250 ILAST=1
03260 GO TO 920
03270 890 NEXPT=-1
03280 900 ITER=ITER+1
03290 920 RETURN
03300 END
03310 SUBROUTINE INVK(X,A,EPS,SIMUL,INDIC,N)
03320 DIMENSION IROW(6),JCOL(6),JORD(6),Y(6),A(6,6),X(6)
03330 MAX=N
03340 IF(INDIC.GE.0)MAX=N+1
03350 IF(N.LE.50) GO TO 5
03360 PRINT 200
03370 SIMUL=0.
03380 RETURN
03390 5 DETER=1
03400 DO 18 K=1,N
03410 KM1=K-1
03420 PIVOT=0.
03430 DO 11 I=1,N
03440 DO 11 J=1,N
03450 IF(K.EQ.1) GO TO 9
03460 DO 8 ISCAN=1,KM1
03470 DO 8 JSCAN=1,KM1
03480 IF(I.EQ.IROW(ISCAN)) GO TO 11
03490 IF(J.EQ.JCOL(JSCAN)) GO TO 11
03500 8 CONTINUE
03510 9 IF(ABS(A(I,J)).LE.ABS(PIVOT)) GO TO 11
03520 PIVOT=A(I,J)
03530 IROW(K)=I
03540 JCOL(K)=J
03550 11 CONTINUE
03560 IF(ABS(PIVOT).GT.EPS) GO TO 13
03570 SIMUL=0.
03580 RETURN
03590 13 IROWK=IROW(K)
03600 JCOLK=JCOL(K)
03610 DETER=DETER*PIVOT
03620 DO 14 J=1,MAX
03630 14 A(IROWK,J)=A(IROWK,J)/PIVOT
```

APPENDIX A (continued)

```

03640 A(IROWK,JCOLK)=1./PIVOT
03650 DO 18 I=1,N
03660 AIJCK=A(I,JCOLK)
03670 IF(I.EQ.IROWK) GO TO 18
03680 A(I,JCOLK)=-AIJCK/PIVOT
03690 DO 17 J=1,MAX
03700 IF(J.NE.JCOLK) A(I,J)=A(I,J)-AIJCK*A(IROWK,J)
03710 17 CONTINUE
03720 18 CONTINUE
03730 DO 20 I=1,N
03740 IROWI=IROW(I)
03750 JCOLI=JCOL(I)
03760 JORD(IROWI)=JCOLI
03770 IF(INDIC.GE.0) X(JCOLI)=A(IROWI,MAX)
03780 20 CONTINUE
03790 24 IF(INDIC.LE.0) GO TO 26
03800 SIMUL=DETER
03810 RETURN
03820 26 DO 28 J=1,N
03830 DO 27 I=1,N
03840 IROWI=IROW(I)
03850 JCOLI=JCOL(I)
03860 27 Y(JCOLI)=A(IROWI,J)
03870 DO 28 I=1,N
03880 28 A(I,J)=Y(I)
03890 DO 30 I=1,N
03900 DO 29 J=1,N
03910 IROWJ=IROW(J)
03920 JCOLJ=JCOL(J)
03930 29 Y(IROWJ)=A(I,JCOLJ)
03940 DO 30 J=1,N
03950 30 A(I,J)=Y(J)
03960 SIMUL=DETER
03970 RETURN
03980 200 FORMAT(1H0,5X,'N TOO BIG')
03990 END
04000 SUBROUTINE GENTNL(PAR)
04010 DIMENSION PAR(800,5),Z(4,99),BDEL(4),NZ(4),YYXP(800)
04020 COMMON/GENTNL/X(800,5),YXP(800),J,N,Z,ITER,BDEL,NOPT
04030+,NOPT2,NZ,NNL,INL,NP,XPY(5),YTH(800),NOUT
04040 133 FORMAT(' TYPE THE INITIAL GUESS AND DELTA')
04050 135 FORMAT(' TYPE THE NUMBER OF FILES TO BE SKIPPED, '//
04060+' THE NUMBER OF DATA POINTS, THE NUMBER OF INDEPENDENT '//
04070+' VARIABLES, THE NUMBER OF LINEAR PARAMETERS TO BE FIT '//
04080+' AND THE OPTION NUMBER.')
04090 IF(ITER.NE.1) GO TO 129
04100 PRINT 135
04110 READ(5,*),NO,N,NP,J,NOPT
04120 IF(NO.EQ.0) GO TO 145
04130 DO 150 I=1,NO
04140 150 READ(1,*) YYXP(I),(PAR(I,K),K=1,NP)
04150 145 DO 130 I=1,N

```

APPENDIX A (continued)

```

04160 READ(1,*) YYXP(I),(PAR(I,K),K=1,NP)
04170 130 YXP(I)=YYXP(I)
04180 ENTRY GENTEP(PAR)
04190 IF(NOPT.EQ.0) GO TO 128
04200 IF(NOPT.EQ.1) GO TO 129
04210 PRINT 132
04220 132 FORMAT(' TYPE>NNL, SEARCH #, & OUTPUT #')
04230 READ(5,*),NNL,NOPT2,NOUT
04240 IF(NOPT2.EQ.2) GO TO 131
04250 PRINT 134
04260 134 FORMAT(' TYPE THE INITIAL GUESSES')
04270 READ(5,*),(Z(I,1),I=1,NNL)
04280 PRINT 100
04290 100 FORMAT(' TYPE THE NUMBERS OF THE N.L. TERMS IN ORDER')
04300 READ(5,*),(NZ(I),I=1,NNL)
04310 GO TO 129
04320 131 INL=1
04330 IF(NNL.EQ.1) GO TO 99
04340 PRINT 98
04350 98 FORMAT(' WHICH NON-LINEAR PARAMETER IS TO BE FIT?')
04360 READ(5,*), INL
04370 PRINT 134
04380 READ(5,*),(Z(I,1),I=1,NNL)
04390 PRINT 410
04400 410 FORMAT(' TYPE DELTA')
04410 READ(5,*) BDEL(1)
04420 DO 10 I=2,99
04430 DO 10 KJK=1,NNL
04440 10 Z(KJK,I)=Z(KJK,1)
04450 GO TO 129
04460 99 PRINT 133
04470 READ(5,*),Z(INL,1),BDEL(1)
04480 GO TO 129
04490 128 DO 390 I=1,N
04500 X(I,1)=1.0
04510 X(I,2)=PAR(I,1)
04520 X(I,3)=PAR(I,1)*PAR(I,1)
04530 X(I,4)=PAR(I,1)*X(I,3)
04540 X(I,5)=X(I,3)*X(I,3)
04550 390 CONTINUE
04560 RETURN
04570 C*****SPECIAL REGRESSION EQUATION FORMS GO HERE***** EQUATION 7
04580 129 DO 290 I=1,N
04590 ARG1=PAR(I,1)*Z(I,ITER)
04600 IF(ABS(ARG1).GE.100)ARG4=0.
04610 IF(ABS(ARG1).LT.100)ARG4=EXP(-ARG1)
04620 X(I,1)=1.-ARG4
04630 X(I,2)=1.
04640 290 CONTINUE
04650 RETURN
04660 END
READY.

```

APPENDIX A (concluded)

```
04570C*****SPECIAL REGRESSION EQUATION FORMS GO HERE***** EQUATION 5
04580 129 AK=Z(1,ITER)
04590 AN=Z(2,ITER)
04600 DO 290 I=1,N
04610 PAP1=PAR(I,1)-T0
04620 T1=0.
04630 T2=0.
04640 T3=0.
04650 ARG=UZ**(1.-AN)/(AK*(1.-AN))
04660 IF(PAR1.GE.ARG.AND.AN.LE.1)GO TO 289
04670 ARG=1.+AK*PAR1*(AN-1.)*UZ**(AN-1.)
04680 T1=ARG**(1./(1.-AN))
04690 T2=PAR1*UZ**(AN-1.)*ARG**(AN/(1.-AN))
04700 T3=AK*T2*(1.+(AN-1.)*ALOG(UZ))/
04710+(AN-1.)*ALOG(ARG)*T1/((1.-AN)*(1.-AN))
04720 289 X(1,1)=1.-T1
04730 X(1,2)=T2
04740 X(1,3)=T3
04750 290 CONTINUE
04760 RETURN
04770 END
-END OF FILE-
?
```


APPENDIX B

Computer Program for the Jander Equation (Equation 13)

```

0: DIM Z[100,10],A[10,10],Y[100],X[100],C[10],R[10],D[10],T[10],F[100]
1: DIM Q[2,2],M[6],S[6],I[2],B[4],S$[80],X$[80],Y$[80],G[2],Q[2],E[4],F[2]
2: ENT "TYPE # OF DATA POINTS",L
3: LDM:SFG 1;DEG:PCLA;LBL " " ;CFG 0;1)P
4: ENT "TYPE ORDER OF FIT",N;N+1)N)H
5: ENT "ENTER FINAL WEIGHT",W
6: FOR I=1 TO L
7: ENT Y[I],X[I]
8: NEXT I
9: "LIST":SPC ;PRT "DATA POINTS:";SPC ;PRT "I","Y[I]","X[I]"
10: FOR I=1 TO L
11: FXD 0;PRT I;FLT 9;PRT Y[I],X[I]
12: NEXT I
13: -1)I
14: ENT "CORRECT POINT #",I
15: IF I=-1;JMP 3
16: IF I=0;GTO "LIST"
17: ENT Y[I],X[I];0)I;JMP -3
18: SPC ;SPC ;PRT "I";PRT "ALPHA[I]";PRT "X[I]"
19: FOR I=1 TO L
20:  $(1 - (1 - Y[I]/W)^{(1/3)})^2 Y[I]$ 
21: FXD 0;PRT I;FLT 9;PRT Y[I],X[I]
22: NEXT I
23: "CALL":CLL "MAT"
24: SPC ;PRT "COEFFICIENTS:";FLT 9;APRT C
25: CLL "PRD"
26: -1)A;ENT "NEW ORDER? J=",A
27: IF A=-1;A+1)N)H;GTO "CALL"
28: SFG 0;0)A;ENT "LIST PREDICTED VALUES?1=YES,0=NO",A
29: IF A=0;JMP 2
30: CLL "PRD"
31: 0)A;ENT "LIST OTHER PREDICTED VALUES?",A
32: IF A=0;JMP 8
33: FLT 9;1)L;SPC ;PRT "Y[I]","X[I]";SPC
34: ENT X[I]
35: IF X[I]=-9.9E-99;JMP 5
36: CLL "MAT"
37: CLL "PRD"
38: PRT X[I];SPC
39: -9.9E-99)X[I];JMP -5
40: GTO 87
41: "MAT":RDM Z[L,N],A[N,N],R[N],C[N],T[N],D[N];INA A,R
42: FOR I=1 TO L
43: FOR D=1 TO N
44: IF D=1;1)Z[I,1];JMP 2
45:  $X[I]^{(D-1)}Z[I,D]$ 
46: NEXT D
47: NEXT I
48: IF FLG0;RET
49: FOR D=1 TO N
50: FOR K=1 TO N
51: FOR I=1 TO L
52:  $Z[I,D]Z[I,K]+A[D,K])A[D,K]$ 
53: NEXT I

```

APPENDIX B (concluded)

```

14: NEXT K
15: NEXT D
16: INV A>A
17: FOR D=1 TO N
18: FOR I=1 TO L
19: Z[I,D]Y[I]+R[D]>R[D]
20: NEXT I
21: NEXT D
22: MAT A>R>C
23: RET
24: "PRD":0>R>S>T
25: IF FLG0;IF FLG1;IF L>1;PRT "PREDICTED VALUES";FLT 9;SPC
26: FOR I=1 TO L
27: 0>P[I]
28: FOR D=1 TO N
29: Z[I,D]C[D]+P[I]>P[I]
30: NEXT D
31: IF FLG0;IF FLG1;PRT P[I];JMP 1
32: (Y[I]-P[I])^2+S>S;Y[I]+T>T;Y[I]Y[I]+R>R
33: NEXT I
34: IF FLG0;RET
35:  $\sqrt{(1-S/(R-TT/L))}>R$ 
36: FLT 6;PRT "SS=";S
37:  $\sqrt{S/(L-N)}>S$ 
38: PRT "SE=";S;FXD 7;PRT "R =",R
39: FOR I=1 TO N
40: IF A[I,1]<0;PRT "SINGULAR!";DEEP
41: S>\ABS(A[I,1])>D[I]
42: C[I]/D[I]>T[I]
43: NEXT I
44: SPC ;FXD 2;PRT "T STATISTICS:";APRT T
45: FLT 3;PRT "DELTA:";APRT D
46: S>U;R>V;RET

```

APPENDIX C

Computer Program for the Phase Boundary Model (Equation 16)

```

0: DIM Z[100,10],A[10,10],Y[100],X[100],C[10],R[10],D[10],T[10],P[100]
1: DIM Q[2,2],M[6],S[6],I[2],B[4],SS[80],XS[80],YS[80],G[2],Q[2],E[4],F[2]
2: ENT "TYPE # OF DATA POINTS",L
3: L)M;SFG 1;DEG;PCLR;LBL " ";CFG 0;1)P
4: ENT "TYPE ORDER OF FIT",N;N+1)N)H
5: ENT "ENTER FINAL WEIGHT",W
6: FOR I=1 TO L
7: ENT Y[I],X[I]
8: NEXT I
9: "LIST":SPC ;PRT "DATA POINTS:";SPC ;PRT "I","Y[I]","X[I]"
10: FOR I=1 TO L
11: FXD 0;PRT I;FLT 9;PRT Y[I],X[I]
12: NEXT I
13: -1)I
14: ENT "CORRECT POINT #",I
15: IF I=-1;JMP 3
16: IF I=0;GTO "LIST"
17: ENT Y[I],X[I];0)I;JMP -3
18: SPC ;SPC ;PRT "I";PRT "ALPHA[I]";PRT "X[I]"
19: FOR I=1 TO L
20: 1-(1-Y[I]/W)^(1/3))Y[I]
21: FXD 0;PRT I;FLT 9;PRT Y[I],X[I]
22: NEXT I
23: "CALL":CLL 'MAT'
24: SPC ;PRT "COEFFICIENTS:";FLT 9;A)PRT C
25: CLL 'PRD'
26: -1)A;ENT "NEW ORDER? J=",A
27: IF A=-1;A+1)N)H;GTO "CALL"
28: SFG 0;0)A;ENT "LIST PREDICTED VALUES?1=YES,0=NO",A
29: IF A=0;JMP 2
30: CLL 'PRD'
31: 0)A;ENT "LIST OTHER PREDICTED VALUES?",A
32: IF A=0;JMP 8
33: FLT 9;1)I;SPC ;PRT "Y[I]","X[I]";SPC
34: ENT X[I]
35: IF X[I]=-9.9E-99;JMP 5
36: CLL 'MAT'
37: CLL 'PRD'
38: PRT X[I];SPC
39: -9.9E-99)X[I];JMP -5
40: GTO 87
41: "MAT":DIM Z[L,N];A[N,N],R[N],C[N],T[N],D[N];INA A,R
42: FOR I=1 TO L
43: FOR D=1 TO N
44: IF D=1;1)Z[I,1];JMP 2
45: X[I]^(D-1))Z[I,D]
46: NEXT D
47: NEXT I
48: IF FLG0;RET
49: FOR D=1 TO N
50: FOR K=1 TO N
51: FOR I=1 TO L
52: Z[I,D]Z[I,K]+A[D,K])A[D,K]

```

APPENDIX C (concluded)

```

53: NEXT I
54: NEXT K
55: NEXT D
56: INV A)A
57: FOR D=1 TO N
58: FOR I=1 TO L
59: Z[I,D]Y[I]+R[D]R[D]
60: NEXT I
61: NEXT D
62: MAT A)R)C
63: RET
64: "PRD":0)R)S)T
65: IF FLG0;IF FLG1;IF L=1;PRT "PREDICTED VALUES";FLT 9;SPC
66: FOR I=1 TO L
67: U)P[I]
68: FOR D=1 TO N
69: Z[I,D]C[D]+P[I])P[I]
70: NEXT D
71: IF FLG0;IF FLG1;PRT P[I];JMP 1
72: (Y[I]-P[I])^2+S)S;Y[I]+T)T;Y[I]Y[I]+R)R
73: NEXT I
74: IF FLG0;RET
75:  $\sqrt{1-S/(R-TT/L)}$ )R
76: FLT 6;PRT "SS=";S
77:  $\sqrt{S/(L-N)}$ )S
78: PRT "SE=";S;FXD 7;PRT "R =",R
79: FOR I=1 TO N
80: IF A[I,I]<0;PRT "SINGULAR!";BEEP
81: S)ABS(A[I,I])D[I]
82: C[I]/D[I])T[I]
83: NEXT I
84: SPC;FXD 2;PRT "T STATISTICS:";APRT T
85: FLT 3;PRT "DELTAS:";APRT D
86: S)U)R)Y;RET

```